Energy-efficient Neuromorphic Technologies for Scientific Computing

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Large artificial intelligence models supported by digital architectures are facing a memory and power efficiency wall. Models with trillions of parameters need supercomputers with hundreds of thousands of processors and GWh of energy per training, a financial and environmental cost that is unstainable beyond-exascale. The current digital hardware is orders of magnitude less efficient than computation performed by the brain. Recent neuroscience studies emphasize that the characteristic structure of the brain networks is key to reducing the energetic costs of computation in the brain. New brain-inspired computing approaches and new analog hardware are needed to bridge the gap. This project draws inspiration from the hippocampus, a core brain region that supports learning, memory and navigation, to develop networks that can perform learning and adaptation at scale in an energy efficient fashion and under limited hardware constraints. Two key concepts from neuroscience, i.e. spontaneous resting-state dynamics and cell assemblies, seem to underpin the efficiency, self-regulation and robustness to noise and variability of the biological neuronal circuits. In this work, they will be explored in an integrative fashion using biologically-plausible models with a goal towards analog circuit translation. The research is driven by three main objectives and uses neuronal models derived from the rodent hippocampus, one of the most studied brain regions. The emergence of spontaneous resting-state dynamics in hardware-relevant network models will be investigated. The results will be utilized to explore energy efficient cell assemblies formation in such networks. The algorithmic insights will be translated to neuromorphic circuits that have resting-state dynamics and pattern classification capabilities. In conjunction with transistor circuitry tape-outs, novel analog devices with tunable time constants will be investigated to support the neuronal and synaptic diversity in the biologically-realistic system. This project will bring neuroscience insights to develop neuromorphic technology capable of analyzing large and/or incomplete data of relevance to DOE in an energy-efficient, fast and robust way.

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

A High-Luminosity Active Nuclear Target for Recoil Tagging Measurements

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Understanding the quark and gluon substructure of helium-4 – a light, and tightly-bound nucleus – is a fundamental goal of nuclear physics. The properties of helium-4 emerging from the dynamics of quarks and gluons can be studied in electron beam scattering experiments where the helium-4 remains intact. These experiments require the scattered electron, the low energy recoiling helium-4 nucleus, and any additional produced particles to be detected simultaneously amid a high radiation background. This project will explore and develop a novel active helium-4 target as a detector system based on linear arrays of superconducting nanowire single-photon detectors (SNSPDs) and cryogenic readout technology. Significant R&D will be conducted to demonstrate a prototype of this first-of-its-kind concept of a cryogenic target system operating as a novel "photon time projection chamber". Such a transformative target system could be used in high beam intensity experiments at Thomas Jefferson National Accelerator Facility (TJNAF), including the proposed Solenoidal Large Intensity Device (SoLID) experiment. The project will make use of state-of-the-art micro-fabrication materials and accelerator test facilities at Argonne National Laboratory.

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

Toward Quantum Imaging of Nuclei

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The atomic nucleus emerges from interacting quantum particles called quarks and gluons, but how this happens remains unknown. This might be elucidated with quantum-level "images" of their position, orbital motion, spin alignment, and entanglement. This quantum imaging represents a cornerstone at the Thomas Jefferson National Accelerator Facility. This project will extend this research from its current focus on studying isolated protons and neutrons to the realm of complex nuclei, where theoretical models hint at new phenomena. Experiments will use a high-intensity, high-energy electron beam to probe a wide range of nuclear targets, from lithium to lead. Key studies will involve measuring the angles of the scattered electrons and other particles and how they depend on the spin state of electrons or nuclei. This project seeks to establish a solid experimental foundation for the quantum imaging of the atomic nucleus.

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

Deciphering Complex Chemical Reaction Dynamics Induced by Non-Equilibrium Microplasma Discharges at High Pressures

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Microplasma, confined to dimensions on the scale of millimeters or smaller, demonstrates remarkable stability even under high pressures, facilitating self-sustained and continuous operation. This stability is attributed to the efficient energy transfer within the confined space, leading to heightened ionization and excitation processes. With their cost-effectiveness, ease of operation, simplified hardware design, and portability, microplasmas find applications across diverse fields, including materials processing, sensing, energy generation, environmental remediation, and chemical synthesis. Understanding the intricate dynamics of ions, electrons, metastable species, and excited atomic and molecular species within transient streamers and early afterglow regimes of microplasma, particularly under atmospheric and above-atmospheric pressures, is imperative for unlocking its potential in complex reaction dynamics. At elevated pressures, where the electron mean free path approaches the inter-electrode gap, quenching processes emerge as dominant factors.

The proposed research endeavors to delve into electron-impact ionization and fragmentation of molecules, such as methane and ammonia, within the microplasma environment. Additionally, the investigation will explore the influence of Rydberg molecules on plasma chemistry and subsequent chemical reactions. This research aims to unveil novel chemical pathways in gas-phase systems by harnessing the unique characteristics of electrons, ions, and Rydberg molecules within a high-pressure non-equilibrium microplasma. Over a five-year span, the research trajectory will commence with focused studies on well-established gases like helium and/or argon during the initial two years. Subsequently, the scope will expand to encompass investigations into air, methane, and ammonia systems, particularly in the context of energy applications, in the latter three years. Through this progressive approach, the research aims to deepen our understanding of microplasma chemistry and its potential for transformative applications in various domains.

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

Who Lives, Who Dies, Who Cares?
Using Soil Microbial Demographics to Predict Carbon Transformation

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Due to their abundance and ubiquitousness, microorganisms shape the Earth's global cycles of important nutrients such as carbon, nitrogen, and phosphorus as they reproduce and die over time. Fundamental aspects of these processes can be studied by culturing individual microbes in the laboratory. However, measuring these processes in wild microbial communities that cannot be cultured has proved challenging until recently. This project aims to significantly advance our understanding of microbial population growth and mortality rates and their critical roles in soil biogeochemical cycles, especially carbon cycling. The project employs high throughput approaches to test if and how microbes utilize a broad diversity of carbon compounds that mimic those found in their natural soil habitat. Different "omics" analyses are conducted on soils from multiple incubations along with a technique called quantitative stable isotope probing (qSIP) to track microbial activities and the fate of organic compounds as they are utilized and modified by the microbes. One of the goals of the project is to develop a publicly accessible, comprehensive qSIP database to enable advanced analysis of microbial growth and mortality while taking into account the environmental conditions at the time of each experiment. Sophisticated computational and machine learning approaches are used to test and refine ecological theories across different ecosystems. This endeavor is expected to offer critical insights into how carbon substrates affect microbial processes, influencing soil organic matter dynamics and carbon storage. Through its innovative approach and integration of multiple data types, this research will fill critical knowledge gaps and contribute essential data for quantitative models that link microbial activity to broad-scale ecological processes. Ultimately, this project's findings could lead to improved soil management strategies and carbon sequestration techniques, and aid in efforts to mitigate climate change by enhancing soil health and productivity.

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

Multi-channel access to Generalized Parton Distributions

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This project aims to explore the multidimensional structure of the nucleon (proton or neutron) in terms of its internal constituents, called “partons” (quarks and gluons), from an experimental and phenomenological point of view. Several new and dedicated experiments will be developed at Jefferson Lab Hall C. Experimental data will be analyzed to expand the global data accessing Generalized Parton Distributions (GPDs), which are functions parametrizing this internal structure. GPDs contain the relation between parton’s longitudinal momentum and transverse position. The final step will be to produce multi-channel/multi-observable fits of functions of the GPDs. What is unique in this approach is that novel reactions that will be measured will access for the first-time kinematics enabling a 3-dimensional interpretation (“tomography”) of the quark and gluon distributions. These measurements will also enable assessing whether GPDs are universal functions, a milestone in nuclear physics. This project will involve experimental work: detector R&D and assembly, simulations, data taking, data analysis; and phenomenological work: impact studies, interpretation of the results, fits and modeling, and development of event generators. It will have a major impact on assessing GPDs’ universality, bringing new and independent constraints to GPD models, constraining the full kinematic phase-space of the GPDs, which is needed for tomographic interpretations, and obtaining novel information on the spatial and momentum distributions of quarks in the nucleon.

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

Attosecond Metrology for Electron and X-ray Beams

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Probing the rapid motion of electrons within molecules requires making measurements on an attosecond timescale. Recently, free electron lasers facilities (FELs) have developed powerful attosecond x-ray sources by selectively lasing on a single spike within a much longer electron beam. The single-spike FEL operates in a novel regime where the x-rays develop *partial longitudinal coherence* due to slippage effects. The coherence implies a stable, seed-like structure (relative to the electron beam), which can be used to shape the x-ray pulse in downstream amplification stages. In principle, this enables attosecond pulses with higher peak power, two colors, improved stability, and shorter pulse lengths. But the physics underlying this process remains largely unexplored, because diagnostics capable of resolving the FEL instability on an attosecond timescale do not exist. This program will build a photoelectron streaking diagnostic in which the space-charge field of the electron beam provides the streaking momentum. Because the same electron beam is used both to generate and to streak the x-rays, the diagnostic will be intrinsically synchronous and able to reconstruct the first-order coherence properties of the x-ray beam. Such synchronous metrology is required to directly access the physics of a single-spike FEL, and the insights learned will help push the boundaries of FEL performance. Shot-by-shot information from the new diagnostic can then be used for online optimization of attosecond FELs.

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

Phosphine-Modified Cationic Co(II) Precatalysts for Hydroformylation at Mild Conditions

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Carbon monoxide is a cheap and abundant carbon source used to produce fuels and various commodities. While historically produced through energy-intensive processes such as steam-reforming, advances in CO production from biomass gasification and via CO2 reduction allow for CO to be now viewed as a renewable carbon source. The capture and conversion of carbon to generate products critical to society (fuels, polymers, pharmaceuticals) remain a significant scientific challenge for the 21st century. Toward the goal of lowering carbon emissions, the efficient use of CO represents a lynchpin between renewable sources of carbon and producing the commodities on which we rely. However, many of the large-scale processes that leverage CO demand high temperatures and pressures and have large energy demands. One of the largest is hydroformylation, which converts alkenes, H2, and CO into aldehydes at over 10 million metric tons annually. Discovered nearly 100 years ago, this process is commercially catalyzed by either Co(I) or Rh(I) carbonyl complexes, sometimes supported by ancillary phosphine ligands. Whereas Co(I) catalysts have the advantage of being based on an earth-abundant metal, higher temperatures and pressures are required, and decomposition to Co metal can yield alkene hydrogenation side reactions, which have little value. Rh catalysts are active at lower pressures (30 bar *vs* 100 bar) but inherently use precious metals while also suffering from their decomposition pathways. Recently, a Co(II) precatalyst for hydroformylation was discovered with unique properties. The resulting catalysis occurs at milder conditions, with activity near that of Rh(I), no decomposition is reported, and minimal alkene hydrogenation is observed. These new precatalysts have the potential to use cheap Co-based catalysts to achieve conditions similar to Rh and with comparable rates. However, as Co(II) hydroformylation precatalysts remain an emerging class of complexes, little is known about controlling the reactivity and the nature of the active catalytic species.

In this project, we seek to develop this novel Co(II) precatalyst further. We will determine the structure of the active catalyst through various *in situ* spectroscopic methods. We will create a structure/activity relationship to elucidate the key features of the ligand field that are critical to catalytic activity and selectivity. We will also expand the principles of the Co(II) systems to comparable base metals of intermediate oxidation states. The goal of this work is to identify the key structural and electronic factors that allow Co(II) precatalysts to generate these unique hydroformylation catalysts. It will also represent the initial efforts to broaden the scope of catalyst reactivity to other base metal complexes. More broadly, this work will advance the development of base metal catalysts and our understanding of how precatalysts of intermediate oxidation states can yield active and metastable catalysts under reducing conditions.

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

Observing and understanding the role of surface thermal heterogeneity in mesoscale circulations over AMF3 BNF: Implications for land-atmosphere interactions

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When thermal heterogeneity over the land surface is sufficiently pronounced and organized (on the order of kms), it can drive the development of mesoscale circulations which, in turn, can impact boundary layer and cloud development. The realization that these secondary circulations can play a larger role than expected in the climate system is driving a push to improve the sub-grid heterogeneous land-atmosphere coupling in Earth system models. As new coupling parameterizations emerge, there is a need to improve understanding of these circulations and how they are driven by the underlying surface physical environment. Furthermore, it is critical to develop metrics to compare existing observations to evaluate the modeled thermal spatial patterns and the circulations. The third Atmospheric Radiation Measurement (ARM) Mobile Facility in the Bankhead National Forest (AMF3 BNF) provides a unique opportunity to address this need, as it provides an environmental setup that combines spatially organized heterogeneities in soils, land cover, and topography; it has a climate and environment that is favorable for locally driven shallow cumulus clouds; and it has a network of Doppler lidars that makes it plausible to observe the circulations. The overarching objective of this project is to leverage AMF3 BNF to improve understanding of the role of thermal surface heterogeneity in mesoscale circulations. To accomplish this goal, this project will 1) leverage observations to determine the connection between thermal surface heterogeneity and mesoscale circulations; 2) assemble a digital twin of the AMF3 BNF region using Large Eddy Simulations and land surface modeling and compare to observations; 3) perform a sensitivity analysis to understand how the surface drivers of spatial heterogeneity influence the secondary circulations and how these circulations, in turn, impact the surface energy balance.

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

Coherent X-ray Detection of Quantum Correlations in Quantum Many-Body Systems

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Uncovering the role of quantum correlation in electronic phase ordering is of utmost importance to designing improved and reliable quantum materials with novel functionality. This program invests in a new approach to identify and study quantum correlations in solids. Specifically, we will utilize state-of-the-art synchrotron resonant coherent x-ray techniques along with laser excitations to study equilibrium and non-equilibrium critical dynamics of electron correlations with nanometer and nanosecond resolutions. Then quantum witness methods will be employed to quantify the degree of multipartite entanglement from the measured dynamical structure factor. A time-resolved pump-probe capability will be implemented at the Coherent Hard X-ray Scattering (CHX) beamline at National Synchrotron Light Source II at Brookhaven National Laboratory. The coherent x-ray interference patterns diffracted from quantum materials reflect their complex spatial texture of charge and spins. By tracking the interference pattern with time, we will gain both spatial and temporal information on phases of matter. This program will lead to a detailed understanding of how coexisting quantum phases share the density of states at phase boundaries, ultimately leading to the ability to design new quantum materials with stable topological phases.

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

Ultrafast Terahertz Scanning Tunneling Microscopy of Atomic Defects in Complex Materials

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In complex materials, microscopic interactions lead to surprising emergent phenomena. Among these, the Kagome compounds are characterized by a lattice of corner-sharing triangles similar to a basket-weave pattern in which the orientation of interacting electron spins is geometrically frustrated. This frustration, together with electron-electron correlations and topology, leads to exotic charge density waves and superconductivity. Atomic defects in the Kagome lattice such as single-atom vacancies may couple to these ordered states, providing a means to both investigate their underlying cause and, potentially, control them.

Ultrafast materials science uses impulsive excitation by laser pulses to perturb emergent order, allowing the relevant microscopic mechanisms to be unraveled in the time domain. This research will investigate atomic defects in Kagome materials with simultaneous atomic spatial resolution and ultrafast temporal resolution using lightwave-driven terahertz scanning tunneling microscopy (THz-STM). THz-STM uses the oscillating electric field of single-cycle THz pulses to coherently control quantum tunneling of electrons between a tip and sample. Pump-probe THz-STM imaging experiments will capture femtosecond snapshots of charge ordering around single-atom defects in Kagome materials following optical excitation. Terahertz scanning tunneling spectroscopy and terahertz time-domain spectroscopy on the atomic scale will supplement these movies by revealing the key processes underlying coupling between the emergent order and defects. Finally, the prospect of using strong THz fields at the tip apex to locally control the emergent order will be explored.

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

Broad-Spectrum Light-Harvesting and Energy Transfer in Bioinspired Nanocluster Assemblies

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This project advances the fundamental solar photochemistry of few-atom metal nanoclusters (NCs), which are promising for artificial light-harvesting systems that mimic natural photosynthesis. A significant body of theoretical work has illustrated the promise of NCs for increasing the efficiency and range of resonance energy transfer, which is a key step in harvesting solar energy. However, experimental studies to verify these predictions have been hindered by the major challenge of creating well-controlled nanoscale architectures of NCs. This research overcomes this long-standing challenge by harnessing new capabilities in bioinspired programmable assembly of DNA-stabilized silver nanoclusters (Ag_N-DNAs). DNA-directed atomically precise NCs architectures will be assembled using programmable DNA base pairing and then experimentally investigated to understand how resonance energy transfer efficiency is influenced by factors including the distance between NCs, as well as NC size and geometry. Comparison of experimental results and theoretical modeling will test the hypothesis that plasmon-like coupling can enhance resonance energy transfer between NCs. Next, the unique DNA-encoded properties of Ag_N-DNAs will be used to design and assemble NC architectures for broad-spectrum light harvesting and to investigate the upper limit of resonance energy transfer distance and energy down-conversion. Finally, hybrid architectures of Ag_N-DNAs and carbon nanotubes will be studied to understand how chirality influences energy transfer and whether NC donors can generate photoinduced current in carbon nanotubes. This research will result in general design rules to guide the development of NC-based materials for critical applications in solar energy harvesting and solar fuels, of interest to the DOE Solar Photochemistry Program. This work is also expected to lead to new materials systems that enhance the collection and transfer of solar energy.

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

Disentangling the factors controlling the emission of bioparticles that act as ice nucleating particles

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Ice nucleating particles (INPs) affect cloud radiative properties and precipitation through their ability to initiate primary ice formation. Primary ice formation is a critical step required for important cloud microphysical processes that govern cloud phase and other downstream properties. Bioparticles (defined as solid airborne particles derived from biological organisms, including microorganisms and biological material fragments) are thought to be a key contributor to ambient INP populations in certain regions due to their high ice nucleation activity at warm temperatures but currently are not included in most global and regional models. Despite their importance, the identities of and factors controlling the emission of bioparticles that act as INPs (bio-INPs), along with their downstream effects on clouds, are not well understood.

This project seeks to improve the ability to predict INP concentrations and variability in regional and global models by improving process understanding of bio-INP emissions using a three-part plan. First, laboratory measurements using instruments designed to measure bioparticles and INPs will be collected. Those measurements will be used to develop machine learning (ML) tools for classifying bioparticles in the ambient atmosphere. Second, samples will be collected at a remote vegetated site in the southeastern United States and returned to the laboratory for analysis. The previously developed ML tools will be used to generate a long-term dataset of bioparticle and bio-INP concentrations with high time resolution. Finally, the relationship between environmental factors and bioparticle and bio-INP emissions will be examined. ML techniques will be used to analyze the dataset of ambient bio-INP concentrations to derive and test quantitative relationships between bio-INP emissions and environmental factors.

This project will improve the understanding of the extent to which bioparticles control warm INP populations in the ambient atmosphere as well as identify factors that can be used to predict their concentrations and variability. The process knowledge developed from this project will be used to improve the emission schemes of bio-INPs, leading to increased accuracy in INP predictions by state-of-the-art Earth system models.

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

Microbial Metabolic Controls on Soil Carbon Dynamics through Root-Microbe-Soil Interactions: Connecting Molecular Processes to Ecosystem-level Impacts

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In land ecosystems, plants fix carbon dioxide through photosynthesis and convert it into organic compounds that constitute their cell walls and other biomass components. Some of these organic compounds are also released into the soil through the plant's roots. The fate of this carbon fixed in plant biomass and root deposits is determined by soil microbial communities. Microbes either degrade it and release it back to the atmosphere as carbon dioxide or transform it into microbial biomass and soil organic matter. Lipids are key components of soil organic matter and play a crucial role in microbial metabolism. However, they are the least understood biomolecules in soil ecosystems. This project investigates how microbial processes centered around lipids influence the persistence of carbon in soils. Deep soils associated with bioenergy sorghum roots are being studied to identify lipid-centric microbial strategies as well as metabolic interactions among plants, bacteria, fungi, and viruses that impact the molecular composition and durability of soil carbon. The research integrates field observations with laboratory experiments to identify general patterns of microbial lipid processes that affect soil organic carbon. One of the goals of this project is to build a publicly available database of soil lipids to promote widespread adoption of soil lipidomics and foster collaboration and sharing knowledge among the research community. This project will advance BER's mission in bioenergy and the environment by identifying key lipid-related microbial metabolic strategies, interkingdom interactions, and ecosystem-level outcomes, achieving a functional understanding of soil microbiomes and plant-microbe interactions that are important for long-term soil carbon storage.

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

Simulating nuclear physics with nuclear spin qudits

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The Standard Model of particle physics is described by gauge theories in which “gauge bosons” mediate interactions between matter particles (“fermions”). Simulations of phenomena in the standard model are performed with lattice gauge theories in which space is discretized to enable efficient computer simulation. Even so, the simulations quickly become intractable on classical computers, limiting the ability to predict the spectra and scattering properties of, e.g., nuclear matter. Quantum computers – based on inherently quantum-mechanical binary digits called “qubits” – show great promise for simulating the dynamics of lattice gauge theories. However, like classical computers, their binary nature severely limits their ability to simulate the high-dimensional spaces of quarks and gluons which have flavor, color, and spin degrees of freedom. Accordingly, quantum hardware that can be operated with larger quantum digits, generically called “qudits”, instead of qubits provides an opportunity to advance our understand of lattice gauge theories and their application to nuclear matter, called “quantum chromodynamics” (QCD). This project will leverage 4- and 8-dimensional spaces of neutral ytterbium-171 atoms to implement quantum computing algorithms that simulate quantum electrodynamics (QED) and QCD. This research will utilize an electronic qubit, a nuclear spin qubit, and a motional qubit all within a single atom where each can be controlled independently. A universal gate set will be constructed for this multi-qubit encoding and used to realize circuits that simulate electron-positron scattering and the low-energy spectrum of two-flavor mesons. More broadly, the hardware efficiency of this approach will carry over to quantum computing and networking applications.

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

Fine-grained Theory and Robust Algorithms for Randomized Numerical Linear Algebra

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Randomized algorithms have gained increased prominence within numerical linear algebra, and they play a key role in an ever-expanding range of problems driven by a breadth of scientific applications. Randomized algorithms promise to accelerate pervasive computational kernels (such as low-rank approximation and solving least squares problems) within scientific computing while simultaneously providing rigorous theoretical guarantees. Consequently, in the generic case these methods have received an enormous amount of theoretical analysis, and many strong results have been developed. However, the matrices that arise from applications are often highly structured and there has been significantly less analysis of randomized algorithms with respect to such structures.

This project will directly address the development and deployment of randomized algorithms for problems from domain science. This will include the development of adaptive algorithms that leverage the best of modern randomized algorithms while retaining certain advantages of classical algorithms. They will leverage randomization to ensure robustness and computational efficiency, while also including strategies that adapt to problem structure as they are being run. Complementing these algorithmic advances, this project will develop a collection of fine-grained theoretical results that refine our understanding of randomized algorithms. Prior results often obfuscate the nuances of specific problems, making it difficult for randomized algorithms to effectively exploit the nature of a specific problem. Newly developed results will explicitly incorporate bounds that adapt to common (application motivated) structures and provide a more nuanced landscape of theoretical guarantees. Ultimately, this project will provide a comprehensive picture of the relative performance of randomized and deterministic methods that enables practitioners to select appropriate algorithms. As a central motivation for studying randomized algorithms for structured matrices is that they arise in problems of scientific interest, this project will feature an undercurrent of research objectives in three key domains: computational physics, data science, and deep learning.

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

Adaptive multiscale modeling using pseudospectral wavepackets

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This project will develop a suite of methods for the efficient and accurate numerical simulation and modeling of multiscale, multiphysics systems. Traditional numerical methods often rely on simple component functions that are largely agnostic to both the underlying physics and the emergent features of the field variables being solved for. On the other hand, tailored basis functions, while problem-specific and more accurate, typically require pre-existing high-fidelity data to identify, and can only be defined numerically on discrete meshes, thereby losing some of the computational advantages of pre-defined analytic basis functions. This project seeks the best of both worlds: functions to use within numerical simulation methods that are highly efficient at representing pertinent phenomena without the need for existing high-fidelity data, while also possessing closed-form analytic descriptions. This objective will be achieved by leveraging advances in operator pseudospectral theory and projection-based modeling approaches. This methodology will first be applied to develop nonlinear reduced-order models that are accurate and adaptive. Next, these methods will be used for closure modeling in the solution of time-averaged equations. Finally, the methodology will be applied for the high-fidelity simulation of multiscale systems. The methods will be tested and validated across a range of example problems, including fluid and thermofluid systems that exhibit turbulence, geometrical complexity, and fluid-structure interaction.

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

Multi-Tiered Algorithms for Solving Extreme-Scale Inverse Problems Emerging from New Experiments

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Technological advancements at DOE experimental facilities are enabling new measurements of complex phenomena and specimens with unprecedented detail. However, the ever-increasing extreme scales involved in analyzing these emerging experiments are surpassing our current ability to solve the inverse problem of reconstructing important scientific information from the data at the speed, accuracy, and robustness needed to enable scientific breakthroughs. To fully realize the potential of these state-of-the-art experiments, advanced high-performance computing systems need to be coupled with fundamentally new mathematical insights and algorithmic approaches to solve complex inverse problems at the required scales.

This proposal seeks to develop new mathematical algorithms for solving inverse problems from experiments at the following emerging extreme scales:

- Data rate. Data is being produced faster than can be loaded into memory or transferred to storage, requiring large compression, leading to information loss and inaccuracies in inversion. (i)
- Resolution elements. Experiments are making measurements at unprecedented resolution, requiring unparalleled inversion accuracy to reconstruct. (ii)
- Physical complexity. The complexity of the physics involved in new experiments is skyrocketing, requiring new methods to efficiently simulate and invert. (iii)
- Problem sensitivity. New experiments are measuring weaker signals, often buried under noise. Physical limitations can prevent full parameter sampling, leading to inversion ill-conditioning. (iv)
- Turnaround time. Quick results are required to enable real-time steering of experiments and optimal use of expensive experimental resources. (v)

To address these scales, we propose to develop new multi-tiered inversion frameworks, which are based on decomposing very complex inverse problems into a series of simpler subproblems, for which optimal mathematical and algorithmic solutions can be developed to effectively target the specific physics and scales of the inversion. As demonstrated by the PI's Multi-Tiered Iterative Projection (M-TIP) technique, multi-tiered inversion schemes are able to leverage advanced methods in machine learning, optimization, linear algebra, harmonic analysis, and statistics to solve much more complex inverse problems than traditional approaches. As a result, M-TIP has allowed us to solve many open problems in inverting data for emerging DOE experiments at LCLS, APS, ALS, NSLS-II, and NCEM, including enabling real-time single-particle analysis at LCLS through the ExaFEL ECP.

Here we will leverage and expand upon the M-TIP framework to develop fundamentally new algorithmic approaches that enable inversion at our targeted scales. This work includes:

Machine-learning-augmented inversion frameworks capable of accurately and efficiently encoding new physics and constraints (addresses scales ii,iii,iv,v).

Statistically-constrained parameter optimization techniques to automatically determine accurate noise models and regularization weights during inversion (addresses scales ii,iv,v).

Data-compression modeling in inversion to enable accurate reconstructions from highly compressed data (addresses scales i,ii,iv,v).

These approaches will be implemented and integrated into M-TIP and our other inversion codes to enable their immediate use in solving inverse problems from experiments data. By leveraging ASCR supercomputers, this work will create the computational capability to address emerging practical barriers in analyzing new extreme-scale experiments, ultimately enabling a host of new scientific breakthroughs throughout DOE facilities. Finally, our proposed mathematics and algorithms will establish fundamentally new research pathways in hybrid machine-learning/optimization, optimization-based automation, data-compression modelling, and algorithmic frameworks that can holistically combine these advances to tackle a wide range of grand scientific challenges at scale.

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

Multiscale Modeling of Heteroepitaxial Interfaces for Scalable Thin-Film Solar Cell Applications

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Thin-film photovoltaic devices consist of a multilayer architecture, for which charge-carrier transport across the interfaces plays a crucial role in minimizing the associated recombination losses and achieving high solar conversion efficiencies. To achieve insight-driven engineering and optimization of thin-film solar cells, a high-level characterization that gives a local, electronic, and chemical picture of the interface properties is needed. However, owing to their narrow widths and their often non-crystalline structures, interfaces are difficult to resolve or access by purely experimental means. Atomistic modeling and simulation are therefore ideally suited to complement experiments but there is a need for more efficient multiscale methods, that can operate at larger time and size scales. Two main challenges of simulating realistic interface models level remain: (i) the simulation cell must be sufficiently large to accommodate the incommensurate nature of the system and include misfit-induced structural modifications and (ii) the final structure must not be influenced artificially by the starting structure. With the emergence of machine learning interatomic potentials (MLIPs), we are now at the threshold of achieving efficient atomistic simulations with DFT-level accuracy.

This project aims to develop and implement a multi-scale modeling environment (integrating advanced first-principles DFT calculations, ab initio molecular dynamics (MD), and classical MD simulations accelerated by high-accuracy machine learning interatomic potentials) to simulate large-scale realistic interfaces. We will establish a universal set of reliable and transferable MLIPs for large-scale simulated amorphization and recrystallization molecular dynamics that will evolve the complex microstructural features observed experimentally at perovskite/charge transport layer interfaces, including interfacial reconstructions, and defects such as dislocations, grain boundaries, vacancies, and interstitials. We will also establish rational molecular design principles and structure-property relationships needed to provide experimental guidance for selecting passivation ligands to improve stability and performance. We will perform a microkinetic simulation of temperature-programmed desorption (TPD) to predict the desorption temperatures of selected passivation molecules at perovskite surfaces. The detailed atomic level information will be experimentally tested and used to enhance the perovskite solar cell technology. The precise understanding of the microscopic structure of interfaces and the mechanisms of interfacial phenomena obtained from the work, will not only help to identify specific bottlenecks to the performance and stability of photovoltaic devices but enable an insight-driven optimization of interface properties to achieve more efficient and stable solar cells.

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

Next Generation X-ray Magnetic Measurements at Ultra-High Pressures

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Magnetic interactions are one of the key ingredients towards realizing novel properties in quantum materials, including several candidates for spintronics, a critical energy relevant technology. Physical pressure is a well-known route to tune magnetic interactions through the control of interatomic distances and bond angles. Pressure-driven magnetic quantum phase transitions thus provide a unique path to driving and understanding novel phenomena not readily accessible at ambient conditions. The goal of this project is to build a new X-ray Emission Spectroscopy instrument, named MagXES, that leverages the polarization dependence in x-ray emission to increase the sensitivity of magnetism-dependent x-ray measurements by as much as two orders of magnitude, enabling high-throughput measurements of magnetism and electronic properties at extreme pressures. This development will be complemented with the use of nanofabrication tools to tailor the high-pressure environment, which will extend the accessible pressure range and enable novel multi-modal electrical transport measurements. MagXES is designed to take full advantage of the sub-micrometer beam size, advanced x-ray polarization control, high magnetic field, and low temperature capabilities of the new POLAR beamline at the upgraded Advanced Photon Source (APS). By investigating the correlation between electronic and magnetic properties in emergent phenomena at high pressure, this research will contribute to the understanding of novel quantum systems. Beyond the APS, the developed high-pressure methodology will largely benefit the exploration of quantum materials at extreme conditions.

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

Innovative X-Ray Diagnostics for Diverse Fusion Environments

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The goal of this project is to develop an integrated set of innovative X-ray diagnostics that will transform the current measurements of basic plasma processes and meet the complex and challenging need for future magnetic fusion energy (MFE) and inertial fusion energy (IFE) experiments including burning plasmas. There are four thrusts of proposed diagnostic innovations: 1) 1D high resolution X-ray spectrometers based on novel aspherical crystal shapes for simultaneous achievements of high spatial and spectral resolutions and high throughput, 2) 2D X-ray imaging system that consists of dual spherical crystals for stigmatic imaging, 3) radiation-hardened X-ray spectroscopy, and 4) crosscutting connections between inertial confinement fusion (ICF)/IFE and magnetic confinement fusion (MCF)/MFE. Significant efforts will be devoted to absolute calibrations of all proposed X-ray diagnostics. With extensive experiences and ample resources in X-ray diagnostics development, the team is aiming at an innovation center for developing the next generation of X-ray spectrometers and imagers ready for burning plasmas and fusion power plants. The proposed X-ray diagnostics, once developed in the laboratory, will be applied to tackle important physics problems including direct measurements of material mixing for energy gain enhancement for IFE and active system control at burning plasma conditions for MFE.

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

Enabling Scientific Data-Driven Modeling from Heterogeneous, Multi-Model, Massive, and Distributed Datasets

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Scientific Machine Learning (SciML) has emerged as a collection of techniques that, by combining data and numerical methods, can achieve excellent results in learning tasks unsuited or too time intensive for humans. Unfortunately, while classical ML applications, e.g., speech and object recognition, usually enjoy an abundance of data, science and engineering problems are often characterized by sparse data. For scientific predictions, the data sparsity translates to a limited exploration of the high-dimensional parameter space, which in turn limits the quality and accuracy of the resulting models. In principle, the data sparsity could be mitigated by leveraging the large amounts of data routinely produced and stored in scientific laboratories, e.g., U.S. Department of Energy's national laboratories; however, these datasets are generated from different physical experiments or numerical models that span different experimental configurations and model parameters, i.e., they are heterogeneous. Consequently, these heterogeneous data cannot be directly employed to augment sparse high-fidelity data.

In this project, we propose to develop domain-aware SciML methods with quantifiable uncertainty that i) mine multiple modalities of heterogeneous and distributed information available and stored across enterprises, ii) discover their underlying common representation with high-fidelity data through lower dimensional parametrizations, and iii) fuse them to enable challenging scientific tasks and predictions. The project vision is realized by combining multi-model dimension reduction and manifold learning strategies, multi-model data-fusion approaches for heterogeneous data, and novel uncertainty quantification workflows to account for epistemic and aleatoric uncertainty generated through the data reduction, compression, curation, and fusion. Furthermore, we will design SciML methods to operate in a federated learning fashion such that the transfer of the training datasets across storage locations can be reduced or significantly minimized. We will demonstrate these novel tools on an array of complex scientific and engineering problems including, but not limited to, climate, fusion, and wind energy applications.

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

Machine Learning for New Physics and Microelectronics at the Energy Frontier

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A broad exploration of particles and their interactions at the energy frontier is essential for a better understanding of the fundamental universe. Machine learning (ML) and microelectronics are cross-cutting technologies that can be leveraged in this exploration to enhance the scientific discovery potential at collider experiments. This research will employ ML across software and hardware to improve new physics searches in the ATLAS (A Toroidal LHC ApparatuS) experiment at the Large Hadron Collider (LHC), located at the European Organization for Nuclear Research (CERN) near Geneva, Switzerland. Advanced ML-based anomaly detection (AD) methods will be developed and deployed in offline data analysis, facilitating model-independent searches for beyond the Standard Model signatures. In the ATLAS trigger system, online AD will be implemented for the real-time classification of anomalous collision events, yielding a novel dataset that can be analyzed to probe uncovered regions of phase space for new physics. Moreover, to enable intelligence at the front-end, ML-based detector readout will be pursued in the context of embedded Field Programmable Gate Arrays, advancing microelectronics R&D for future state-of-the-art detector concepts. Results from this research will inform experimental designs at next-generation energy frontier facilities, such as the Future Circular Collider proposed to be hosted at CERN with international collaboration. Together these efforts are expected to provide a new approach for exploring the unknown in particle physics, while simultaneously developing key interdisciplinary technologies and capabilities.

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

Understanding the Role of Itinerant Electrons and Inhomogeneity in Magnetic Van der Waals Materials

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Magnetic materials are essential for various modern technologies. Recently, metallic van der Waals (vdW) magnets have gained significant attention as they can be easily engineered into thin crystals, facilitating their integration into devices and switches. Because these materials are also metallic, itinerant conduction electrons play a pivotal role in mediating magnetic interactions within these systems. The interplay between metallicity and magnetism enables the electrical control of the magnetic structure, which is a cornerstone for future spintronic technologies. Yet, the fundamental mechanisms by which itinerant electrons interact with spins and influence magnetic structures are not yet fully understood. In many cases, key technological properties like ferromagnetism above room temperature or electrical control inherently require disorder across different length scales, from the atomic to the meso-scale. This research project is dedicated to investigating the role of itinerant electrons and inhomogeneity in prominent magnetic vdW materials. It specifically employs scanning tunneling microscopy combined with spectroscopy and spin-polarized measurements, to study the spatial variations of charge, spin and structural properties within metallic vdW materials. Specific goals include investigating the role of itinerant electrons and inhomogeneity in enhancing ferromagnetic transition temperatures and in enabling the electric control of local magnetic structures. This research project will advance our understanding of the fundamental interplay between charge and spin degrees of freedom at the nano- and meso-scales in materials that are expected to play a major role in the development of controllable quantum systems.

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

Universality in Quantum Gravity and Beyond

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One of the most important open questions about the fundamental laws of our Universe is how to reconcile quantum mechanics with gravity. Traditionally, the path to answering this question has relied on finding a unified UV complete theory incorporating all known fundamental forces. Recently, there has been a tremendous number of developments, from a better understanding of how information escapes the interior of black holes to exact gravitational path integral computations of BPS black hole degeneracies, that show that detailed observables in quantum gravity can oftentimes be reliably studied directly in the low-energy theory without a detailed knowledge of the UV completion. This project will combine a multitude of interdisciplinary tools, from the abstract tool of supersymmetric localization to the numerical tool of semidefinite programming, to study universal quantum properties of gravitational theories and their strongly coupled duals with the hope of addressing some of the most pressing questions in quantum gravity. Are black holes described by ordinary quantum systems? If so, can we explain the emergence of a discrete Hilbert space of black hole microstates starting from gravitational variables? When do gravitational observables receive large quantum corrections, and when can the low energy theory make quantitative predictions about these corrections? Can the techniques we developed also be used to study universal features in strongly interacting quantum systems independent of their relation to holography?

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

Color Centers in Noise-Free Hosts for Quantum Sensing and Communication Applications

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The advent of quantum technologies heralds the introduction of novel capabilities, such as high-precision magnetic field sensing and the ability to store and communicate quantum information over long distances. These technologies leverage quantum emitters to encode quantum information or monitor environmental changes. Despite their transformative potential, the widespread adoption of these technologies is impeded by the scarcity of materials in which electron spins exhibit long coherence times. In the best host materials, magnetic interactions between the nuclei and electron spins induce fluctuations in electron energy levels, leading to decoherence. While isotopic purification can address this issue, it remains costly and difficult to scale.

This project explores cerium oxide as a host material for optically active quantum bits. The naturally abundant isotopes of oxygen and cerium, the two components of cerium oxide, lack magnetic nuclei, potentially enabling long coherence times without the need for isotopic purification. The large bandgap of cerium oxide, its compatibility with various substrates, and its biosafety further enhance its suitability for a broad spectrum of applications. We will employ density functional studies to identify promising emitters and use pulsed laser deposition to grow high-quality single-crystal films. We aim to synthesize the predicted emitters in these crystals through doping and ion irradiation and characterize their optical and spin properties using magneto-optical measurements. The success of this project will uniquely contribute to the advancement of quantum information science by unlocking a scalable, optically active qubit platform. Our research on these emitters can yield high-resolution magnetic field sensors capable of imaging large areas, surpassing the capabilities of existing technology. Additionally, the project will explore the cooperative phenomena arising from interactions between rare-earth dopants in cerium oxide, potentially opening new avenues for quantum information storage or the emulation of many-body effects using these dopants.

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

Probing Two-Dimensional Quantum Materials with Flying Electron Qubits

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Strongly correlated electronic phases in two-dimensional (2D) quantum materials, such as exfoliated few-layer van der Waals (vdW) materials, have attracted enormous attention in recent years. To understand these materials, innovative probing techniques may reach unexplored regimes and provide unexpected insights. In this project, we will utilize our recent accomplishment in quantum information science (QIS) – the long-coherence high-fidelity electron-on-solid-neon (eNe) qubit platform – to develop a quantum-enabled scanning probe microscopy (SPM). With this technique, 2D quantum materials under investigation will be transferred onto a superconducting quantum circuit and coated with a noninvasive layer of solid Ne. A single electron qubit flying above the solid Ne can be transported, trapped, controlled, and read out by the quantum circuit. The spin states of the qubit electron will strongly interact with the spin or current states of the material electrons and shed light on the local magnetic, topological, and superconducting orders approaching zero temperature. The eNe-SPM can facilitate QIS-inspired material discovery, design, and synthesis and define a new paradigm for quantum information science in material science and engineering (QIS-MSE).

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

Learning to Adaptively Manage Heterogeneous Scientific Workloads on Heterogeneous Clusters

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Computational science applications are growing ever more diverse, driven in part by the growing prevalence of large-scale machine learning applications that aim to analyze ever-growing amounts of scientific data. These applications' computing needs are equally diverse: for example, small-scale simulations may need only a few CPU cores to complete in a reasonable amount of time, but some machine learning training tasks my require dozens of the most advanced GPUs. Such diversity raises significant challenges in ensuring that each application has the computing resources that it needs to ensure acceptable performance.

Recent work in computer systems proposes to first split applications into constituent tasks and then provision computing resources for each task, so as to optimize the overall application performance. Typically, this process is conducted within a (super)computing cluster, so the provisioned computing resources for an application's tasks may reside at different, interconnected, and heterogeneous physical machines. These task placement methods, however, quickly grow infeasible as the number of tasks, number of applications, and size of the computing cluster grow, especially when applications and clusters are highly heterogeneous. Working at a large scale, however, may come with a hidden benefit: large-scale workloads may be broken into more constituent tasks, which may reveal local task similarities. This project is based on the key insight that even tasks and machines that appear heterogeneous may exhibit hidden, underlying similarities in their resource requirements and performance characteristics. The goal of the project is to design, implement, and evaluate new algorithms to discover and track such hidden similarities, exploiting them to schedule and place heterogeneous scientific computing workloads in heterogeneous supercomputing clusters. In doing so, we will be able to develop adaptive and uncertainty-aware placement and scheduling algorithms, ensuring that scientific computing workloads receive the resources they need in today's increasingly large-scale and heterogeneous environments.

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

Quantum Field Theory in Our Universe

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Cosmology is a study of correlations. By measuring the correlations between structures in the universe, like galaxies in the night sky, we determine both the contents of the universe and how it evolved. Further, by tracing these correlations back in time, we infer that they originated as quantum fluctuations during a pre-Hot Big Bang epoch of quasi-exponential expansion, which we call cosmic inflation. The details of this early-universe phase remain deeply mysterious, and we only have access to it via the correlations that it generated. Understanding the origins of structure in the universe therefore requires us to understand quantum correlations in cosmological spacetimes. This is the domain of quantum field theory, and this project will develop new field-theoretic tools to study the universe at its earliest moments and highest energies.

The goal of this project is to study quantum field theory in cosmological spacetimes, like our own, by focusing directly on the observable correlations that are generated by cosmological time evolution. These correlations must be consistent with fundamental physics principles, and these consistency constraints are sufficiently stringent that they can often be used to reconstruct (or "bootstrap") the correlations directly. This project will further develop this bootstrap approach to cosmological quantum field theory by exploring how the physics of time evolution is encoded in cosmological observables, and by mapping the space of consistent theories in cosmology. These new insights will help refine our understanding of the dynamics of the universe, and will help make progress on critical questions in cosmology.

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

Improved Calibration of Xenon-Based Dark Matter and Neutrino Experiments By Simultaneously Measuring Different Types of Electron Recoil Backgrounds

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Background rejection is paramount in the search for the elusive dark matter signal. In the dual-phase liquid/gas xenon time projection chamber which has emerged as one of the best technologies in direct detection, these backgrounds mostly arise from electromagnetic (electron and photon) interactions producing electronic recoils inside the detectors. Their responses, if not properly understood, could leak into the dark matter nuclear recoil signal region of interest and be mis-identified as dark matter signals. Our current estimates are that 99.0-99.9% of the background interactions from electrons or photons can be rejected at 50% nuclear recoil acceptance. However, these estimates were derived from recoil measurements using a single beta-decay source (producing high energy electrons) with the assumption that the same response applies for photon interactions. Although some experimental data and theoretical models suggested that electron recoil responses in liquid xenon are different between electron and photon interactions, and also vary with the amount of energy deposited and the drift field, this was not further investigated. As current xenon detectors such as LUX-ZEPLIN are leading the field and new ones are being planned to probe new parameter spaces drawing us closer to a potential discovery, every assumption should be tested to avoid a false discovery claim. Moreover, the remaining electronic-recoil backgrounds from double-beta decay, electron captures, internal conversions, and Auger electrons should also be properly understood and be accounted for while extracting a potential dark matter signal. This proposal is about conducting detailed, simultaneous measurements with small-scale xenon detectors of the liquid xenon responses to all these various electronic recoil backgrounds at different energies and drift fields. These measurements will then be fed back into the simulations of the micro-physics of xenon detectors to properly take into account the complete responses of the detector to these backgrounds to not only improve the sensitivities of current leading experiment such as LUX-ZEPLIN and future xenon experiments looking for dark matter, but also for neutrinoless double-beta decay and other rare physics.

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

Pore-Confinement Effects on Mineral Crystallization Behaviors in Geologic Multiphase Flow Systems

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The objective of this research is to quantify the impact of multiphase flow dynamics, specifically flow rate and partial water saturation states, on mineral nucleation and crystallization reactions in nano- and micro-porous geologic media. The project focuses on the formation of carbonate minerals and water-soluble hydrous minerals within vesicular basalt pore structures and 2D/3D "dual-porosity" microfluidic analogues. Vesicular basalts are porous igneous rocks that contain tight nano-porous matrices punctuated by vesicles and/or microfractures of varied connectivity (e.g., dual porosity). Due to their potential fluid storage capacity, reactivity with carbon dioxide (CO_2), and relative global abundance, vesicular basalts are targeted in recent and upcoming government and industrial subsurface carbon mineralization pilots. Carbon mineralization is a promising long-term CO_2 storage strategy, whereby carbon dioxide is trapped in the form of dissolved carbonate and bicarbonate ions and eventually converted to carbonate minerals through crystallization reactions. The influence of the distribution of capillary water and water films on supersaturation and subsequent secondary mineral crystallization morphologies and growth rates in these systems is not yet well understood. The project leverages subsurface vesicular basalt samples of varied alteration and pore connectivity subjected to natural (i.e., long-term) and engineered (i.e., short-term) CO_2-rich multiphase flow regimes. Multimodal sample imaging and measurement techniques, including nuclear magnetic resonance (NMR), are leveraged to characterize and create digital representations of pore confinements and alteration states. Computational fluid dynamics (CFD) methods are used to quantify the evolution of multiphase flow and fluid-mineral interactions in those domains. Parallel microfluidic experiments yield fundamental relationships and controlled CFD benchmarks that isolate multiphase flow controls on short-term crystallization dynamics. Hydrous minerals (e.g., halite, gypsum, hydrated copper sulfate) are used as scaled proxies for fast and low-temperature experimental investigation of an extended multiphase flow-crystallization parameter space. Findings from the research objectives are applicable to enhancing carbon mineralization in a host of subsurface basaltic and other mafic/ultramafic rocks as well as subsurface sedimentary formations, soils, mine tailings/heap mines, cements, and packed bed reactors. The work is also of importance to understanding multiphase flow controls on rock diagenesis, maintaining flow path connectivity in enhanced geothermal systems, and halite salt precipitation during carbon storage operations.

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

An Innovative (n, xn) Measurement Capability for Fusion Reactors, Fast Reactors, Radiochemical Diagnostics, and Astrophysics

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Fusion reactor technology has rapidly matured over the last decade. Reliance on highly-uncertain nuclear data for neutron-induced reactions near and above 14 MeV incident neutron energy has grown in tandem, especially experimentally-challenging and poorly-understood (n,2n) and (n,3n) reactions. Specifically, the ^{9}Be and ^{208}Pb(n,2n) reactions are essential for fusion reactor operation through their use as neutron breeder nuclei to enhance tritium production through the ^{6}Li(n,t)α reaction , though reactions on ^{52}Cr, ^{93}Nb, ^{181}Ta, ^{197}Au, and ^{203}Tl and many other nuclei are also important for neutron flux diagnostics. This project will develop a unique and revolutionary capability for measuring the (n,2n) and (n,3n) reaction data by directly measuring the energy of just one emitted neutron from these reactions without neutron time-of-flight (TOF) techniques. This method will utilize emergent ^{7}Li-enriched Cs_2LiYCl_6:Ce (CLYC-7) detectors within n-n or higher-order neutron coincidences observed from (n, xn) reactions to break the neutron TOF degeneracies that have hindered differential measurements of neutrons emitted from these reactions at continuous (white) neutron sources. An array of large-volume CLYC-7 detectors will be purchased and installed in the Correlated Gamma-Neutron Array for sCattering (CoGNAC) array of dual n-γ detectors at the Los Alamos Neutron Science Center white neutron source. High-priority measurements on ^{9}Be, ^{181}Ta, and ^{208}Pb will be performed during the course of this project, leading to a sustained campaign of (n, xn) measurements supporting multiple DOE and NNSA missions.

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

Using Crystallographic Defects to Control Emergent Behavior in Quantum Materials

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The presence of entanglement in strongly correlated quantum materials underlies their potential for next-generation technologies with applications ranging from quantum computers to sensors to solid-state devices. But the same entanglement also poses challenges for theory, prohibiting efficient generic simulations on classical computers and complicating our classical intuition. A compounding challenge for correlated quantum theory is set by defects and other types of quenched disorder. These are often ignored but are always present in real materials. In materials such as alloys and doped compounds, disorder is intrinsic, and its properties are in part controllable. This offers a tuning handle. Here we pose the question: Can disorder in correlated quantum materials be useful for identifying, generating, and controlling desirable emergent behavior?

In this project we address this question by constructing original theoretical models that allow us to describe novel behavior. Our approach combines a diverse theoretical toolbox ranging from analytical quantum field theory techniques to diagonalization and tensor network numerics. We supplement this toolbox with collaborations with experimentalists to disseminate and apply the developed abstract theories and to identify and resolve experimental puzzles in current and next generation compounds. A longstanding puzzle involves the highly entangled Quantum Spin Liquid (QSL) phases of strongly correlated magnetic insulators. QSLs offer a combination of exciting emergent features (codes for robust quantum computing, gauge photons, anyons) together with relative theoretical control and experimental realizability, making QSLs the ideal platform for investigating entanglement-driven emergence. But QSL materials are inherently difficult to identify due to their fluctuating ("liquid") spins. This is made even more challenging by crystallographic defects since both, clean QSLs and trivial disordered systems, typically show broadly featureless spectra.

To address these issues, we pursue three objectives: (1) Demonstrate the creation of a certain QSL from weak disorder and construct a full theory, with important implications for controlling emergent behavior using defects, and for quantum information processing. (2) Construct a theory for predicting a class of defect effects in QSLs, which may enable disordered QSLs to be experimentally identified and manipulated. (3) Construct theories that address the dichotomy between global and local experimental probes in materials with local defects, with implications for their design and interpretation with disorder.

Understanding disorder in strongly correlated quantum materials is an important and urgent task for developing next generation technologies for energy applications. This project constructs original theoretical frameworks that address this task. The outcome of this research is to guide new theoretical concepts and experimental probes to uncover how crystallographic defects can identify, generate, and control emergent quantum behavior.

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

Wasted Space?: Visualizing Rare Earth Element Ligand and Analyte Access within Porous Materials

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Rare earth elements (REEs) are critical components for green technologies that must be separated from complex mixtures such as naturally mineralized mined ores or recycled sources before use. Current approaches to extract REEs use harsh solvents resulting in a high carbon footprint and environmental cost. Biological- and bio-inspired molecules on solid supports are a promising alternative to selectively separate REEs. Biomolecules offer the tunability of Nature's toolbox. Just as well-known biological membrane proteins can select between sodium, potassium, and calcium, natural proteins have evolved to selectively adsorb REE ions. Yet, protein-based REE separations on solid supports have thus far been studied using ensemble techniques that are unable to directly probe molecular phenomena at surfaces, resulting in top down, trial-and-error optimization. In order to transform REE separation science from the bottom up, variations in the physical molecular dynamics that occur under realistic separation pressure conditions are measured using single-REE-ion microscopy. Binding events of interest include interactions between REE ions to high affinity, larger protein ligands and to smaller, engineerable, lower affinity peptide ligands immobilized in porous materials. Lanmodulin and peptide ligand size are varied to evaluate how the interior of porous materials is under-utilized in separations based on the steric differences between the ligand and material pores. Molecular information will therefore inform the design and development of new, more efficient REE separations to extract these critical elements to support the clean energy infrastructure.

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

Realizing Functionality in Graphene-Based Quantum Materials via Addressing their Atomic-Scale Properties

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New digital and quantum information processing strategies based on modifying existing physical paradigms represent key research directions dictating the main vectors of progress in modern condensed matter physics. These are motivated mainly by (1) overcoming the physical limits in developing existing CMOS technologies, and (2) novel emerging applications mainly related to quantum computing. In this respect, low-dimensional solid-state systems attract much attention, as recent scientific developments in their synthesis in hierarchical heterostructures enable realizing quantum-mechanical-originating effects such as dissipationless transport in topologically protected edge states.

Precise and rational synthesis of quantum materials realizes the emergent properties that derive from controlling their exact atomic-level architectures. On the other hand, the functionality that results from such atomic-scale control of quantum materials requires similar precision in developing local addressing tools for its practical realization. In this case, scanning tunneling microscopy (STM)-based techniques are the first methods for atomically precise mapping of local topography and distribution of electronic or spin density of states. However, a knowledge gap exists between the characterization of given nanosystems and testing their expected functional properties, even in prototypical applications. As a result, a common problem exists: how to understand the relation between *the local signatures* of the emerging quantum properties, e.g., in the density of states from the STM experiment, and the *mesoscale quantum behavior*, e.g., in electronic transport?

The program addresses this issue and *proposes a rational approach to understanding functionality in low-dimensional graphene-based quantum materials.* We will combine atomically precise on-surface synthesis strategies and in-situ advanced scanning probe microscopy-based methods to reveal the origins of their mesoscale characteristics. These complementary activities are based on our unique expertise in (1) atomically precise synthesis of graphene-based quantum materials, i.e., on substrates providing electronic decoupling, and (2) developing STM-based techniques, including atomically precise multi-probe scanning tunneling microscopy and spectroscopy.

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

Nuclear Reaction Theory with Quantified Uncertainties

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The impact of experimental data on our understanding of nuclear processes is gauged only to the extent that such data can be meaningfully compared to theoretical predictions. Since a significant portion of nuclear data comes from nuclear reaction experiments it is imperative that a predictive reaction theory with quantified uncertainties is formulated, to fully take advantage of high-precision measurements. The goal of this proposal is to combine a first-principle theory of nuclear reactions with verified statistical methods to arrive at a predictive modeling of nuclear reactions with quantified uncertainties. Such a theory will provide stringent constraints and realistic covariances for difficult-to-measure nuclear reaction observables. At the same time, this research will demonstrate how elusive emergent phenomena connect to the fundamental nuclear interaction. Finally, by combining available experimental data with theoretical predictions across reaction networks, this work will produce evaluations for astrophysically-relevant reaction cross sections, as well as observables related to nuclear clustering. Thus, this work will provide a first ever evaluation of thermonuclear reactions at the network level that originates in an uncertainty-quantified microscopic reaction theory.

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

Machine Learning-Enabled Monitoring of Metallic Solutes via X-ray Absorption Spectroscopy in Molten Salt Fusion Blankets

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Recent advances in high-temperature superconductors enable compact, high-field fusion systems that can be deployed in a timely manner for achieving commercial fusion. Here, molten salts are a promising class of fusion blankets that can breed and recover tritium to sustain deuterium-tritium fusion reaction, shield magnets against radiation, and efficiently transfer large amounts of heat to cool the first wall. However, utilizing molten salts in a fusion energy system remains a grand challenge owing to their continuously evolving potential to corrode structural metals, precipitate metallic foulants, and emit volatile metal halides during operation. As such, online monitoring and control of salt chemistry and metal dissolution is crucial for the safe and reliable operation of a fusion power plant. The objectives of this project are to address these needs by 1) developing new tools for monitoring the oxidation states and structures of molten salts with unprecedented spatial resolution, 2) learning the extended structural morphologies and distributions of solvated species that will be found in prototypical fusion systems, and 3) learning the relationships between solute-salt structure and reduction potential. New approaches are proposed that combine recent advances and push the boundaries of machine learning-assisted atomistic simulation, deep learning-based spectral analysis, and high-throughput laboratory-based X-ray absorption spectroscopy, to maximize online measurement efficiency and information recovery. Methods will be validated using synchrotron experiments, and a clear understanding of solvation structures leading to corrosion and precipitation will be developed for structural metals and reducing agents in fusion salts for the first time. As such, this work will help resolve long-standing challenges that have impeded real-time understanding of chemical transformations in molten salts and enable their use in future fusion energy technologies.

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

Incorporating Kinetic Effects in Fluid Models of Low Temperature Plasmas via Machine Learning

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Computational modeling of low temperature plasmas (LTPs) is critical for many technology areas including manufacturing of computer chips, medical treatments, and the synthesis of nanomaterials. For LTPs, particle-in-cell (PIC) Monte Carlo collision simulations is the highest-fidelity technique commonly used. In these models, electrons and ions are treated kinetically – meaning there are no assumptions about their velocity distributions. However, even the massively parallel kinetic codes rarely reach the time scales, length scales, and dimensionality of most real problems. As a result, many of these problems have been examined using fluid models with approximations (e.g., Maxwellian distributions, drift-diffusion fluxes, local mean energy approximation). This project aims to develop and evaluate methods to use machine learning to bridge the gap between kinetic Monte Carlo simulations and fluid-based models for LTPs. These new techniques will enable simulations that extend to fluid time and length scales but include physics that are normally only present in kinetic simulations. This approach will reduce computational time by several orders of magnitude compared to purely kinetic simulations. The method will be applied to explore kinetic effects in atmospheric pressure streamer propagation, a problem in which the high collision frequency makes kinetic simulations computationally prohibitive. These methods would transform computational modeling of LTPs more broadly, enabling an improved understanding of the underlying physics and chemistry that is critical for chemical conversion, semiconductor processing, plasma medicine, and many other areas.

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

Reveal the Structure-Dynamics Relationship in Solution-Phase Photoredox Catalysis with Explainable Machine Learning

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Bimolecular photoinduced electron transfer in the solution phase is fundamental for energy science applications, such as photovoltaics, artificial photosynthesis, and photoredox catalysis. Understanding how the chemical structures of electron donors and acceptors impact the photoinduced electron transfer dynamics is crucial for improving photoredox catalysis efficiency. However, traditional theories for bimolecular electron transfer do not explicitly account for essential structural parameters like the mutual orientation of donor and acceptor molecules. Consequently, there are no established guidelines for designing photoredox catalysts to enhance charge transfer efficiency in specific reactions. This project exploits a data-driven approach to reveal the structure-dynamics relationship in solution-phase photoredox catalysis, using a photopolymerization reaction as the model system. This objective can be achieved by implementing an automated data pipeline for molecular dynamics simulations of photoinduced electron transfer between a fixed electron donor and various photoredox catalyst candidates in explicit solvent environments. Explainable machine learning models can then extract the structure-dynamics relationships from the simulation data, addressing fundamental questions about how catalyst structures dictate donor-catalyst orientation/separation and how these factors influence charge transfer and catalytic efficiency. This project promises transformative discoveries in the field of photoredox catalysis, enabling energy-efficient and eco-conscious chemical reactions. The strong connection to DOE-operated high-performance computing facilities will further enhance the impact of advanced computing on complex condensed-phase and interfacial molecular science.

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

Narrowing the Human-AI Knowledge Gap through Audience-Aware Visualization

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The increasing reliance on artificial intelligence (AI) systems, particularly deep neural network models, to tackle critical scientific problems has exposed a growing knowledge disparity between machines and humans. Machine knowledge is encoded in network parameters and latent representations, which are inaccessible to users. In contrast, human knowledge is expressed through natural language, high-level concepts, and logical reasoning, making it difficult to communicate effectively with machines when solving scientific problems. This machine-user knowledge gap raises crucial questions: (1) how can users interpret and extract knowledge from machines to gain scientific insights, and (2) how can users effectively convey their intentions and understanding to machines for model steering and improvements?

Objective: Bridging machine learning (ML) and visualization research, this project will create an adaptive and audience-aware visualization framework that supports machine-human knowledge exchanges. The established framework will reveal the model's internal logic, inject user knowledge back into the model, and address the differences in users' knowledge levels and their distinct goals.

Method: To achieve this vision of effective human-AI knowledge exchange, I propose three interconnected research directions: **(1) Extract knowledge from models to inform diverse audiences:** I will develop adaptive visualization approaches that adjust to the needs of different audience groups (e.g., ML researchers, domain scientists, policymakers/public) by providing insights about the AI models at varying levels of complexity; (**2) Inject user knowledge and convey intention to models:** I will maximize the efficiency of human feedback to machines by developing methods to generalize user annotations to the machine, and I will develop a framework to translate user intentions expressed in natural language into composable instructions to machines; and **(3) Identify the shared abstraction between machine and human:** I will explore techniques to map out the shared semantic abstractions that will be understandable for human users yet accessible and controllable in the ML pipeline. This abstraction will form a universal backbone for human-AI knowledge exchange and democratize access to complex black-box ML systems and enable researchers from diverse backgrounds to contribute to interpretability and alignment research.

Impact: This proposal addresses fundamental challenges in developing intelligent approaches for adaptive, context-aware visualization of scientific data and AI, as well as science communication, both of which are priority research directions (PRDs) identified by ASCR in the basic research needs report for visualization for scientific discovery, decision-making, and communication. By developing novel techniques that combine ML with intuitive and interactive visualizations, I will provide domain experts with the tools and insights necessary to understand, interpret, and align AI models with their domain knowledge to facilitate discovery. Through close integration with Lawrence Livermore National Laboratory projects, I will demonstrate immediate benefits for ML applications in material science, physics, and biology. With a forward-looking research agenda, the proposed research will also yield long-term impacts in AI-driven discovery, scientific foundation models, and AI safety.

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

Neutron Scattering Studies of Nanoscopic Structure and Dynamics of Single Ion Conducting Polymer Blend Electrolytes

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The ongoing development of rechargeable batteries with increased energy density is critical to continue the growth in the electrification of mobile technologies. To achieve these goals, new electrolytes must be developed that possess fast ion transport characterized by high ionic conductivity and high cation transference number (the fraction of ions that carry current), a combination of properties typically not found in a single material. Therefore, we propose a novel battery electrolyte system known as single ion conducting polymer blend electrolytes (SIPBEs), which are binary mixtures of an ion-containing polymer and an ion-conducting polymer. The ion-containing polymer contains Li^+ counter ions that induce mixing with the ion-conducting polymer generating robust miscible blends. Although it is well-known that ion transport in polymer electrolytes is intrinsically linked to the polymer self-assembly and segmental dynamics, the ion transport mechanism in multicomponent polymer systems remains an open question. We will use neutron scattering to study the nanoscopic structure and dynamics of a SIPBE model system. Through selective isotopic labeling, neutron scattering is the only technique capable of probing the static and dynamic behavior of each polymer component individually with nanoscopic resolution. Fundamental insights generated from this work will develop a novel class of Li metal battery electrolytes accompanied by a theoretical framework to describe the thermodynamics and ion transport mechanism of the multicomponent polymer system. While we will focus on a single model system, the insights gained from the developed theoretical model can be applied broadly to guide material design of optimized battery electrolytes for various battery chemistries including “Beyond Li” chemistries (i.e., sodium, magnesium batteries).

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

Development of a Novel High Count Rate, High Resolution Neutron Camera with Advanced Gamma Discrimination Capabilities

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Neutrons are powerful nondestructive probes of the structure and dynamics of materials. They play a unique role in developing new materials due to the unique nature and features of neutrons, enabling insight into materials no other probe can. New materials are much needed to provide technology-enabling properties, including polymers, pharmaceuticals, biological membranes, batteries, solar cells, novel superconductors, and magnets.

Oak Ridge National Laboratory (ORNL) hosts two of the most powerful neutron sources in the world, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR). These world-class neutron sources currently support over 30 neutron scattering instruments designed for specific experiments that require tailored and sometimes unique neutron detector configurations. Detecting thermal and cold neutrons is challenging because of their low kinetic energy, low absorption cross-sections for most materials, and lack of charge. As neutron sources become more powerful, and next-generation neutron techniques more sensitive, current neutron detector technology is being pushed past fundamental limits of count rate, spatial resolution, and signal-to-noise ratio. The objective of this project is to develop a general-purpose neutron detector, suited to a wide range of scattering instruments, to meet these future requirements.

This detector will be based on current Anger camera technologies that use a scintillator layer to convert low-energy thermal neutrons into thousands of visible photons along with an array of silicon photomultipliers to localize the neutron absorption position. Improvements in both the neutron-converting layer (scintillator) and read-out electronics will allow seamless, unlimited tiling for building a modular detector array of sizes from tens to thousands of square centimeters. Hardware, firmware (programable logic), and software will be designed to allow for simultaneous neutron detection at separate locations on the detector as well as maximum count rates greater than 1 million per second. The ability to reject gamma radiation, which is unavoidably produced during neutron scattering experiments, is crucial for observing extremely weak but scientifically important signatures for many experiments. Gamma discrimination will be advanced via hardware-implemented pulse analysis and by using a novel, ORNL-developed multilayer scintillator that relies on the differences in electron and ion energy deposition to reduce the signal from gamma radiation.

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

Ultrafast Spin Torque Dynamics in van der Waals Magnetic Heterostructures

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This research program aims to achieve space-time visualization and manipulation of nonequilibrium spin, charge, and magnetic orderings using Sagnac interferometry and ultrafast time-resolved Kerr rotation optical microscopies, along with the Quantum Spin-Polarized Low-Energy Electron Microscope, at femtosecond temporal and nanoscale spatial resolutions. The PI and her collaborators will pioneer the development and adaptation of these advanced optical and electron microscopies to demonstrate the excitation and manipulation of nonequilibrium spin and charge orderings in van der Waals magnetic heterostructures driven by electrically-generated spin current and spin transfer torque. The fundamental knowledge established in this program will uncover emergent frontiers of modern condensed matter physics, such as Berry curvature of unoccupied states, topological phases, and long-range chiral spin orderings.

The research effort is organized under two themes. The first theme will be primarily conducted in the PI's lab to investigate space-time correlation of topological spin-torque dynamics in 2D magnets using advanced optical probes. The second theme will be carried out in collaboration with the Quantum Spin-Polarized Low-Energy Electron Microscope (qSPLEEM) user facility at the Lawrence Berkeley Lab Molecular Foundry, with the goal of visualizing nonequilibrium and nonuniform spin and charge orderings in van der Waals magnetic heterostructures.

The fundamental understanding of coupling and dynamics of various quantum degrees of freedom (spins, photons, magnons) at van der Waals interfaces and heterostructures provides a solid scientific foundation that will guide the choice of materials and the design of devices incorporating future spin-based quantum computing and quantum sensing hardware. The success of this proposed program will potentially address some of the most urgent needs for the microelectronic industry, particularly by enabling new forms of energy efficient nonvolatile magnetic memory, low-power computing, high-performance terahertz emitters, and multifunctional hybrid quantum devices with widespread societal impact.

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

Toward an Enhanced Photon Detection System for DUNE Far Detector 3

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The Deep Underground Neutrino Experiment (DUNE) aims to study neutrino oscillations, explore phenomena beyond the standard model of particle physics, and provide clues to explain why the universe does not have equal amounts of matter and antimatter. The photon detection system (PDS) of the DUNE far detector contains components that must operate in challenging, high-voltage environments at cryogenic temperatures. To address these challenges, power-over-fiber (PoF) technology has emerged as a reliable solution. The PoF technology produces electrical power by sending light, typically from a pig-tailed laser diode, through an optical fiber connected to a photovoltaic power converter. South Dakota School of Mines & Technology and Fermilab led the first application of PoF technology in high energy physics, successfully powering DUNE Far Detector 2 PDS prototypes that were located on a high-voltage cathode surface and submerged in liquid argon. This research project aims to enhance the PoF technology through collaboration with Fermilab and industry experts to develop customized solutions that optimize PoF components for harsh conditions. The improved technology will power the novel field-cage-integrated large-area photon detectors proposed for DUNE Far Detector 3. Expanding photon detection coverage will improve energy thresholds, time resolution, and energy resolution, enhancing sensitivities to supernova and solar neutrinos, as well as searches for phenomena beyond the standard model. Additionally, the analysis of charged-particle test-beam data that will be collected with DUNE prototypes located at the European Organization for Nuclear Research (CERN) will improve the understanding of hadron-argon interactions and develop better techniques for particle identification. The results of this project could guide future directions for using PoF technology in other systems operating in challenging environments, such as dark matter and neutrinoless double beta decay experiments. Moreover, the results of the project could benefit quantum and space-exploration technologies by offering a dependable solution with low noise, optimal efficiency and superior isolation.

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

Late-Time Observations of Type Ia Supernovae to Probe Nucleosynthesis in Thermonuclear Explosions

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Stars born with an initial mass approximately eight times or less than that of the Sun will evolve into a white dwarf (WD) star. Some WDs in binary star systems can experience thermonuclear runaway in their cores producing an explosion that fully disrupts and ejects the stellar material, known as a Type Ia supernova (SN Ia). Explosive nucleosynthesis in SNe Ia produces the majority of the iron-group elements (IGEs; e.g., iron, nickel, cobalt) in the Universe. While we know that WDs can explode, precise knowledge of the mechanism that ignites the explosion and the WD binary systems that can be disrupted via thermonuclear runaway eludes us. In the next year, two new experiments that scan the night sky searching for stellar explosions, the La Silla Schmidt Southern Survey (LS4) and the Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST), will each begin. For this DoE Early Career award, we will leverage the incredible synergistic possibilities of LS4 and LSST and connect these two experiments to produce a novel, holistic view of SNe Ia that captures their evolution from just after explosion for multiple years after their thermonuclear ignition. We will build a new machine learning model that uses artificial intelligence to automatically discover stellar explosions in newly acquired LS4 images. Following that, we will couple the observations from LS4 and LSST to constrain which WD systems explode and subsequently conduct three independent probes of explosive nucleosynthesis in SNe Ia, based on early, late, and ultra-late observations of thermonuclear SNe. The novel coupling of a small and large telescope will produce an unprecedented “experiment” that synergistically fuses two separate surveys to execute these disparate lines of inquiry producing the largest systematic study of nucleosynthesis in thermonuclear explosions that has ever been conducted.

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

Exploring Actinide Nanocrystal Growth towards Defining 5f Surface Chemistry

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When particles are very small, down to the nanometer length scale, they display unusual properties not typical of larger materials. Most of the atoms in these structures are at the surface of the particles, which give them different electronic properties. While these unusual properties have been studied in most of the periodic table, little is known about how the electronic properties of the actinides, such as neptunium and plutonium, behave when they become so small. This planned research will study growth pathways of actinide nanoscale particles. Interestingly, the shapes of the particles change depending on the specific actinide species, spanning from thorium through americium, despite having otherwise identical arrangements of atoms. This project will use differences in the shapes and growth pathways of different actinide particles to learn about trends in electronic properties at surfaces across the actinide row. Growth pathways will be determined using a combination of synthesis and the use of advanced X-ray characterization tools. These X-ray characterization tools can provide information about electronic properties and also local bonding characteristics. This project will also inform how to make unprecedented actinide oxide nanoparticles using very small quantities of material. This will enable safe working with radioactive materials and the study of materials that never before have been made into nanoparticles. Meanwhile, students will be trained in working with these exotic materials.

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

Time-Dependent Electronic Structure Theory of Atomic Qubits: Entanglement, Coherence, and Dynamical Response

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Neutral-atom quantum computers (NAQCs) are promising platforms for unlocking advanced quantum computation in analog mode. This transformative innovation could solve significant scientific challenges beyond the reach of conventional classical computing. Achieving this with NAQCs requires a comprehensive physical and quantitative understanding of two-dimensional atomic clusters, the building blocks of these quantum computers. Progress in this direction is essential for enhancing the creation and control of quantum coherences, as well as for the design and operation of groundbreaking NAQCs. However, a crucial unsolved problem is accurately predicting the time evolution of atomic qubits under arbitrary initial states and understanding how this evolution is influenced by driving laser fields and sources of noise. Addressing these points, this project aims to: (1) Advance new cutting-edge theoretical methods for predicting the dynamical response of general quantum states, such as entangled, superimposed, and excited states of NAQC building blocks; (2) Develop highly parallelizable open-source algorithms to numerically describe the time evolution of these atomic clusters under general initial states, laser pulses, and different geometrical settings; and (3) Discover strategies for generating, characterizing, and controlling coherent/entangled states. Additionally, the effect of physical sources of error/noise on the time behavior of atom clusters will be investigated, including ways to mitigate or control them. This work will result in the deployment of flexible, scalable, publicly accessible software to support the critical development of analog quantum computing systems aimed at surpassing the capabilities of conventional classical technologies.

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

Advancing the Lorentzian Frontier: From Collider Physics to Novel Structures in QFT

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The most powerful means of understanding nature at the smallest length scales is with particle colliders. Colliders smash together particles at the highest possible energies, briefly producing new particles through quantum fluctuations, and ultimately leading to complicated sprays of energy in the surrounding detectors. Improving our understanding of the underlying microscopic physics of the Standard Model, and furthering the search for subtle quantum imprints of new physics, therefore relies on our ability to decode these complicated correlations in energy flow.

In quantum field theory, energy flux in collider physics experiments is described by correlation functions of energy flow operators. These operators have recently been found to play a central role in diverse areas of formal quantum field theory and gravity, with applications ranging from non-perturbative constraints on renormalization group flows, to understanding the emergence of causality in the Anti-de Sitter Space / Conformal Field Theory correspondence.

The goal of this research program is to explore both formal aspects, and phenomenological applications, of energy flow operators, and to build bridges between developments in formal quantum field theory and collider phenomenology. The research program will develop new theoretical tools to enable world record precision measurements of parameters of the Standard Model of particle physics, will enhance searches for new physics at colliders, and will uncover novel theoretical structures in quantum field theory and gravity.

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

Topological Classification of Chemical Reactions:
A New Tool to Understand and Manipulate Chemical Reactivity

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We will develop a fundamentally new approach for exploring the quantum mechanical principles of molecules and their reactions by leveraging recent developments in the field of topological physics. This approach has the potential to change the way chemical reactions are understood and manipulated by providing novel tools and concepts for examining the global properties of the potential energy surface using topological methods. The project will focus on three aims: 1) Systematically establishing the use of modern topological concepts such as invariants for molecules; 2) Studying the relationship between changes in topological invariants and reaction dynamics; and 3) Applying the new theory to a model system: cyclization reactions described by the Woodward-Hoffmann rules, to find systematic ways to switch between allowed and forbidden pathways.

The application of topology, a branch of mathematics, to the study of electronic energy bands in crystalline materials has had a revolutionary impact on the field of condensed matter physics; it led to the discovery of new quantum states such as topological insulators and semimetals and was recognized with the 2016 Nobel Prize in Physics. In the context of topological band theory, topological invariants serve as order parameters for crossings between electronic energy levels. These crossings, whether manifesting as isolated points, lines, or surfaces, cause the occurrence of topological surface states. Electrons in these states are protected from scattering, making topological materials attractive for use in the next generation of electronic devices as scattering can limit device performance. Current estimates suggest that approximately 53% of existing crystalline materials might harbor topologically protected electronic states, a statistic that underscores the widespread potential of topological analysis in materials science.

The application of modern topological methods to molecular systems has been largely unexplored, since insights from band theory do not easily translate due to the distinct quantum mechanical descriptions of solids and molecules. Understanding the global properties of the potential energy surface (PES), including the location and connectivity of crossings and avoided crossings, is crucial for developing tools to selectively influence the outcome of chemical reactions. We will bridge this gap by providing new tools to predict and manipulate the outcome of chemical reactions through classifying the global properties of the PES with topological methods. We will focus on experimentally verifiable predictions that will provide the chemical community with a set of theoretical tools for tackling the challenges of chemical synthesis. A long-term outcome of a successful effort will be new tools to predict and manipulate the outcome of chemical reactions by classifying the global properties of the potential energy surface, e.g. crossing points, seams and higher order saddle points through topological methods. The ability to greatly improve cycle-fatigue of electrocyclization based photoswitches would provide a new framework to drive new innovations in chemical synthesis.

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

Enzyme-like Porous Catalysts for Upgrading Biomass Feedstocks

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Biomass is the largest source of renewable carbon, and the ability to refine it into valuable products could significantly reduce petroleum usage. Unfortunately, significant quantities of biomass are wasted because current catalysts struggle to efficiently transform these complex chemicals, like lignin and polyols, into desirable value-added commodities. Enzymes can accomplish many of these challenging reactions in large part due to their multifunctional active sites, but they are fragile and costly. Our objective is to integrate key features of enzymes into solid-state materials to achieve durable, recyclable, and highly efficient heterogeneous catalysts for tackling biomass conversion. However, the design and synthesis of artificial materials that approach the complexity of enzymes is a long-standing challenge. This project leverages recently discovered peptide frameworks, which are porous solid-state materials spontaneously generated from peptide self-assembly. Like enzyme active sites, the pores within these materials have multiple unique functional groups that are permutable, enabling rapid synthesis of elaborate catalyst variants. This project will evolve these scaffolds to enhance the sustainability and efficiency of catalytic processes for aerobic lignin valorization and polyol deoxygenation. Furthermore, the crystallinity of these peptide frameworks provides a unique opportunity to routinely obtain high-resolution structural data that informs the rational design of next-generation catalysts. The expected outcomes of this research are more efficient catalysts for upgrading biomass, versatile tools to precisely manipulate multiple noncovalent interactions, and fundamental structure-activity knowledge for enzyme-like catalyst design.

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

Precision Cyclotron Radiation Emission Spectroscopy for direct neutrino mass measurements

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Neutrinos are the most common particles of known matter. They played a crucial role in shaping the formation of structure in the early universe. Today, they are emitted in huge numbers by the fusion reactions that power the sun. Our fundamental theories predicted that they would be massless, but experiments have shown that they do have a tiny mass: less than one millionth that of electrons! They are so light that no one has yet succeeded in measuring their mass, only in setting an upper limit. We also don't understand the physics that gives rise to neutrino mass; it may be connected to yet-to-be-discovered, extremely heavy particles, or even to the mechanism that caused there to be more matter than antimatter in the universe, enabling our existence. Knowing the mass of neutrinos would improve our understanding of both fundamental physics and of the origins of our universe.

The research funded by this Early Career Award will advance an emerging technique, Cyclotron Radiation Emission Spectroscopy (CRES), to pave the way to measuring the neutrino mass. To learn about neutrino mass, we observe the radioactive decay of tritium, which produces an electron and an anti-neutrino (which has the same mass as a regular-matter neutrino). We cannot detect the neutrinos directly, but by precisely measuring the energy of the electrons that are produced, we can deduce how much energy from the decay is going into creating the neutrino mass, following $E=mc^2$. With the CRES technique, rather than measuring the electrons' energies by letting them slam into a solid detector as in previous detection techniques, we use an antenna to pick up the extremely faint radio waves that each single electron produces as it moves in a magnetic field. The frequency of these radio waves tells us the electron's energy, a link caused by Einstein’s special relativity.

Recently, with the Project 8 Collaboration, we published the first neutrino-mass measurement using CRES. It demonstrated CRES's excellent energy precision and powerful background-noise suppression. To become sensitive to even smaller neutrino masses, we must make the experimental apparatus larger to observe more decays, and we must also measure electron energies more precisely than ever before. Using a new resonant-cavity-based detector that is compatible with this scaling-up, we will measure the energies of electrons emitted by ^{83m}Kr internal-conversion decay with a goal of reaching 0.3 eV resolution, more than three times better precision than in our previous work. We will also improve precision by developing magnetometry, energy-calibration, and analysis techniques to make use of signal features to reconstruct, and correct for, the tiny differences in the magnetic fields experienced by individual electrons. These improvements will play a crucial role in making it possible to reach our targeted sensitivity to ten-times-lower neutrino mass than the limit set by current experiments. This will yield insight into how the universe became what it is today.

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

Modeling the Molecular Mechanisms of Interfacial Welding in Self-Healing Polymers

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Intrinsically self-healing polymers are plastics that rapidly repair damage when two broken interfaces are brought into contact. Self-healing plastics have garnered interest as sustainable plastic alternatives because they can be repaired and reused, reducing the accumulation of plastic waste. However, designing self-healing plastics remains challenging because the molecular mechanisms governing self-healing remain poorly understood in many polymer systems. We lack this knowledge because self-healing occurs at nanoscale polymer interfaces, and experiments cannot easily access these details while interfaces are welding together. The objective of our project is to combine molecular dynamics simulations and mechanical welding experiments to identify the molecular mechanisms that mediate self-healing in polymers with precisely controlled chemical sequences. Molecular simulations can directly resolve the molecular-scale details of polymer interfaces and relate them to the time-dependent recovery of mechanical strength measured in experiments. This combined approach will build fundamental relationships relating the chemical structure of polymer chains to the speed at which they recover specific mechanical properties like strength, stiffness, and yield stress during interfacial welding. Our findings will guide the molecular design and synthesis of new self-healing plastics with improved durability and repairability.

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

Quantum Computing and Machine Learning for Enhanced Understanding of Fracture Flow

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Understanding fluid flow through complex fracture networks is essential to advance energy systems such as hydraulic fracturing, enhanced geothermal systems, carbon sequestration, and hydrogen storage. Traditional numerical methods struggle to model these networks because of the wide range of fracture sizes and their complex interconnections. This research utilizes machine learning and quantum computing to address these challenges. By training advanced machine learning models, the project will create fast, accurate simulations of reactive transport processes across multiple scales, significantly reducing computational costs while maintaining high accuracy. Quantum computing will be employed to explore the potential of solving large systems of fracture flow equations that are currently intractable with classical computers, providing insights into the role of small-scale fractures that are neglected in classical simulations. Quantum algorithms for seismic wave propagation will also be studied, aiming to enhance interpretation of seismic data and improve models of subsurface dynamics. While quantum computing holds promise, this work aims to estimate the quantum resources required and optimize algorithms to make them practical for application to fractured systems in the coming years. This research aligns with the mission to develop advanced computational methods for subsurface energy applications, supporting the clean energy transition.

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

Searching for Strongly Coupled Dark Matter at the LHC with Unsupervised and Generative AI

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The nature of dark matter remains one of the outstanding questions in particle physics. New models of strongly coupled hidden sectors akin to standard model (SM) quantum chromodynamics (QCD), called "dark QCD", predict invisible, composite dark matter candidates that are only accessible at colliders. These models are associated with several novel phenomena, notably semivisible jets, which contain a mixture of visible particles and invisible dark matter. Data acquired from the third physics run of the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland provide an unparalleled opportunity to execute a model-independent strategy motivated by the complexity of dark QCD. At the Compact Muon Solenoid (CMS) experiment, unsupervised artificial intelligence (AI) will be employed to record interesting or "anomalous" events at the trigger level, as well as to reject SM background jets. Semi-supervised, interpretable AI will reconstruct the mass of the dark matter particles from the semivisible jets, providing an observable signature independent of how the dark sector couples to the SM. Once this search is complete, combinations of semivisible jets and other dark QCD phenomena will be scanned to identify models that have not yet been covered in order to motivate future CMS searches at the high-luminosity LHC. Exploring this broad model space requires large simulated event samples, which are prohibitive to produce with the current software. Diffusion models, a leading generative AI technique, will be trained to replace and enhance detector simulation, providing competitive quality while substantially reducing computation. The algorithm inference will be accelerated on graphics processing unit (GPU) coprocessors, such as those at high performance computing (HPC) centers, accessed as a service to maximize portability, flexibility, and throughput, while minimizing cost. The outcomes from this research are expected to have theoretical impact and practical relevance throughout the field of particle physics while simultaneously advancing feasibility and design studies for future colliders.

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

Co-designed Quantum Many-Body Suite for Deciphering Quantum Phenomena in Complex Molecular Systems

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Complex molecular systems, particularly the quantum phenomena they exhibit, present significant challenges due to limitations in integrating current theories, computational methods, and the experimental observations. The core scientific challenge is to accurately model quantum exchanges of charge, spin, and energy, which are crucial across various disciplines. Examples include understanding how molecules with specific structures can transport quantum states, how water shows unique quantum behaviors over time, and how molecules interact with light and vibrations at the quantum level. Gaining insight into these systems-level behaviors and emergent functionalities will facilitate the manipulation of information and energy transport in a wide range of fields such as catalysis and quantum information science.

Towards this goal, this project will develop an innovative and comprehensive quantum many-body suite. This suite aims to overcome the challenge of simulating system-level behaviors with precise control over accuracy, ensuring computational efficiency and sustainability. The project will leverage our experience developing computational chemistry capabilities at Pacific Northwest National Laboratory, and the synergy among advanced theories in quantum chemistry, physics, and mathematics alongside state-of-the-art computing technologies and leading-edge experimental methods. This integrated approach will enable more detailed study of specific complex molecular systems in detail.

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

Exclusive Reactions at the EIC with Far-Forward Superconducting Nanowire Detectors

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Superconducting nanowire detectors, known for their exceptional speed and precision, are widely used in quantum information science and nanophotonics to count individual photons at high rates with minimal noise. However, their use in other fields, such as nuclear physics, is rare and not yet fully exploited. This research aims to adapt this quantum technology into a fully functional charged particle detector for the upcoming Electron-Ion Collider at Brookhaven National Laboratory capable. This research project will develop superconducting nanowire sensor arrays and integrated cryogenic electronics components, to detect and identify particles in the harsh environment of the accelerator where the detection is very close to the high intensity circulating beams far from the collision point. Successfully creating this technology will significantly enhance the nuclear physics research program at accelerator facilities and contribute valuable knowledge to the field of quantum sensors by understanding how they operate under a variety of conditions, including high magnetic field environments.

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

Investigating the Fundamental Properties of the Heaviest Elements

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The Periodic Table of Elements (PTE), one of science's biggest celebrities, might need revisions. It is well-recognized, even by elementary students, that the PTE elegantly organizes the elements by their chemical properties. But what if the chart adorning classroom walls is wrong? The Superheavy Elements (SHEs, Z > 103) were added to the PTE by increasing proton number at the bottom of the d-block. Yet, the suggested "signature" d-electron configurations and associated chemical behaviors indicated by these placements may be significantly different from the true properties of these elements due to the onset of relativistic effects. In the past, studying the chemical properties of SHEs has been tough - they don't exist naturally on Earth and need to be created one atom at a time in nuclear physics labs. They are also highly radioactive with short lifespans, making their properties hard to pin down. This research program aims to re-evaluate the placements of these elusive elements by probing the accessibility and reactivity of each element's signature d-electron configuration. The first step will be to examine the accessibility of the d^1 and d^2 electron configurations of Lr (Z = 103) and Rf (Z = 104), respectively. It has been shown, in systematic gas-phase studies of elements more accessible than SHEs, that metal ions with ground state or low-lying d^1 or d^2 electron configurations would form distinct molecular products if reacted with alkane gases such as methane, ethane, etc. To perform similar studies on SHEs, a new experimental technique has been developed at Berkeley Lab utilizing the Berkeley Gas-Filled Separator and FIONA devices. This technique allows for the direct assessment of SHE ion reactivity using atom-at-a-time gas-phase measurements. Now, SHE ions can be contained within an ion trap while reactive gases are added, enabling chemical reactions to occur. The resulting species are then directly identified by their mass-to-charge ratio. Observing the specific molecular species produced from these reactions with alkane gases will reveal the true d-character of these heavy elements and help determine their correct positions on the PTE.

This research was selected for funding by the Offices of Basic Energy Sciences and Nuclear Physics.

Investigating the interactive impact of long-term warming and altered precipitation on grassland nitrifying communities

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Nitrogen is a major limiting nutrient for living organisms in many natural and agricultural ecosystems. Soil microorganisms play critical roles in the global nitrogen cycle. Microorganisms such as archaea and bacteria that are able to oxidize ammonia to nitrite and then to nitrate, are called nitrifiers. These microorganisms control the inventory and transformation of reactive nitrogen species in soils. Nitrifiers also contribute to nitrogen losses by producing the powerful greenhouse gas nitrous oxide and as nitrate moves from the soil into groundwater. Understanding how environmental and climatic variables control nitrifier abundance and activity is essential for achieving a sustainable bioenergy economy and maintaining healthy soil ecosystems amidst rapid climate change. Leveraging a long-term experimental field simulation system established in 2009 at a US Great Plains tallgrass prairie in central Oklahoma, this research combines fieldwork and laboratory studies to investigate the interactive effects of climate warming and altered precipitation on the diversity, structure, and activities of soil nitrifiers, the nitrification process, and the associated nitrous oxide production. Using an integrated approach that includes culture-based ecophysiological characterizations, multi-omics technologies, stable isotope probing, and high-throughput droplet microfluidics, this project aims to elucidate the physiological, molecular, and ecological mechanisms controlling the responses of soil nitrifiers to climate change. This work will expand our understanding of the impact of anthropogenic climate change on microorganisms involved in the nitrogen cycle and the corresponding microbial feedback to soil biogeochemistry, nutrient dynamics, and greenhouse gas emissions.

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

Understanding and Controlling Light and Spin Dynamics in Chiral Hybrid Semiconductors

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Semiconductor spintronics aims to advance the evolution of next generation low-power electronics, information processing, communication, and storage. In order for spintronic devices to fulfill the demands for high-speed, high-density, and low-power electronic components, innovations in materials design and processes are essential. The spin generation and manipulation in GaAs is feasible due to a strong spin-orbit coupling (SOC), however, the spin lifetime is relatively short. Whereas in graphene and diamond with weak SOC, longer spin lifetimes are observed. Materials possessing both strong SOC and prolonged spin lifetimes represent an ideal yet rare category for spintronic applications, offering an exciting prospect for the development of unconventional semiconductors. To fill this gap, this project will be subdivided into two tasks: (1) advancing new organic-inorganic chiral semiconductors with tailored chiroptical properties, and (2) subsequently obtaining optical control and manipulation of spin dynamics without the need for an external magnetic field through ultrafast spectroscopy measurements. Achieving the objectives of this project requires a strong synergy between materials design and synthesis using a solution-processable approach and advanced characterization of optical and spin dynamics in the materials. This accomplishment will enable the control and characterization of chiral semiconductors, providing guidelines for designing superior solution-processable spintronic materials.

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

Searching for New Physics with Real-time Anomaly Detection

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An extremely vast array of searches for physics beyond the Standard Model (BSM) have been performed during the lifetime of the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) near Geneva, Switzerland. Although certain tantalizing hints exist, BSM physics remains elusive. As a result, it is becoming increasingly necessary to question the typical paradigms and methods used in new physics searches at the LHC. Modern artificial intelligence and machine learning (AI/ML) techniques, specifically those under the umbrella of "anomaly detection" (AD), are now capable of enabling searches that do not rely on assumptions about the nature of BSM physics. Such AD techniques are especially necessary in cases where the form that BSM physics may take does not agree with existing theoretical models and where current strategies are highly unlikely to produce a future discovery. The prospects for a discovery with traditional analysis methods are even weaker in scenarios where BSM physics occupies a region of phase space that is not selected by existing experimental trigger methods. In this case, a new observation will not occur through larger datasets or more advanced data analysis, but instead only through improved triggering capabilities. The integration of real-time AD into the ATLAS (A Toroidal LHC ApparatuS) detector's trigger at the LHC will be combined with sophisticated AD-based search methods that are designed in conjunction with those used in the trigger. The comprehensive application of AD at all stages of data collection and analysis will maximize the potential for scientific discoveries and provide sensitivity to new physics that would otherwise go entirely undetected at the LHC. Moreover, this research will make extensive use of recent advances in the deployment of AI/ML on field-programmable gate arrays (FPGAs) to improve the efficacy of the complex ATLAS trigger framework as well as facilitate broader improvements in AI/ML that can enhance subsequent data analysis capabilities. The techniques and tools developed for real-time AD are also expected to have profound implications for on-detector data compression at both current and future particle physics experiments.

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

Chemical and Loading Rate Controls on Fracture: Toward a Universal 'Phase-Diagram' of Factors Controlling Fracture Networks from Creep to Dynamic Failure

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A boulder slowly falling apart in the desert, stimulation of bedrock in geothermal wells, and an asteroid impact – all of these are examples of fracture in rocks, but the *rate* of fracturing or cracking goes across twelve orders of magnitude ($<10^{-8}$ m/s to $>10^{3}$ m/s). If these were lengths, this range of magnitudes is the difference of a size of less than the head of a pin (1 mm) vs. the distance to the moon (4 trillion mm). Despite how common fractures are and their broad use in engineered systems, no systematic experimental study or theoretical framework exists for the full range of deformation rates, or detailed understanding of the molecular mechanisms that control the fracture-scale observations. This research fills that gap. Across the full range of fracture rates, the project combines physical experiments that control the factors that drive fracture (chemical reactions vs. mechanically pulling the material apart), and simulations of the processes at the molecular scale. Ultimately, the experiments and simulations will be used to test a concept that could unite the full range of deformation together into a unified framework.

Fractures form when a narrow tip is levered open – the tip concentrates stress, providing a preferred location for the material to rupture. At high rates, the molecular bonds holding the rock together are being mechanically torn apart. At the highest rates, the fracture propagates near the speed of sound – the limit of rate of fracture propagation – and excess energy is used up either fracturing the rock away from the main fracture or in 'tearing' liquids like water off the fracture surfaces. At the lowest rates, the stretching of molecular bonds at the crack tip allows water to more easily break bonds at the tip – this is a process called stress corrosion. Intermediate (quasistatic) rates lead to single fracture planes. Complicating the picture above, if the crack tip is repeatedly stressed, or fatigued, then small flaws will randomly add up around the fracture tip and in the rest of the material, forming a volume that is damaged which allows fractures to move forward.

This study fractures silicate rocks across the full spectrum of deformation rates, exploring the impact of different types and sizes of flaws, chemical reaction rates, and surface tension on the energy required to break the material. The study places fracturing processes into a unified framework *independent of* rate by quantifying how different factors dissipate energy during fracturing, either away from the crack tip or in the crack tip. This is analogous to using a prybar to break apart pieces of particle board vs. pieces of hickory. The study proposes that rocks don't care about the process and rate that breaks them, just the efficiency of being broken.

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

Chiral Dynamics in Asymmetric Catalysts Probed by X-rays

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Chirality, or the lack of inversion symmetry, is very common in nature and is found on all scales, from the shape of galaxies to certain properties of subatomic particles. It is crucial across a broad array of open questions in chemistry, including both fundamental problems and applied challenges. In this program, we will develop new X-ray spectroscopy techniques to explore chirality as it occurs in molecules. These techniques will provide a qualitatively new type of element-sensitive local information that will help scientists understand the structure and evolution of chirality at the atomic level. Specifically, we aim to understand the process of asymmetric catalysis, in which chirality is transferred from a chiral molecule to an achiral one.

Current techniques can detect whether a molecule is chiral but are less successful at detecting where and how chirality is induced. To access that mechanistic information, we will develop chirality-sensitive ultrafast X-ray spectroscopies. These have become feasible due to recent improvements at large-scale X-ray light sources, that now provide adequate energy, brightness, time resolution, stability, and polarization control. We will carry out experiments both on simple, well-known chiral molecules and on chiral transition-metal catalysts. These experiments will be complemented by theoretical and modeling work.

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

Scalable Additive Manufacturing of Spherical Foam Targets for Inertial Fusion Energy

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Nuclear fusion promises clean, reliable, safe, and abundant energy with minimal radiation risks. The 2022 fusion ignition demonstration at the National Ignition Facility marked a critical milestone toward achieving the goal of producing net energy via inertial fusion. However, major scientific and technological barriers remain in making inertial fusion energy (IFE) an economically viable source of electricity. One of the biggest hurdles is the cost and production rate of the spherical fuel containers, which are known as targets. For fusion to be economically competitive, targets must be produced at a fraction of the current cost and at much higher speeds. At present, target manufacturing is slow and expensive due to the need for extreme precision. This project aims to transform IFE target manufacturing from a low-volume, expensive effort into a cost-effective, mass-production enterprise. This will be achieved by generating the processing science for a scalable additive manufacturing (AM) approach for producing foam targets using the two-photon polymerization (2PP) technique. This technique uses light to process material with nanoscale precision. Although 2PP can achieve the extreme precision needed for IFE targets, it currently suffers from uncontrolled defects and low production rates. These challenges will be overcome by studying and eliminating defects, increasing production rates, and reducing costs through novel light projection techniques. By transforming 2PP into a fast layer-by-layer process and developing models to predict the processing outcomes, this project seeks to create a scalable, affordable, and ultra-precise IFE target manufacturing approach. The resulting manufacturing capability will enable novel experimental and computational physics studies of target yield performance with advanced foam-based target designs. Furthermore, the manufacturing science knowledge generated in this work will pave the way for commercially viable fusion energy by enabling the industrial-scale production of IFE targets.

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

Hydrodynamics as a Platform to Harness Emergent Properties of Quantum Materials

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Transport measurements are incredibly sensitive tools for examining the emerging low-energy, long-wavelength features of quantum materials. Unfortunately, very few methods exist to calculate transport properties in strongly correlated materials without making unjustified assumptions about quasiparticles and their scattering. In this context, the formalism of hydrodynamics stands out as a non-perturbative method which works even better in the presence of strong interactions. In this project, we develop new theoretical formalism to (1) find new materials exhibiting hydrodynamic transport and predict smoking-gun signatures of this regime, (2) surpass the limitations of semiclassical calculations by exploiting connections with the growth of operator complexity in quantum systems, and (3) explore unique features of hydrodynamic transport by exploiting non-linear, topological, and geometrical effects.

In the first thrust, we use numerical methods to calculate the electron-electron scattering operator for realistic band structures obtained from first principles, and use it to make quantitative predictions about experiments which are sensitive probes of the hierarchy of relaxation timescales in correlated metals, namely (1) ultrasound attenuation, (2) the angle-dependent magnetoresistance, (3) the temperature scaling of the resistivity, and (4) non-linear transport as a probe of Berry curvature multipoles. In the second thrust, we use the connection between Krylov operator growth and quantum transport to derive general properties of transport in correlated materials which depend only on universal features of the Krylov description of quantum dynamics. In the third trust, we develop a combination of theoretical tools (from the Navier-Stokes equation to lattice Boltzmann simulations) to study how the interplay between non-linear, topological, and geometrical effects contributes to the emergence of novel phenomena in hydrodynamic metals.

The research program will advance the field of viscous electronics which has shown promise for applications in low-energy electronics, optoelectronics, and plasmonics. It will also produce new tools to predict transport properties of quantum materials, including a detailed understanding of the hierarchy of relaxation time scales in correlated metals. The research program will be complemented by an educational mission centered around student mentorship and training, with a special emphasis on fostering greater involvement of underrepresented minorities in physics.

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

Atomistic Information Theory of Materials Synthesis and Free Energy Landscapes

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Atomic-scale control of synthesis can enable the production of materials with structures and properties unachievable by conventional routes. While determining which structures should be synthesized is now a mature task within computational science, predicting how to synthesize them is challenging with computational methods, particularly at the atomistic scale. This project will develop a theoretical framework to obtain and control free energy pathways relevant for materials synthesis. By building on recent advances in machine learning potentials, high-throughput simulations, synthesis prediction, and statistical thermodynamics, this work will: (1) propose an atomistic information theory to simplify calculations of free energies landscapes; (2) rationalize crystallization and precursor selection in inorganic synthesis using information as a surrogate for free energies; (3) compute kinetic phase diagrams to inform advanced manufacturing approaches; and (4) elucidate mechanisms of synthesis for seed-assisted crystallization of inorganic materials, interfaces, and amorphous systems. Complementing property prediction methods or materials design pipelines, this project proposes a first-principles approach to synthesis simulation by focusing on large-scale quantification of entropy and its surrogate metrics. Along with atomistic simulations, the work will deliver a computational counterpart to *in situ* characterization methods for synthesis and theoretical models that rationalize processing conditions for transformative manufacturing.

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

Reducing the core-edge integration gaps in tokamaks with novel divertor geometries and plasma configurations

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This project will provide two-dimensional quantitative divertor detachment characterization for a range of existing and proposed DIII-D divertor geometries, targeting core-edge integration issues in tokamaks via new diagnostics, experimental analysis, and simulations on the DIII-D National Fusion Facility. One of the main challenges faced by magnetic fusion energy devices is the integration of a high-performance core with a divertor plasma compatible with the survival of the divertor and first wall materials. Future reactors will rely on impurity seeding to achieve divertor detachment and reduce steady state and transient heat fluxes onto plasma-facing components. The DIII-D National Fusion Facility is pursuing an upgrade plan to test new divertors for improved detachment front stability, develop new plasma scenarios based on negative triangularity shaping, and change the wall materials to reduce the extrapolation gap to future fusion power plants. Enabled by new spectroscopic capabilities—together with the existing suite of unique DIII-D divertor diagnostics and the anticipated divertor upgrades—this research program will address core edge integration questions essential for future devices, derive empirical detachment scalings, experimentally verify capabilities of the new divertor/wall upgrades to optimize the divertor radiation front while avoiding transient re-attachment and act to validate boundary codes in divertor regimes closer to those expected in a reactor. This research will develop new fast 2D ultraviolet-visible spectroscopy and ultraviolet spectroscopic imaging diagnostics for determining seeded impurity densities and radiation dynamics and steady-state and time-dependent simulation capabilities benchmarked on the DIII-D tokamak that will aid in the extrapolation towards a tokamak-based fusion power plant.

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

Dynamically Switching Polymer Networks using Transmutable Nanoparticles as Crosslinks

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Bio-inspired, self-repairing properties for polymeric materials prolong the lifetime of materials against physical damage. The translation of such fundamental biological principles to materials systems is important for advancing the versatility and energy efficiency of modern materials. This research will apply interfacial engineering and self-assembly strategies to synthesize a multi-component polymeric material that displays reversible mechanical adaptability. We will achieve this goal through the judicious design of transmutable nanoparticles as polymer crosslinks that can reversibly control the interfacial nanoscale bond dynamics and network topology at junctions. Positive cooperativity via multivalent interactions enhances the bond strength of underlying weak monovalent interactions in polymer networks, but it also slows down the bond exchange kinetics and self-repairing efficiency. Our strategy will mitigate this effect by manipulating the extent of positive cooperativity by controlling the number and type of interfacial interactions using an external stimulus and providing a synthetic route to reach two (or more) distinct equilibrium states. Overcoming this key drawback of self-repairing polymers using nanotechnology will enable the design of sustainable materials for a wide range of applications relevant to energy technologies, including bio-inspired mechanics, photoactuators, and advanced packaging, and, more broadly, the basic science underpinning the role of nanoscale bond dynamics in multi-component polymer networks.

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

Light-Driven Proximity Control of Designer Moiré Nanomaterials

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Exposing quantum materials to intense electromagnetic stimulation can induce novel emergent phenomena that are unattainable in thermodynamic equilibrium. In recent years, extensive experimental work has aimed to discover new quantum phases driven by ultrafast laser pulses, which can enhance our knowledge of quantum many-body systems out of equilibrium and enrich the possibilities for next-generation quantum technologies. However, we lack a systematic understanding of how nonequilibrium quantum phases emerge, what forms they can take, and how to control them. A promising approach to bridge this knowledge gap and foster new technological developments is to integrate ultrafast control techniques with nanomaterial systems that possess flat electronic bands, since they possess rich quantum phases, high sensitivity to small perturbations, and versatile equilibrium control knobs that can unlock new territory for nonequilibrium exploration.

This project will develop and deploy novel ultrafast driving protocols to realize nonequilibrium electronic and magnetic phases in two-dimensional (2D) moiré nanomaterials. Femtosecond laser excitation can generate rapid light-induced effects in different 2D materials, including charge/spin dynamics and phase transitions. Our strategy is to use tailored laser pulses to photo-excite 2D materials in proximity to a moiré bilayer, which can quickly modify the moiré parameters in a non-local fashion. Specifically, we will harness interlayer charge transfer, photo-induced insulator-to-metal transitions, and ultrafast magnetization dynamics to generate rapid doping, screening changes, and magnetic exchange field control in a target moiré material. These three ultrafast “proximity pumping” protocols will be combined with traditional photodoping control and equilibrium moiré tuning knobs, such as electrostatic doping and electric field, to systematically investigate the response of 2D moiré magnetism and correlated insulating states far from equilibrium. This research will address fundamental questions about moiré quantum materials, enable new functionalities for quantum optoelectronics, and establish a strategy for precisely tailoring light and matter to create, understand, and control nonequilibrium phases.

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

UNSHADE: Understanding and Modeling of Shallow to Deep Convection Transition

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Moist convection, a key component in cloud formation, precipitation, and energy transport, is critical to understanding and modeling weather and climate. Moist convection undergoes several stages, evolving from shallow clouds to deep precipitating convection. The shallow to deep convection transition is subject to considerable variability, influenced by factors such as atmospheric thermodynamics, large-scale flows, land-atmosphere interactions, and the dynamics of the planetary boundary layer. Climate models frequently struggle with accurately capturing shallow to deep convection transition, often hastening the transition phase and triggering deep convection prematurely, sometimes hours earlier than observations. Such premature activation contributes to significant inaccuracies in the timing and intensity of convective processes. This, in turn, misrepresents the diurnal cycle of precipitation and the cloud radiative effects, leading to substantial biases in the hydrological cycle and the Earth's energy budget as predicted by these models.

Accurately modeling the shallow to deep convection transition requires understanding the complex interplay of multiple factors, such as the atmospheric thermodynamic state and updraft characteristics, including their width and turbulent kinetic energy. The non-linear nature of these interactions complicates both the quantification of individual contributions and the development of accurate models that depict the evolution of convection. This project addresses these challenges by using observational data from the Atmospheric Radiation Measurement (ARM) Mobile Facility at the Bankhead National Forest (AMF3-BNF). We will employ advanced machine learning techniques to preprocess this data and develop models that quantify the factors contributing to the shallow to deep convection transition. The AMF3-BNF site is ideal for this research due to its comprehensive monitoring capabilities of the land surface, planetary boundary layer, and lower free troposphere.

The UNSHADE project aims to clarify the role of various factors in the convection transition using modern machine learning methods. By incorporating these insights into climate models, the project aims to refine predictions of the diurnal cycle of moist convection, improving the accuracy of hydrological cycle and Earth's energy budget forecasts. Additionally, UNSHADE will develop machine learning-based tools for data preprocessing, which will be integrated into the ARM data system to enhance research on land-atmosphere interactions, planetary boundary layer dynamics, and deep convection.

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

Mind the Gap: Direct Probing Room Temperature Topological Spin Textures with Multi-modal Electron Microscopy

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Topological spin textures such as skyrmions are particle-like objects consisting of swirling spins that have the potential to revolutionize information and related technologies. Two-dimensional (2D) van der Waals (vdW) magnetic materials offer a unique platform for exploring novel magnetic and topological phases, owing to their highly tunable crystal symmetries and magnetic interactions within and across the vdW gap. Room temperature stabilization of topological spin textures opens opportunities for spintronics applications based on atomically thin vdW crystals. This research project will develop innovative techniques based on four-dimensional scanning transmission electron microscopy (4D-STEM) to directly measure the spin and lattice structures and understand the interplay between real-space topology, crystal symmetry breaking, and magnetism. Specifically, the goal is to investigate how the topological spin textures beyond skyrmion are stabilized at room temperature through intercalated magnetic atoms within the vdW gap. Furthermore, this research will manipulate emergent spin textures and elucidate the mechanisms of their transformation, using in-situ 4D-STEM with electrical and temperature measurements within nanodevices. The findings are expected to provide a foundational understanding of the underlying physics that governs these complex materials, thereby enabling the design and manipulation of quantum materials for future technological applications.

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

Spin Dynamics of Molecular Qubits

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Molecules with unpaired electrons can serve as the building blocks of the next-generation artificial systems for quantum information processing. Such molecular qubits have a well-defined molecular structure, which can be tuned with remarkable precision. Molecular qubits employ the electronic spin, an intrinsic quantum property of the electron, to encode quantum information. However, interactions of the electronic spin with molecular vibrations disrupt the coherent motion of the spin, destroying the stored quantum information. Molecular qubits are thus a fruitful playground to address fundamental questions on the loss of quantum coherence as a result of the interactions of quantum systems with their environment. By developing and applying theoretical and computational methods, this research aims to derive a comprehensive first-principles microscopic model of the decoherence processes that destroy the electronic spin coherence in molecules. The model will include both traditional spin-vibrational interactions, resulting from the vibrational modulation of static spin interactions, and novel spin-vibrational interactions, resulting from the finite-velocity atomic motion, like the spin-vibrational orbit coupling. Using the first-principles model, this research will uncover how molecular composition, geometry, electronic structure, and vibrational motion work together to determine the spin coherence of molecular spin systems. The new theoretical methods will be employed to directly simulate the spin dynamics of structurally diverse molecular qubit candidates, charting the road to enhanced electronic spin coherence at elevated temperatures in early-transition-metal molecular qubits. The theoretical approaches will also be applied to understand spin coherence in optically controlled electronic spin qubits, which employ the interaction of molecules with light to manipulate the electronic spin, and to describe the spin dynamics of molecular qubits in complex chemical systems. Beyond enabling the structural tunability of the coherent properties of molecular spin systems, this research will define strategies to create and manipulate quantum states for quantum information processing of molecular coherent systems in diverse chemical environments and in a wide temperature range.

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

Application of Additive Manufacturing to Target Fabrication

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Innovation in target fabrication approaches is needed for isotope production to meet increased demands for radionuclides and evolution of accelerator facilities that will have higher intensity beams. In most cases of isotope production, full dissolution of the target is not desirable as it slows down the radiochemical isolation of the product, can decrease the specific activity, and at times, introduce complex or hazardous chemical processes for hard-to-dissolve metals. Additive manufacturing (AM) allows for careful tuning of the composition and geometry of a final component through feedstock design and particle consolidation approach. Specifically, the ability to tune the composition will be leveraged in this work by creating custom multi-element feedstocks to avoid full target dissolution. The approach will apply four objectives to three radionuclide production test cases: 1) synthesize and characterize feedstock, 2) deposit feedstock on the substrate and characterize, 3) irradiate samples, and 4) isolate and characterize product radionuclides. This work will directly address the need for novel methods for isotope production with innovation in target fabrication using additive manufacturing. Successful demonstration of new target production approaches will benefit the isotope production community as well as the specific fields that use these isotopes including nuclear medicine, forensics, physics, and more.

This research was selected for funding by the Office of Isotope R&D and Production.

Radiation Transport in Laser-produced Extreme Ultraviolet Plasma Light Sources

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Extreme ultraviolet lithography (EUVL) is a key enabler of the ongoing technology transition from a microelectronic to a nanoelectronic semiconductor industry. Such transition is needed to sustain Moore's law and continue to shrink transistor characteristic feature size. EUVL light sources use laser-produced plasmas on tin targets, where molten tin droplets are ablated by a pulsed CO2 laser to generate plasma that emits intense light at 13.5 nm (92 eV). The sole global supplier (ASML Holding) produces EUVL machines that have enabled the current 5-nm process node era in semiconductor manufacturing. However, chip makers are seeking higher throughput (about 200 exposed wafers per hour) which requires a power output of 600 W at 13.5 nm that is beyond the current capabilities of the commercial machines. The low conversion efficiency (CE) of laser pulse to EUV radiation, presently at 3-6%, is a significant limiting factor. To achieve the theoretical maximum CE of 20%, replacing CO2 lasers with Nd:YAG lasers is being explored. Nd:YAG lasers offer better wall-plug efficiency, compactness, and advanced pulse shaping capabilities, which could potentially increase CE. However, plasmas produced by Nd:YAG lasers have higher densities, making them opaque to EUV radiation and requiring the transport of EUV radiation from high-density to low-density regions, thereby reducing CE. While theoretical models suggest mechanisms for this radiation transport, experimental validation is lacking. This project aims to leverage ultrafast optical diagnostics, such as collective Thomson scattering, optical emission spectroscopy, and x-ray betatron imaging, to study opacity and radiation transport during laser-tin target interactions. This research will validate fundamental scaling laws and pave the way for future light sources at even shorter wavelengths (~6.7 nm, Blue-X technology), which are expected to use targets such as gadolinium instead of tin.

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

Role of Energy in Continuous Dielectrophoretic Molecular Separations

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This project is developing predictive models for dielectrophoretic separations. Dielectrophoresis is a type of force whereby charged and non-charged species undergo separation in the presence of a non-uniform electric field. Current models that explain these separations do not align with experimental observations by up to two orders of magnitude. To reconcile this discrepancy, a new model that incorporates properties of the solution is being developed. Key to this is acquiring and correlating local solution property data and field strength using a continuum model. Four objectives are sought. First, the continuum model of dielectrophoretic transport is being validated for colloidal particle solutions. Second, the validity of this model is being extended to the molecular scale. Next, an understanding between separations throughput and efficiency is sought so that the final objective, which focuses on understanding and quantifying the sensitivity of dielectrophoretic separations by observing several challenging separations such as the rare earth series and chiral solutions, is achieved. The completion of these objectives is enabled by a unique experimental approach that permits real time, spatially resolved spectroscopy measurements of solution composition between and around electrodes while controlling initial concentrations, field strengths and gradients, and flow rates. In so doing, advancements in and expansion of this non-thermal separation mechanism are likely.

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

Synthesis and Structure-Property Relationships in the New Family of Porous Metal Halide Semiconductors (PMHS)

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Semiconductor materials are the core components of almost every electronic device currently utilized for terrestrial and space applications. With the advancement of technology, there is a demand for next-generation materials that feature multiple functionalities besides excellent optoelectronic properties. In particular, the generation of porosity in fully inorganic semiconductors not only improved their optoelectronic features, enabled bandgap tuning, and enhanced photoconductivity but also rendered them proper for uncharted applications, such as photocatalysis and energy storage. Motivated by these synthetic challenges, we recently developed a new family of materials, namely porous metal halide semiconductors (PMHS). Utilization of molecular cages as structure-directing agents and counter-cations rendered PMHS porous and water-stable for over 1.5 years without impacting their optoelectronic properties. While this stability performance is unparalleled for hybrid semiconductors, the reasons behind it remain unclear. Interestingly, the fact that these compounds can indeed be rendered porous opens new avenues in material design, as, in addition to the currently available customization of optoelectronic and mechanical properties, it is now possible to fine-tune the porosity. Therefore, this project's focus is to expand the pallet of PMHS materials, allowing a deeper dive into the understanding of the structural factors that dictate stability and how porosity impacts their optoelectronic and ionic properties. The development of PMHS materials will address current hybrid semiconductors' deficiencies towards commercialization, fostering a competitive and sustainable economy. Corresponding PMHS can be tailored to target applications such as lithium-free solid-state batteries, water purification, and disinfection, water-stable antibacterial coatings on personal protective equipment and medical devices, CO_2 reduction, and hydrogen evolution (HER) reaction for the generation of clean fuels.

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

Modulation of Light-Harvesting by Endogenous Switches and Fuses in the Phycobilisomes

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From solar cell design to engineered crops to biofuel production, human technologies for harvesting and harnessing solar energy are inevitably inspired by (or co-opt) the elegant, diverse photosynthetic systems found in nature. Like naturally evolved systems, our technologies must operate in ever-changing sunlight and environmental conditions, which can result in photodamage or reduced efficiency. Plants, algae, and cyanobacteria have all evolved sophisticated ways to protect themselves from excess sunlight and tune photosynthetic output by safely dissipating or rerouting energy when needed.

To learn design principles that could mimic these capabilities, we must first understand the underlying molecular mechanisms that govern natural photoprotection and photoadaptation. The research will focus on understanding and learning to control such mechanisms in the phycobilisome, which is the main light-harvesting antenna protein complex of cyanobacteria.

Recent single-complex and single-molecule level studies of phycobilisomes have revealed surprising evidence of photodynamics originating on multiple length scales – from single pigments, to structural rearrangements, to interactions with other proteins such as the Orange Carotenoid Protein (OCP). Although OCP is known to quench the phycobilisome and recently its binding site for one species has been discovered, the dynamics and detailed mechanism of quenching are still not well understood, and where it binds to other phycobilisome architectures is not known.

The goals of the research are to (1) discover the molecular origin of the different photophysical states of phycobilisomes with and without quenching, using single-particle spectroscopic measurements of their properties and dynamics, (2) test the hypothesis that these states are induced by changes in incident light or other environmental parameters to learn whether they are indeed photoadaptive or photoprotective, and (3) determine to what degree we can exert control over these mechanisms. Building a mechanistic bottom-up view of the intrinsic photodynamic sophistication of phycobilisomes is essential for extending our biological understanding of photosynthesis, and provides highly complementary insights to more traditional research approaches. The outcomes of the research will impact future advances in alternative energy technologies and engineering crops for food security.

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

Continuous Redox-Mediated Electrochemical Liquid-Liquid Extraction for Critical Element Recovery

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Platinum group metals (PGMs) are used in many modern technologies but are difficult to recover and purify because of their low natural abundance, complex and environmentally dependent chemical states, and structural similarity. Electrochemical approaches offer a promising pathway to promote selective separation of PGM for their recovery while also reducing waste generated and enabling reusability. This project investigates how the structure of homogeneous redox-active extractants can be tuned to affect the selective separation of PGM chloro-anions under electrochemical control. Insight into both short- and long-range interactions are sought through a combination of single-site design and controllable surfactant self-assembly to maximize selectivity, regeneration, and uptake of PGM ions. The scientific objectives include the synthesis of soluble, electrochemically responsive molecules that selectively bind to PGMs; the mechanistic evaluation of how metals and extractants distribute between different liquid phases and assemble at interfaces using advanced operando techniques; and the selection of electrolytes and solvents for enhanced conductivity. This project, which focuses on establishing molecular design principles for developing new continuous electrochemical separations for critical element recovery, has the potential to advance understanding of non-thermal separation mechanisms.

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

Accelerated Robotic Design of Energy Materials (ACE lab)

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Chirality describes a property where an object or molecule is not superimposable on its mirror image. It is fundamental to the processes of life, and is ubiquitous in Nature e.g. nucleic acids, amino acids, and sugars. Chiral semiconductors can enable control over spin, charge, and light without the need for magnetic components. Such materials would be pivotal for next-generation technologies spanning quantum computing, encryption, and drug screening. Although there are numerous organic chiral molecules, their structural softness and poor electrical properties prevent them from wide-spread application. Recently, hybrid organic-inorganic perovskite semiconductors have emerged as new class of chiral semiconductors combining asymmetry with outstanding optoelectronic properties. However, their optical properties associated with the chiral molecules (chiroptical properties) are currently too weak for practical applications. Thus, to harness the full potential of chiral perovskites requires not only a fundamental understanding of synthesis-process-structure-chiroptical activity relationships but also a systematic search of the multidimensional compositional parameter space.

This project aims to uncover structure-chiroptical activity relationships to significantly enhance chiroptical properties and to discover new chiral perovskites by developing the Accelerated Robotic Design of Energy Materials (ACE) lab. ACE lab integrates robotics and real-time data collection with the use of machine learning-driven data interpretation and decision-making to accelerate progress of this promising material class. ACE lab will be a next-generation robotic platform operating autonomously to directly optimize properties with real-time characterization feedback allowing for in-the-fly learning and control. Success of this project impacts the deployment of advanced technologies. Once this research project is accomplished, the ACE lab concept can be naturally expanded to engage a broader materials science community to systematically contribute to the fundamental understanding of oxides, inorganic, organic, and hybrid semiconductors. ACE lab will be established at the Molecular Foundry User Facility at Lawrence Berkeley National Lab (LBNL) and thus, will be accessible for the broad materials science community, in addition to providing a state-of-the-art multidisciplinary training platform for the future workforce.

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

Quantum Control for Nuclear EDM Experiments

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Two of the biggest questions in physics converge in nuclear physics: why, in the early universe, is more matter created than anti-matter, given that they are otherwise so similar? And, why is the interaction that binds a nucleus together (the strong force) the same if time runs backwards, while the interaction that governs nuclear decay (the weak force) is not? The detection of the first intrinsic nuclear electric dipole moment would go a long way towards resolving both of these mysteries. The project here is to maximize the "quantum advantage" of the next generation of nuclear EDM searches by extending their coherent integration time. Our research will focus on the super-position state of the xenon-129 nuclear spin, whose coherence time we aim to extend by as much as a factor of 35, to the theoretical limit set by decoherence of the stationary states. We will use a combination of precision measurement techniques to tune away non-linear interactions, and quantum control techniques to ensure the optimal superposition state is created every time. Each improvement to the integration time will directly improve the sensitivity of the next xenon EDM measurement, planned for 2026 at LANL, by an equal factor.

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

Advancing the Quantum Magnetism Frontier in the Topology Era

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Topology is now firmly established as one of the organizing core principles for our understanding of quantum phases of matter. This is not only true for insulators and metals that are well-described by single-particle physics, but also extends to materials with strong correlations, such as magnets and superconductors. The goal of this project is to advance the theory of topological magnetism and bridge the gap between formal classifications of magnetic topological phases, which are known, and identifying, interrogating, and controlling such phases in real materials, which remains a key challenge. This is in fact a broader challenge for topological phases with strong interactions and stems in part from the formidable effort often required to gain insight into the behavior of materials which exhibit strong correlations between electrons. Several new frontiers in quantum magnetism, which have exposed unexplored properties of magnetic materials, offer a highly compelling opportunity to advance our understanding of correlations and topology. These include the observation and control of magnetism in layered van der Waals materials, even down to monolayer systems, and the discovery of new types of magnets - referred to as "altermagnets" - which provide unexpected venues for topological magnetism. The design of this project leverages and further advances these developments in key areas. The central objectives include developing methods to study, characterize, and predict the experimentally accessible charge and magnetic excitations in topological magnetic metals and insulators, and the exploration of pathways for realizing new topological phases by quantum and thermal melting of unconventional magnetic order. In a broad sense, this project offers a roadmap for advancing our understanding of magnetism in the topology era to fruitfully connect and exploit the realms of ideas, models, and materials.

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

Polymer Origami – A Blueprint for Hierarchical Folding of Sequence-Controlled Multiblock Copolymers

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Advances in chemistry have produced a class of multiblock polymers constructed via combining sequence-controlled oligomeric blocks and flexible amorphous blocks. These polymers are of interest due to their ability to self-organize into 2D nanosheets and simple 3D polyhedra. Such directed chain folding is reminiscent of biopolymers folding into proteins ubiquitously found throughout Nature. While not as structurally sophisticated, this class of polymers provides a model platform for studies aimed at translating complexities intrinsic to biological systems to synthetic materials. Successfully converting Nature's blueprint for protein folding to operate on synthetic polymers will open unprecedented avenues for their applications in stimuli-responsive, filtration, and catalytic materials.

The bottleneck in designing polymer folding, however, lies in parameter space complexity. Many of the polymer subunits utilized in synthesis possess complex shapes and sizes. As a result, folding prediction requires an understanding of the interplay between geometry, connectivity, and directional interactions in sculpting the assembled structures. Our proposal will address this challenge in materials design by combining theory and simulation to elucidate the driving forces governing polymer folding. Insights from our works will be leveraged to design a library of polymers for immediate synthesis. These designs include porous nanostructures for separation or catalytic applications as well as reconfigurable morphologies for usage as actuators in soft robotics. Our work will not only establish polymer origami as a synthetic analog of protein folding, but also highlight universal principles that underpin macromolecular folding processes. The latter means that our findings can complement approaches being used for protein engineering, providing transformative impacts beyond polymer self-assembly.

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

HYBRID DIGITAL-ANALOG QUANTUM SIMULATIONS OF NUCLEAR REACTIONS IN THE NOISY INTERMEDIATE-SCALE QUANTUM ERA

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The physics of atomic nuclei is crucial to understanding the origin of visible matter, the lifecycle of stars, developing novel medical radiotherapies, enabling robust and safe nuclear energy, and ensuring our national security and nuclear forensics. Unfortunately, nuclear physics is complicated, especially when it comes to extremely short-lived, highly radioactive nuclei, which are exceedingly difficult to measure in a lab or predictively model with modern theoretical tools while still being extremely important to the applications above. This project will develop the theory and tools needed to predict the properties of such nuclei on near-term quantum computers that will come online within the next decade. Exploiting the exponentially growing computational space that quantum computers offer, the research will enable fully microscopic prediction of nuclear properties that are impossible, even in the post-exascale era, with classical high-performance computing. By treating quantum computers as digitally controllable analog simulators, efficient simulations will be realized, making full use of available modern and near-term quantum resources. This research will develop these novel hybrid digital-analog simulations of nuclear dynamics, rooting dynamics within effective field theories and deriving the optimal mapping between the nuclear dynamics and the physical dynamics of the quantum platform.

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

Developing low-threshold liquid argon time projection chambers with photo-sensitive dopants for dark matter and neutrino experiments

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Liquid argon is an often-used material for detecting fundamental particles due to the large signals it makes when particles deposit energy in it. Its inexpensive price, transparency, and purity allow liquid argon detectors to be scaled to very large sizes, up to hundreds or thousands of tons, making it a powerful tool for measuring rare fundamental particle interactions that can ionize the argon target. A particular kind of liquid argon detector, a time projection chamber (TPC) equipped with photodetectors, is sensitive to scintillation light and ionization electrons produced in these interactions and can therefore measure low-energy signals. This project will explore the possibility of enhancing the performance of these detectors by doping the liquid argon with so-called “photo-sensitive” dopants that have ionization energies lower than argon, and thus allow lower-energy interactions to produce detectable ionization electron signals. These dopants may also convert some of the scintillation photons produced in the interaction to additional ionization electrons, which are more efficiently measured in a TPC. Furthermore, because the dopants are rich in hydrogen—the lightest element there is—they may increase sensitivity to interactions with very low-mass dark matter particles, neutrons, or neutrinos. This project addresses several technical challenges to building doped-argon detectors and explores the impact of dopants on low-energy signals, paving the way for future dark matter and neutrino experiments, among other potential applications.

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

Tuning Electrocatalytic Reduction of Plasma Pre-Activated CO_2 Toward Multicarbon Products

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Upgrading CO_2 to chemicals and fuels could provide a scalable strategy for mitigating climate change. Electrochemical conversion of CO_2 with water under mild conditions that are compatible with renewable energy could provide a low-carbon approach compared to alternatives that require H_2 or high temperature and pressure. However, electrocatalytic CO_2 reduction with H_2O (CO_2R) is rate-limited by the CO_2 or CO activation step. This limitation also constrains catalyst design to favor CO_2/CO activation at the expense of tuning catalytic pathways toward high-value multicarbon products. Nonthermal plasma has accomplished CO_2 conversion at atmospheric pressure, but the non-selective nature of plasma makes it challenging to control the subsequent conversion to valuable products.

This project will unlock new electrocatalyst design spaces for multicarbon product generation using CO_2/CO pre-activation with nonthermal plasma. We hypothesize that by applying nonthermal plasma in CO_2R for the first time as an approach that is outside the conventional scope of catalyst development, we may help solve outstanding challenges in electrocatalytic CO_2 upgrading to high-value products. This strategy would address the limitations of existing approaches to electrocatalytic CO_2R by decoupling reactant/intermediate activation and product formation using plasma pre-activation, opening a wider design space for electrocatalysts optimized for selective product generation further along the reaction pathway. Based on coupling plasma with electrocatalysts across a novel engineered interface, the proposed research will uncover new reaction pathways, materials, and catalyst design strategies for electrocatalytic reduction of pre-activated CO_2 to C_{3+} products. The results are expected to have broad implications for development of new classes of electrocatalysts for CO_2 reduction, as well as for opening new methods for upgrading molecules possessing strong chemical bonds.

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

Mechanisms of Non-Equilibrium Ion Dynamics in Radiation Tolerant Alloys

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This project will advance the frontiers of knowledge that underpin our nation's fusion energy capabilities by addressing one of the key limiting factors of a viable pilot plant; the survivability of plasma facing materials. One of the main challenges in understanding the cumulative effects of radiation damage in structural and functional materials lies in the ultrafast dynamics after an energetic collision with the lattice. Our limited scientific understanding of degradation and component lifetime predictions when exposed to these environments stands as a roadblock to commercially available inertial and magnetic confinement fusion energy power plants. The extremely fast timescale (10^{-11}s) and large excess of energy (10^4 - 10^7eV) imparted into the material during neutron and charge particle exposure are inadequately described by the assumptions of equilibrium dynamics. It is hypothesized that primary recoil damage and defect recombination involve high-energy, non-equilibrium electronic excitations that alter the potential energy surface and subsequent ion dynamics. This activates fundamentally different damage accumulation mechanisms and populations than those inferred from simple equilibrium theories in metals. Downstream phenomena emerging at longer length and time scales (chemical segregation, mechanical response, and thermal transport) are intimately linked to these initial transient non-equilibrium behaviors. The material selection to test these theories on reflect leading candidates for plasma facing (WReOs) and structural components (Oxide dispersoid strengthened steels). Work done here to unveil the fundamental radiation damage accumulation mechanisms and advancement of our modeling and simulation capability transcends the specific technical application where this effort will generate a wake of research efforts centered on matter in extreme environments where many modern science and engineering challenges lie.

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

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Machine-Learning Enabled Field-level Inference for Primordial Gravitational Wave Discovery

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Inflation is a leading paradigm for describing the earliest moments of the universe. The search for a key signature from inflation, imprints of primordial gravitational waves (PGW) on the B-mode polarization of the cosmic microwave background (CMB), is a major goal of many current- and next-generation CMB experiments. SPT-3G and BICEP/Keck are two leading experiments in this search: with SPT-3G providing a template of the lensing B modes to delens the BICEP/Keck maps, thus removing a major contaminant to the PGW B-mode search. The planned work enables the incorporation of otherwise foreground-contaminated temperature data in an optimal lensing estimate by approximating the probability distributions of extragalactic foreground fields using generative neural networks. The trained generative network will be part of a hybrid analytic and simulation-based likelihood when performing cosmological parameter inference on million-pixel maps. The gain in precision on PGWs B modes from including the SPT-3G temperature data is equivalent to a substantial extension to the SPT-3G survey time. This project will produce leading constraints on PGWs with data from the two most established experiments in this search, SPT-3G and BICEP/Keck. The techniques developed will be broadly applicable and impactful for the cosmology community for analyses of survey data on small scales such as those from DESI and Rubin-LSST in the present and CMB-S4 in the future.

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

Randomized Algorithms for Multiscale Electromagnetic and Multiphysics Problems

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This research aims to develop, implement, validate, and apply parallel randomized algorithms for solving large-scale and multiscale problems in electromagnetics and multiphysics. These problems, governed by Fredholm integral equations (IEs) of the first or second kind or by partial differential equations (PDEs) of the elliptical, parabolic, or hyperbolic type, are crucial in understanding electromagnetic and optical wave interactions with matter. Such interactions are fundamental to numerous modern sciences and technologies, involving high-frequency wave radiation, transmission, propagation, and scattering in complex media and their interaction with charged particles.

Numerical modeling and simulation are vital for research and development in these areas, but the multiphysics, multiscale, and nonlinear interactions between electromagnetics and other physical phenomena present significant challenges to existing deterministic numerical methods. This research aims to overcome these challenges by developing novel parallelized randomized algorithms for IEs and PDEs, enhancing the simulation efficiency of traditional deterministic algorithms. The project's major scope includes:

1. Developing randomized IE solvers using randomized factorization, matrix compression, and projection techniques for large-scale electromagnetic scattering and radiation problems.

2. Creating randomized hyperbolic and parabolic PDE solvers for multiscale electromagnetic and multiphysics problems.

3. Designing efficient parallel randomized solvers for large-scale computations based on the UPC++ library.

The expected outcomes of this project include hybrid deterministic-randomized scientific computing methodologies, leading to revolutionary simulation tools with enabling modeling and design capabilities that do not currently exist.

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

Light Harvesting Photoenzymes for Energy Conversion

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Enzymes that require a steady flux of light for catalysis are known as photoenzymes. By capitalizing on efficient visible light harvesting mechanisms resulting from millions of years of evolution, natural photoenzymes utilize clean solar energy to enable otherwise challenging and biologically important chemical processes. The pursuit of fundamental physical biosciences underlying sunlight-driven photoenzymes will greatly advance basic energy research. We detail an interdisciplinary research program centered around the study of a new class of naturally occurring flavin-dependent photoenzymes, namely fatty acid photodecarboxylases derived from algae. Combining biochemistry, biophysics, protein engineering, photochemistry, and bioinformatic methods, we will shed light on the fundamental flavoenzymology and photophysics underlying fatty acid photodecarboxylase-catalyzed reactions. Fueled by clean solar energy, improved flavophotoenzymes will allow the conversion of abundant and easily accessible bio-derived building blocks into useful products.

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

Understanding Elevated Temperature Plasticity in Refractory Complex Concentrated Alloys

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This research aims to advance our fundamental understanding of high-temperature deformation of an important new class of refractory elements-based concentrated solid solutions known as refractory complex concentrated alloys (RCCAs). These materials exhibit high melting points and elevated-temperature strength, which provide an exciting new framework to develop structural materials that surpass the capabilities of current-generation Ni-base superalloys that are widely used in energy, environment, and defense industries. This project will develop an understanding of the factors and mechanisms that control the elevated temperature strength and creep deformation by a combination of controlled-environment mechanical testing as well as in-situ neutron diffraction and 4-dimensional scanning transmission electron microscopy (4DSTEM) experiments. Specifically, this research will utilize these advanced tools to investigate the motion and evolution of defects that govern plasticity in RCCAs across multiple length scales, including local atomic environments that control vacancy and dislocation motion, and mesoscale dislocation structures that evolve during continued plastic deformation. The important insights obtained from the research will set the stage for the discovery and design of new RCCAs with enhanced high-temperature strength and creep resistance for structural applications under extreme conditions.

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

Advancing Edge Physics and Modeling towards Fusion Pilot Plants

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The periphery of toroidal magnetic confinement fusion plasma, commonly known as the edge or boundary plasma, plays a crucial role in the performance and sustainability of magnetic fusion reactors, including fusion pilot plants (FPPs). Recognizing its importance, the study of edge plasmas, particularly in tokamak devices, has been a significant component of magnetic fusion energy (MFE) research for over three decades. Despite this, critical issues, such as edge plasma exhaust in the presence of stochastic magnetic fields, remain unresolved due to the complexity of the problem. Moreover, existing edge models, tailored for specific research objectives, are neither optimized for modern computing hardware, software, and numerical algorithms nor suited for FPP-relevant applications, such as efficient core-edge-SOL integration and automated divertor design and optimization. This project will first develop a modeling framework with built-in capabilities that facilitate sensitivity studies and design optimization for FPPs as well as new edge transport and turbulence models for multiple magnetic configurations upon this framework, and then better understand and quantify edge plasma exhaust dynamics within a stochastic magnetic field, either externally applied, self-generated or both, through theoretical analysis and numerical simulations enabled by these new models. This work aims to address critical R&D topics such as core-edge integration, particle and heat exhaust, boundary turbulent transport, and plasma-wall interaction and to bridge the gap between current magnetized fusion plasma research and the ongoing and upcoming public and private efforts on FPP research.

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

Genome-Scale Modeling of Microbial Members in the Rhizosphere under Fluctuating pH and Temperature

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Comprehensive understanding of the metabolism of soil microorganisms and their interactions with other microbes and with plant roots is a major challenge in environmental microbiome research. Achieving a predictive understanding of these processes from the molecular to the ecosystem scale will have a huge impact on carbon sequestration in soils, bioenergy crop productivity, and the global nutrient cycling. This research focuses on developing mathematical models and high-throughput validation experiments for the five most abundant soil bacteria to understand their metabolism in response to changes in pH and temperature. These two environmental variables have been shown to play a key role in plant productivity, both in natural environments and in agroecosystems. Once these pH and temperature genome-scale models are built and validated, they can be used to perform simulations to further understand –and eventually control– the necessary metabolic processes that affect nutrient synthesis and cycling within different ecosystems. The results of this project will increase our fundamental understanding of relevant soil microorganisms, potentially enabling new model-driven interventions for resilient bioenergy crops and carbon sequestration. This dual experimental and computational project is conducted by a diverse team that includes postdoctoral, graduate, and undergraduate researchers. Members of the team will engage in learning and teaching computational biology activities, thus training the next generation of computational biologists to tackle the most critical challenges in predictive biogeochemistry and environmental microbiome science.

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