Construction of a Background Free, Normal-Ordering Neutrinoless Double Beta Decay Demonstrator

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The experimental quest for the neutrino's true nature, a search dating back to the earliest days of nuclear and particle physics, is now harnessing experiments, machines, and detectors of high precision and massive scale. Observation of a hypothesized unbelievably rare occurrence – a neutrinoless double beta decay of a nucleus -- would indicate that a neutrino is its own antiparticle, and would help to answer fundamental questions about why there is more matter than antimatter in the Universe. Current and planned experiments will only be able to explore certain theories of neutrinoless double beta decay due to coincidental but rare background (i.e., non-signal) data coming from detectors. To fully resolve whether a nucleus can undergo this as-of-yet undetected reaction will require new breakthroughs in detector technology that can reach the elusive "normal ordering" neutrinoless double beta decay regime by eliminating background events. This research program will unify and incorporate the latest developments in nuclear physics R&D into a novel detector capable of demonstrating background-free searches for neutrinoless double beta decay. Notably, this will include sensors capable of detecting, at the single-ion level, Barium++ ions as they are produced by double beta decay in Xenon. Additionally, this detector will synthesize direct ultraviolet light collection and fast optical cameras to enable high resolution, 3D imaging of neutrinoless double beta decay events. Achieving background-free neutrinoless double beta decay searches will enable the Office of Science's high-priority search for neutrinoless double beta decay to reach unprecedented levels of sensitivity.

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

Intelligent Primitives for Scalable Graph Analytics and Learning

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Interactions among entities drive almost all physical, social, and cyber-physical systems on earth. A graph mathematically models an interacting system where a set of vertices represents entities and a set of edges represents their interactions. Since many scientific datasets in chemical, biological, and climate sciences are conveniently modeled as graphs, there is an undeniable need for high-performance and general-purpose graph analysis and machine learning (ML) algorithms and libraries across DOE's scientific domains. The convergence of graph ML methods and domain sciences faces the twin challenges of the diversity of scientific data and the heterogeneity of cyberinfrastructure. We aim to address such challenges by mapping graph algorithms to a handful of intelligent computational kernels that learn from data sparsity and hardware configurations. Relying on the message passing paradigm, we will map many graph ML algorithms to sparse linear algebra operations for which we will develop autotuned and communication-avoiding algorithms that can scale to millions of threads, analyze graphs with trillions of edges, and exhibit portable performance on various computing platforms. This project will also develop flexible and interpretable algorithms for graph embedding and graph neural networks that in turn rely on our intelligent primitives for performance. We will use these algorithms and libraries to solve exascale problems from metagenomics, scientific computing, visualization, and graph machine learning. Thus, this project aims to develop algorithmic foundations for scalable, portable, and usable graph ML algorithms and libraries.

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

Computationally Driven Design and Synthesis for Electron Transfer Materials based on Nonnatural Polymers

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Developing new materials that exhibit control over electron transfer processes is necessary to address challenges in energy production and storage. Nature provides a blueprint for achieving this control through use of protein machinery evolved from archaic modules of small proteins that carry out coupled oxidation and reduction — or redox — reactions. Electrons are transferred from one module to the next within this machinery, with each module containing one or more redox centers. Control is achieved by the sequence of redox centers whose potentials are defined by the local environment within the protein. However, efforts to harness the complex functionality of Nature's modular material design for energy technologies must address the challenge of operating under harsh non-biological conditions. Recent synthetic advances now enable design and synthesis of nanostructured materials from nonnatural, sequence-defined polymers that mimic proteins, but exhibit high stability in such conditions. The purpose of this research is to develop the understanding of structure and function required to incorporate redox centers that mimic the electron transfer function of natural proteins. The focus will be on computational design of individual macromolecular units containing four iron ions and four sulfide ions placed at the vertices of a cubane-type cluster, whose redox potentials are tunable through their local environment. Methods to be used range from quantum to molecular mechanics and coarse grain simulations, specifically as they relate to modeling nonnatural sequence defined polymers and their interactions with redox clusters. Ultimately, these units may be arranged into materials mimicking Nature's exquisite spatial control of electron transfer under non-biological conditions to harness the complex functionality of hierarchical matter.

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

Resolving the *f*-electron Challenge with Scanning Probe Microscopy/Spectroscopy

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The ability to predict the chemical and physical properties of a material is directly related to the structure and interactions of its electrons. For materials comprised of *f*-block elements (the lanthanides and actinides found in the last two rows of the periodic table), the complexity of electronic structure has presented great difficulty in understanding, modelling, and predicting material properties. For this reason, resolving the *f*-electron challenge was identified by the Department of Energy's Basic Energy Sciences program as one of three Grand Challenges to be overcome in order to transform the scientific field. The objectives of this proposed project are to probe the electronic structures of a series of single-crystal actinide (An) carbide, nitride, oxide, and intermetallic samples using scanning tunneling spectroscopy (STS) techniques. Specifically, neptunium (Np), plutonium (Pu), and americium (Am) are targeted due to their unique location in the actinide series of elements, which straddle a transition from itinerant bonding behavior, and localized non-bonding behavior. The instabilities in electronic structure that occur near this transition are thought to be responsible for the complexity of material behaviors observed for derivative compounds of these actinide elements. By performing scanning tunneling spectroscopy (STS) on a range of bulk single crystal actinide intermetallic compounds, a seamless mapping of both the occupied and unoccupied electronic structures of these materials can be obtained using a local probe, providing a means by which their complex chemical and physical properties can be understood. The results thus obtained will be compared to mapping of the electronic structures in these materials obtained by other methods, such as photoemission, X-ray absorption, and X-ray emission spectroscopies. Computational modelling of the electronic structures of these materials will be used to correlate the surface electronic states measured by STS, to bulk electronic states and bonding modes of molecular complexes with analogous bonds relevant to Heavy Element Chemistry (HEC) research.

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

Hybrid Kinetic-Fluid Modeling of Tokamak Disruption Mitigation

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A critical first step toward realizing abundant, carbon-free fusion energy is the self-sustaining, burning plasma ITER experiment. Achieving ITER's goals will require the avoidance or mitigation of disruptions - a rapid loss of the plasma stored energy, and the subsequent runaway electrons - an uncontrolled high-energy beam generated by the disruption. The prevailing mitigation strategy is to rapidly inject additional material to trigger a controlled disruption and dissipate the resulting RE beam. This strategy has proven successful on existing devices, but questions remain on how to optimize the deployment for ITER and next step devices. This presents a clear need for validated predictive modeling to inform mitigation strategies that retire the risks of disruptions and runaway electrons.

The goals of this project are to determine the efficacy of and recommend optimizations for the disruption and runaway electron mitigation system planned for ITER and future reactors. While fluid and kinetic models have separately extended our understanding of disruptions and runaway electrons, less progress has been made to understand their self-consistent, coupled dynamics. In particular, the coupled dynamics are critical for modeling post-disruption, runaway electron generation and mitigation via material injection, where runaway electrons carry the entire plasma current and significantly affect material transport. The project goals will be achieved by developing a self-consistent coupling where fluid fields are calculated simultaneously with the full distribution of kinetic runaway electron orbits. The resulting tool will efficiently and rapidly assess the formation likelihood of runaway electrons and their energy deposition onto the walls of the device to develop practical disruption and runaway electron mitigation solutions.

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

Maximizing Dark Energy Constraints from Next Generation Cosmic Microwave Background Cluster Surveys

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Clusters of galaxies, the largest-gravitationally bound systems in the Universe, are powerful tools with which to constrain cosmological models. Over the past decade, the field has been transformed by the construction of the first cluster samples using data from high-resolution cosmic microwave background (CMB) experiments in which these massive systems are detected via the subtle distortions they imprint on the sky observed at millimeter wavelengths. Current and next generation CMB experiments are poised to continue this revolution by enabling the discovery of 10,000 to 100,000 galaxy clusters. These unprecedented cluster samples will provide critical clues into the nature of dark energy, the mysterious phenomena driving the observed accelerated expansion of the Universe. There are two key requirements for studying dark energy with galaxy clusters: a census of these systems spanning cosmic time and the ability to connect the observed properties of these systems to cosmological models. While these requirements are easy to state, this cosmological census is extremely challenging, and numerous problems remain to be solved to make full use of cluster samples for cosmology.

This Early Career program will address these challenges through an observation- and simulation-based effort focused on obtaining cosmological constraints with a new cluster sample from SPT-3G, an ongoing CMB survey being conducted by the 10 m South Pole Telescope. The close coupling of data and simulation efforts in this program will be critical for achieving tight control over the measurement and modeling biases that currently limit cluster cosmology. The tools developed in this program will enable a significant improvement in cosmological constraints from the SPT-3G dataset, and—perhaps more critically in this era where systematic uncertainties are coming to dominate error budgets over statistical uncertainties—are designed to ensure that these constraints are unbiased. This work will prepare us to leverage the full power of the upcoming cluster samples from the Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST) and CMB-S4 surveys, and thus help to maximize the impact of DOE's investment in these world-class cosmic surveys.

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

Machine learning approaches for spherical tokamak scenario optimization and real-time control

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The PI proposes to develop and demonstrate tools for using machine learning (ML) for optimization of Spherical Tokamak (ST) plasmas and to establish the basis for extending these tools to real-time control of STs. ML algorithms will be used to obtain accelerated simulation capabilities suitable for optimizing actuator trajectories to achieve high performance scenarios. Algorithms for calculating proximity to machine limits and disruptions will ensure trajectories maintain a safe distance from these limits.

While the small size of STs makes efficient use of magnetic fields, it presents space constraints that amplify the problem of handling heat loads and forces, and limits the size of coils for inductive plasma current start up and sustainment. Disruptions compound the heat load and force problems, and strategies to avoid and mitigate them as much as possible are necessary. These challenges make it critical to develop novel tools for prediction, optimization, and active control that can accurately model the plasma response to available actuators while identifying and avoiding machine limits and plasma disruptions. Recent fundamental improvements in machine learning and in computing hardware provide the opportunity to integrate physics modeling and empirical data to make accurate and fast predictions, and to develop rapid optimization algorithms for offline and real-time use. These tools, which will be explored in this work, could have a transformative effect on real-time plasma control and scenario development. The sub-tasks of this project will include:

1. Rapid simulations using ML: Machine learning surrogates for high-fidelity physics models will be used
to accelerate calculations while maintaining high-fidelity. For quantities that are not accurately modeled by available physics models, experimental data will be used to train machine learning models.

2. ML identification of proximity to machine limits, disruptions, and other events: ML algorithms will be used to generate estimates of the safe operating space, free of disruptions and other deleterious events. The identified constraints bounding the safe operating region will be in a form appropriate for use in optimization algorithms.

3. Optimization of actuator trajectories: The rapid, accurate simulation capabilities and the estimates of safe operating space developed in the first two subtasks will enable application of numerical optimization techniques to design actuator trajectories.

4. Implementation of algorithms for control room use: The models and algorithms developed in the first three subtasks will be implemented for control room (between shots) use. As part of this effort, techniques for adapting trained models to newly acquired data will be developed, as well as active learning approaches that will help guide the design of experiments and simulations to simultaneously improve the ML predictive models and ST performance.

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

The Role of Local Chemical Order on Defect Kinetics in Alloys under Irradiation

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As an emerging class of materials, multi-principal element alloys (MPEAs) have attracted increasing attention owing to their extraordinary properties, including diminished radiation defects, enhanced swelling resistance, and suppressed solute segregation when compared to traditional solid solutions. While the fundamental atomic mechanisms and their correlation to the improved radiation performance remain to be elucidated, this project speculates that the hidden local chemical order may be the salient feature that makes MPEAs distinct from traditional alloys, plays a vital role in radiation defect dynamics and kinetics, and contributes to the improved radiation tolerance. The overarching goal of this research is to understand the role of local chemical order on the kinetics of defects in MPEAs under irradiation and to evaluate the mechanistic strategy for controlling radiation defects migration and evolution through tailoring the degree of local ordering at the nanoscale. The research focuses on single-phase MPEAs and addresses the following fundamental questions regarding local ordering: (i) how does the local chemical order influence defect migration, coalescence, and growth; (ii) what are the new atomistic mechanisms and processes enabled by local order that could lead to radiation damage reduction; and (iii) is tuning the degree of local ordering able to promote defect recombination and to alleviate radiation-induced damage accumulation? Specifically, research activities are driven by three mechanistic hypotheses pertaining to the role of local ordering on point defects, defect clusters, and grain boundaries: (1) the presence of local chemical order raises migration energy barriers of point defects and localizes their diffusion; a localized diffusion can promote defects recombination and mitigate defect cluster growth; (2) local chemical order roughens the potential energy landscape, which can locally pin a dislocation loop and reduce its diffusivity; and (3) the introduced local ordering in the grain matrix increases grain boundary migration energy and lowers its mobility. These hypotheses will be evaluated in single-phase MPEAs using integrated theoretical and computational techniques, including molecular dynamics, Monte Carlo, accelerated molecular dynamics, climbing image nudged elastic band method, and a machine learning tool. The modeling and theoretical predictions will be validated by targeted experiments, including energy-dispersive x-ray spectroscopy characterization and in-situ ion irradiation. Evaluation of these hypotheses will advance the fundamental understanding of atomistic mechanisms underlying the extraordinary properties of MPEAs, facilitate material design strategies to manipulate defect behaviors via tailoring nanoscale features, and result in tunable material properties.

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

Towards Robust Cosmology from Large-Scale Structure with Galaxy Surveys

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Cosmology is at an exciting crossroads. Over the last two decades, through a variety of observations, we have put together a standard model of cosmic evolution, the Lambda Cold Dark Matter (LCDM) model, that provides an excellent description of the evolution of the Universe and the structures within it. Recently, however, we are seeing mild tensions in LCDM preferred by the Cosmic Microwave Background (CMB) experiments (a probe of the Universe shortly after the Big Bang) and by galaxy surveys (a probe of the Universe 13.8 billion years after the Big Bang). This research focuses on rigorously addressing this issue for galaxy surveys, as we prepare for the next transformative leap in statistical power coming from the Rubin Observatory's Legacy Survey of Space and Time (LSST), a DOE and National Science Foundation (NSF) partnership. Together with collaborators in the LSST Dark Energy Science Collaboration (DESC), the research team will first complete and validate the LSST cosmology pipelines combining weak lensing and galaxy clustering using simulations. Next the project will re-analyze Stage-III galaxy surveys using this pipeline and combine them together. The results of this analysis will guide our focus for the next decade of dark energy experiments. It will also serve as a critical bridge between Stage-III (Dark Energy Survey) and Stage-IV (LSST) galaxy surveys for transferring knowledge and tools associated with large-scale structure cosmology analyses.

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

Development of PFIB-Xray System with Machine Learning Method to Realize Comprehensive Analysis from Macro- to Nano-scale

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Many scientific questions in materials and biological sciences center around the relationship between hierarchical structures and macroscale functional performance, requiring a unique characterization platform for linking chemical, structural, and functional properties across all relevant length scales. The upcoming upgrade of the Advanced Photon Source (APS) will enable the development of hard x-ray nanoprobes approaching <10 nm spatial resolution. However, upscaling nanoimaging to examine samples beyond the microscopic scale faces many intrinsic challenges. This project will directly address these challenges by developing a Xenon plasma focused ion beam (PFIB) -Xray instrument with associated data analysis methods. The instrument combines an x-ray nanoimaging system and a PFIB probe to allow *in-situ* sample manipulation to facilitate and optimize x-ray imaging from macro- to nano-scale on one integrated platform. Novel data analysis including machine learning methods will be developed to correlate data collected at different scales and extract critical scientific information. With this new technique, one will be able to perform analysis across scales from the level of a functional device to single grains or deeply buried interfaces. A new landscape of scientific applications will be enabled including investigation of performance degradation at various structural levels of perovskite solar cells, multiscale characterization of additively manufactured alloys, imaging of microbe dynamics in undisturbed soil aggregates, and mapping of hierarchical structures in bones or biological tissues. The development of the PFIB-Xray will take advantage of the upcoming APS Upgrade, and in turn fully realize its potential for hard x-ray microscopy.

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

Defining the influence of environmental stress on bioenergy feedstocks at single-cell resolution

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Plant biomass from bioenergy crops is an important resource that enhances energy independence and promotes good environmental stewardship. Environmental stresses such as drought or nutrient deficiency hinder optimal performance of these crops. Therefore, the development of new strategies to improve plant biomass production will require a better understanding of how plants tolerate and respond to environmental stress. Plant responses to drought are complex and involve the coordinated action of many different types of cells with specialized functions. For example, cells that compose stomata (pores in the leaf that open and close to exchange carbon dioxide, oxygen, and water vapor) may respond very differently to drought than cells of the plant vasculature. The objective of this project is to use innovative technologies to measure how individual cells respond to drought and nutrient limitation in two prominent bioenergy crops, sorghum and switchgrass. This will require the construction of large, curated datasets detailing the regulation of genes in hundreds of thousands of individual plant cells. In addition, the planned research will analyze gene expression under drought and nutrient stress using sophisticated plant growth chambers that closely mimic agricultural field conditions. Lastly, this project will investigate the impact of beneficial soil microorganisms on plant growth under stress. The results of this research will significantly advance our foundational knowledge of how plants coordinate their responses to environmental stresses and will ultimately enable us to target genes in specific cells for crop improvement.

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

Resonant Coherent Diffractive Imaging of Quantum Solids

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Electronic symmetry breaking is at the heart of many forms of collective phenomena in quantum solids, including superconductivity, magnetism, and density waves. The inherent competition between these electronic phases and their interplay with disorder often lead to a highly textured landscape across multiple length scales. Visualizing these nanoscale textures is a modern challenge and key to a fundamental understanding of quantum matter, but it suffers from a lack of tailored probes. This research project will address this critical need by combining advanced X-ray coherent ('lensless') imaging methods and resonant soft X-ray scattering into an integrated Resonant Coherent Diffractive Imaging toolset. The main goal is to study the nanoscale organization of quantum phases of matter at length scales between 10 nanometers and 10 microns. These complex spatial textures will be investigated in quantum solids with different forms of collective phenomena: copper oxides and transition metal tellurides (superconductivity and charge-density-waves); rare earth nickelates and van der Waals magnets (antiferromagnetism); and artificial magnets with complex spin textures (skyrmions). Thanks to recent advances in highly coherent X-ray sources, the development of new multiscale imaging techniques is timely and poised to significantly advance our understanding of collective phenomena in complex systems. Looking beyond the horizon of quantum materials, the availability of new coherent X-ray imaging methods provides potentially transformative opportunities for the characterization of a broad class of functional materials (catalysts, batteries, magnetic devices), soft matter, and biological systems.

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

Measuring Key Nuclear Reactions for the Weak r-process

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Where do heavy elements—those heavier than iron, such as gold and europium—come from? For decades, this question has been the subject of intense debate among physicists. The recent first-ever observation of two binary neutron stars colliding and merging suggests that these mergers are responsible for the production of heavy elements via the rapid neutron capture process (r-process). However, observations of ultra-metal-poor stars show that this is not the whole story. Rather, there is strong evidence that there is another r-process site that produces the lightest heavy elements—from strontium to silver—attributable to the r-process. Neutrino-driven winds that follow core-collapse supernova explosions are possible candidates for the production of the weak r-process elements, but unfortunately, none of the relevant reaction rates necessary to constrain astrophysical models are experimentally known. Obtaining direct measurements of these reactions is experimentally challenging because they require unstable neutron-rich beams, which are usually produced at low intensities. The goal of this project is to develop innovative methods of measuring reaction rates important for the production of weak r-process elements, building on a technique recently developed at Argonne National Laboratory's tandem linac accelerator system (ATLAS) for the direct measurement of nuclear reactions using neutron-rich beams. With the development of a powerful active-target detector—a time-projection chamber with three-dimensional tracking and high-rate capabilities—and the implementation of machine learning techniques for data analysis, this research will reduce or remove some of the most important nuclear physics uncertainties associated with the weak r-process and will substantially improve our understanding of nucleosynthesis from neutrino-driven winds in core-collapse supernovae.

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

In-Beam Gamma-Ray Spectroscopy at the Limits of FRIB

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An area of great discovery potential at the Facility for Rare Isotope Beams (FRIB) will be at the neutron driplines, the upper mass limit of existence for each isotope on the periodic table. In this region, the imbalance of neutrons and protons in the nucleus results in the evolution of proton and neutron orbitals, the emergence of collective structure, and the potential for changes in nuclear properties due to the proximity of unbound configurations. The study of nuclei close to the neutron dripline is particularly interesting; these nuclei play a strong role in isotope production in stars and their structure also informs nuclear theory. Establishing how and when large neutron-to-proton ratios in a nucleus require new or modified theoretical tools is a major question in nuclear physics that remains largely unanswered. To move the science forward, data as close to the reachable limits of experiment are essential, requiring targeted measurements and new experimental capabilities. The goal of this research is the study of nuclear structure at the limits of existence through a program of strategic measurements at FRIB. Measurements will focus on the most exotic magnesium, calcium and iron nuclei. In parallel, a thick liquid hydrogen target coupled with charged particle detectors for reaction vertex reconstruction will be developed and deployed to maximize sensitivity for spectroscopy measurements at FRIB.

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

Understanding the Effects of *Populus*—Mycorrhizal Associations on Plant Productivity and Resistance to Abiotic Stress

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Harnessing plant–microbial interactions that occur in bioenergy crop plantations provides an opportunity to create sustainable, multipurpose bioeconomies. In these plantations, globally important biofuel feedstocks can be produced while simultaneously maximizing soil health and mitigating adverse impacts on climate. Over the past two decades, it has become increasingly clear that interactions between plants and microorganisms alter the way in which plants grow and respond to environmental stress. These interactions have been coined "plant holobionts," which are biological units consisting of the plant host plus all of the symbiotic microorganisms associated with the plant. To increase sustainability within biofeedstock plantations, this research is focused on building optimal plant holobionts between biofeedstock trees within the genus *Populus* and fungi that form symbiotic associations (mycorrhizae) with the trees' roots. This will be accomplished by identifying high-performing varieties of *Populus* species and hybrids that are resistant to drought and pairing them with diverse mycorrhizal consortia. This work will examine the ecosystem-level consequences of these assembled *Populus* holobionts to understand how manipulating those interactions influences nutrient cycling and carbon storage in a *Populus* tree plantation. Furthermore, this project will establish a unique collection of plant, microbial, and common garden resources that can be leveraged to engineer the next generation of bioenergy crops.

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

Architecting the Hardware-Software Interface for Neuromorphic Computers

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Neuromorphic computers are emerging computing systems that operate on the principles of the central nervous system. They implement neurons and synapses in hardware, supporting biology-inspired synaptic plasticity. These systems can perform several different types of scientific computations with significantly lower energy footprints compared to a conventional CPU-based computer. Future high-performance neuromorphic computers are expected to aggregate multiple heterogeneous neuromorphic hardware nodes to solve scientific computations that are far too complex for single-node hardware. Despite the progress made on the hardware and technology fronts, the software stacks for these computers have remained largely unexplored. As a result, even a small neuromorphic computer, where neurons and synapses are in the millions, requires an enormous amount of time and expertise to program and visualize results. This complex interface is expected to become a programming bottleneck for systems that can have several orders more neurons and synapses than today's systems. Therefore, there remains a pressing need to architect the hardware-software interface such that these high-performance systems can easily be integrated into the existing workflow at different United States Department of Energy (DOE) Office of Science national laboratories. To address this need, the research will develop virtualization of neuromorphic computers, abstracting the application developers, i.e., the users from the underlying hardware. Specific objectives of this research include 1) hardware-software co-design of the virtual machine interface for neuromorphic computers, 2) managing resources and memory for virtual machines invoked on a neuromorphic computer, 3) supporting concurrent applications with custom priority and security policies, and 4) mitigating security vulnerabilities through application isolation. The proposed research activities will make neuromorphic computers programmable, secure, efficient, and easy-to-use for the broader scientific community of DOE.

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

Scalable Dynamic Scientific Data Reduction

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Lossy compression is critical to the success of today's and future scientific discovery because of the extreme volumes of data produced by scientific applications or instruments. Existing error-bounded lossy compressors, however, suffer from two significant drawbacks: (1) they support only simple error controlling (such as absolute error bound) that does not match the user's requirements for preserving quantities of interest and features; and (2) existing general-purpose data compressors are developed based on static designs without adaptability to the diverse characteristics of application datasets. The overarching goal of this project is to develop a scalable dynamic scientific data reduction (SDR) framework (and practical library/toolkit) that can automatically construct the best-qualified data reduction solution in terms of user requirements and dynamic data characteristics, significantly improving data reduction quality and performance over the existing general-purpose lossy compressors. Four critical thrusts will be explored. (1) SDR will use numerical analysis, machine learning, and deep learning to optimize the specific design for a broad range of data reduction techniques. (2) The project will explore efficient machine learning based search algorithms to determine online the optimal data reduction solution (model and parameters). (3) The project will explore how to satisfy user-requirements (fidelity, speed, reduction ratio) efficiently and accurately. (4) SDR will support multiple parallel heterogeneous environments and will be evaluated comprehensively by using diverse scientific applications on DOE leadership-class supercomputers.

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

Understanding Deep Convective Cloud Kinematic Processes and Their Responses to Aerosols

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Deep convective clouds (DCCs) play an important role in the Earth's energy balance and are prolific rain producers in tropical and mid-latitude regions. The representation of DCCs and their feedback on the global circulation and precipitation represents one of the greatest uncertainties in Earth system models. Among all processes, the aerosol impacts on DCC properties remains particularly poorly understood, limiting the predictability of climate and the water cycle. It has been hypothesized that aerosols, tiny solid or liquid particles suspended in the atmosphere, can help strengthen or invigorate convective storms. In this scenario, an increase in aerosol amount deepens the DCCs through interactions with cloud and precipitation particles, changing the vertical profile of water phase changes and the associated latent heating, which then increases the buoyancy of convective updrafts. A major bottleneck has been the lack of key supporting observations of convective properties to provide clarity of the invigoration processes. Furthermore, the fundamental causal relationships among the highly nonlinear aerosol-DCC-environment interactions are difficult to resolve with traditional statistical methods.

To bridge these critical knowledge gaps in aerosol-convection interactions, we propose a blended observational-modeling framework. The framework combines advanced ground-based observations from the DOE Atmospheric Radiation Measurement facilities, and satellite and reanalysis datasets with innovative machine learning techniques, and high-resolution modeling. The standing hypothesis is that high aerosol amounts promote stronger DCC up- and downdrafts, leading to more vigorous cloud initiation along the convective downdraft boundaries and enhanced convective organization. To test this hypothesis, the project will use several innovative concepts and methods including: (1) evaluation of invigoration hypotheses using unique remote sensing measurements of convective up/downdraft velocities, (2) determination of causal relationships among the aerosol-DCC-environment interactions using a new causal inference framework, (3) identification of the environmental conditions favorable for invigoration using machine learning techniques, and (4) exploration of the underlying invigoration pathways by considering the three-way links between aerosols, the environment, and convective strength through observation-informed high-resolution simulations.

The results from this project will resolve the debate regarding the magnitude and importance of aerosol impacts on DCCs and determine drivers of the aerosol-DCC invigoration hypotheses. As a result, and more fundamentally, the proposed activities will lead to improved understanding of fundamental DCC processes for the improvement of the representation of DCC lifecycles in regional and global models and of the water cycle predictability.

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

Adaptive Synthesis of Nanoporous Membranes by Pathway Directed Self-Assembly

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A new generation of higher performance separation membranes will be critical to ensuring the water, energy, and economic security of the United States in the 21st century. The self-assembly of polymers and other nanomaterials presents an approach to synthesize membranes with tailored nanopore architectures that achieve remarkable improvements in separation performance; however, economically viable strategies for membrane manufacturing by self-assembly have yet to be realized. Directing self-assembly at or near equilibrium can ensure ideal membrane characteristics at the cost of manufacturing scalability. Meanwhile, nonequilibrium solvent-nonsolvent exchange processes for self-assembled membrane fabrication are readily scaled up yet remain extremely challenging to economically optimize. To address this scalability challenge, this research project pursues a transformative synthesis strategy of pathway directed self-assembly, in which industrially scalable processes are rationally designed to follow specific nonequilibrium pathways for the self-assembly of membranes that meet functional design targets. Three specific objectives will be pursued to demonstrate this concept: (1) Analogues of conventional processes for deposition, solvent vapor treatment, and chemical infiltration of soft matter thin films will be developed using ultrasonic spraying, a process already in use at manufacturing scale. (2) Active spray control, real-time nanostructure characterization using synchrotron X-rays, and closed-loop autonomous workflows will be combined to enable adaptive, feedback-controlled spray process tuning. This capability will be used to efficiently survey myriad nonequilibrium assembly pathways, including ones inaccessible through other processing methods. (3) Adaptive spray process tuning will be applied to direct self-assembly pathways towards synthesis of fouling- and organic solvent-resistant membranes with aligned, molecular-scale pores. The advances made in pursuit of these objectives will yield fundamental clarity about nonequilibrium self-assembly processes and introduce a powerful new adaptive synthesis capability to the benefit of Department of Energy facility users.

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

Exotic Probes of Dense Nuclear Matter

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Energetic collisions of nuclei produce a unique phase of matter, called the quark-gluon plasma, where normal particles like protons and neutrons melt down into their constituent parts. As this plasma expands and cools, clusters of three quarks can freeze back into more familiar particles, while larger groups of four, five, or more quarks can coalesce into exotic particles that are not well understood. The rate at which exotic particles form is dependent on the properties of the plasma such as its temperature and density, and also on the structure of the exotic particles themselves. The LHCb experiment at the Large Hadron Collider is uniquely well suited to measure these exotic particles in a wide range of nuclear environments. This project will use LHCb to measure exotic particles produced in both collider and fixed-target collisions, where they will be exposed to different conditions. These measurements will provide new information on the mechanisms by which quarks combine into particles and the fundamentally allowed configurations of quarks that make up visible matter. In addition, these data will be used to guide projections for future studies of exotic particle interactions at the forthcoming Electron-Ion Collider.

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

Verification of Quantum Devices from Emergent Randomness

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As current quantum devices grow more complex, the question of verification becomes increasingly important. Verification refers to tests carried out in order to ascertain how close a quantum device is to its ideal performance limit. This is especially critical for quantum computing and simulation architectures that are not yet error-corrected, which are often referred to as noisy intermediate scale devices. A powerful, and currently leading, method for such verification is to implement a specialized type of random evolution, which generates quantum states or operators that randomly fill the associated state space. However, this type of evolution is not available on many types of quantum devices, including most analog quantum simulators, which have been used to study outstanding questions in quantum many-body physics. To solve this issue, we propose to make use of a very recent and surprising observation: Viewed from the right perspective, generic chaotic many-body evolution will produce randomly distributed quantum states, even without specialized control sequences. We call this phenomenon emergent randomness. We propose to use emergent randomness as a widely available tool for device verification, thereby generalizing existing protocols to a much broader class of quantum devices as well as to shorter evolution times and illuminating the limitations of randomness-based verification more generally.

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

Spacetime Emergence from Quantum Gravity: Perturbative and Nonperturbative Aspects

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The black hole interior is one of the most mysterious and poorly understood phenomena of modern physics, partly because it is simultaneously described by gravity and quantum mechanics. The two theories, both of which have undergone rigorous empirical testing, disagree on a fundamental point: whether information about the region behind the event horizon can escape and be decoded by an observer outside of the black hole. The conflicting predictions are known as the Black Hole Information Paradox, a foundational puzzle in the quest for a quantum theory of gravity: a theory that can simultaneously describe the black hole interior and the dynamics of the big bang. In recent years, a synergy of tools from quantum information theory and gravitational physics have catalyzed a new era of progress on this paradox. This research project capitalizes on the interplay between gravitational phenomena such as gravitational lensing and information theoretic input such as a quantification of the computational complexity of quantum tasks. These connections will be used to both work towards a resolution of the Information Paradox and to leverage this progress into new insights on the quantum nature of spacetime.

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

Frontend Implementation of AI-Machine Learning Neural Networks for On-Detector Radiation-Hard Edge Compute

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Highly granular, large area sensors generate voluminous amounts of experimental data, while still relying on increasingly inadequate conventional means of data transfer. Traditionally readout integrated circuits (chips) are used to amplify the analog signal generated by sensors and convert it to digital signals. Processing this data at the source, as close to the sensor as possible is more efficient than the transmission of data across long networks to data centers. Artificial Intelligence (AI) Machine Learning (ML) using deep neural networks (NN) has been demonstrated as a powerful tool for data compression, processing, and analysis in various applications.

Efficiency is especially critical in High Luminosity Large Hadron Collider (HL-LHC) applications where both power and bandwidth are extremely limited resources. Other challenges include real-time latency constraints, operation in extreme radiation environments, and space limitations. Transforming raw data into higher-level physics information by utilizing ML can result in a reduction of data transfer by orders of magnitude.

Optimized AI instrumentation relies on co-design: the idea that system constraints, algorithm development, and hardware implementation inform and guide each other in complementary ways. ML uses large experimental data sets to create a model which excels in tasks requiring pattern recognition, anomaly detection and prediction. The development of an on-chip, efficient AI implementation begins with algorithm performance and design, tailored to the constraints of the system. While digital ML processing can achieve data reduction, taking advantage of neuromorphic, mixed analog-digital signal processing and in-memory compute techniques will enable super-efficient data processing. The objective of this research program is to develop a hardware-software codesign methodology and demonstrate novel detector instrumentation.

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

Cathode R&D for high intensity electron source in support of EIC

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The future Electron-Ion Collider (EIC) is a unique high-energy, high-luminosity polarized collider that will be one of the most challenging and exciting accelerator complexes ever built. The EIC will be a discovery machine that collides electrons with protons and nuclei to produce snapshots of those particles' internal structure. It will provide answers to the mysteries of matter related to our understanding the origin of mass, structure, and binding of the atomic nuclei. To maintain a high luminosity in the EIC, it is desirable to cool the hadron beams to improve the collision rate. Electron cooling is a promising technique to achieve this goal. This technique requires an electron source that can continuously produce electron beams with low emittance, high average current and high bunch charge. Multi-alkali antimonide photocathodes have proven to be highly effective in meeting these challenges. This research is aiming at growing nearly perfect crystals of alkali antimonides with assistance of a variety of characterization tools and evaluate the performance of the bulk grown crystals as photocathodes. Further, the effort will test these cathodes alongside traditionally grown cathodes for high current operation, both to evaluate performance and to characterize failure mechanisms. These efforts are expected to lead to a dramatic improvement of the material quantum efficiency (QE), with a goal of reproducible production of cathodes with high operational QE and lifetimes at least twice that of traditional cathodes. Furthermore, this research will explore and evaluate the various protective mechanisms brought up by the community in recent years, including 2-D material encapsulation and nano-structure enhancement, under high current operation conditions. The success of this work will yield the ideal photocathode material with better QE and longer lifetime for high current applications for EIC. It has the potential to create both a scientific breakthrough in understanding the properties of photocathode materials, and a technological breakthrough in extending the operational lifetime of cathodes for electron coolers. Ultimately this will improve luminosity and decrease downtime for the flagship machines in nuclear physics.

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

Prediction of Breakdown in Air and Solid Dielectrics:
A Complete Plasma Model from Discharge Initiation to Flashover

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A major challenge for most of the present day technologies and the technologies of the future is the compact and reliable design of insulation systems for their electrical components. Although controlled low-temperature plasma or non-thermal plasma in air at atmospheric pressure are of interest for a variety of technologies, a sudden occurrence of such plasma or discharge in an insulation system is highly undesirable. Such discharges can lead to an electrical breakdown or flashover, resulting in a complete failure of the insulation system. Currently, there is not a complete model of all the discharges that can result in the breakdown of an insulation system. For non-thermal plasma, there have been studies that focus on only one mechanism or just the transition from one discharge mechanism to another. For thermal plasma, studies have also been done focused on just the conditions following the occurrence of an electric arc or flashover. In both cases, a systematic study leading to a complete model comprising all discharge mechanisms is missing. To address this gap, a complete plasma model for both thermal and non-thermal plasmas will be developed using a hydrodynamic approach. The project aims to build the model sequentially, supported by experimental diagnostics covering a wide range of parameters. The model is expected to answer the question of whether or not there will be a breakdown for a given complex geometry of electrodes and insulation systems under a given voltage waveform. The work has the potential to address industrial applications and is of great importance to higher voltage systems.

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

Theory of the Femtosecond and Attosecond Dynamics of Molecules in Complex Regions of their Potential Landscapes

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The capture and transfer of energy by complex molecular structures, developed over millennia by evolution or engineered meticulously by scientists, is a remarkable phenomenon. At some scale of complexity, molecules gain the ability to control this process and direct the energy to accomplish useful tasks. This project seeks an answer to the question of where this scale begins, and specifically whether very energetic excitations in relatively simple molecules can be controlled. Lasers are our best tool to controllably add energy into molecules, and this project investigates the excitations and the subsequent dynamics produced by recently developed laser pulses with durations on the femtosecond (10^{-15} seconds) and attosecond (10^{-18} seconds) timescales. These pulses approach the natural timescale of the motion of electrons in molecules and can excite localized motion of electrons or atoms in molecules. The question of whether chemical reactions can be controlled with lasers has been explored in detail, especially for the ground state and the first few electronic excited states of molecules. While these initial questions were met with some successes and many struggles, recent progress in the field has seen the laser-induced formation of chemical bonds and the control of fragmentation in strong fields. These successes, and the ability to use attosecond pulses to prepare molecules in excited states higher in the energy spectrum, renew the promise of exerting specific control over molecules and their transformations. High-lying excited states in molecules, which are relatively unexplored, have different coupling regimes, transition timescales, and state densities compared to the ground state and first few excited states. The unique properties of high-lying excited states provide new targets that can be used to control the flow of energy in excited molecules. Importantly, the theoretical tools to describe the energetic excitations and their control are also at the forefront of method development. This project takes advantage of recent advances in the areas of quantum optimal control theory, electronic structure including ionizing states, and nuclear dynamics in order to describe excitations with attosecond pulses and develop the control schemes that can exploit them. The methods developed in this project push forward the abilities to compute dynamics in these systems and to provide unprecedented control of molecules.

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

Precise Chain Conformation and Dynamics Control for Conjugated Polymers in Organic Electronic Thin Film Devices

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Organic electronics based on semiconducting polymers are important for a broad range of next-generation renewable energy applications. Precise control of polymer conformation is critical for the device performance. However, it remains a great challenge to manipulate thin film morphologies for specific electronic and optical properties required for end-use products. The goal of this research is to enhance the knowledge base for efficiently and precisely controlling the processing of semiconducting polymers to increase device performance. The project will utilize various neutron and X-ray sources along with computational infrastructure to probe the structure and dynamics of polymers both in solution and thin films. High-throughput instrumentation, combined with machine-learning, will accelerate the understanding of the relationship between processing and device morphology. Ultimately, the project will 1) develop new high-performance semiconducting polymers with controllable morphologies; 2) advance neutron scattering for characterizing thin-film devices; and 3) elucidate the effect of various solution processing conditions on device performance for technologies such as photovoltaics, highly efficient light-emitting diodes, water purification, and solid electrolytes for energy storage.

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

Harnessing the Large Hadron Collider with New Insights in Real-Time Data Processing and Artificial Intelligence

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The next two decades of scientific research at the Large Hadron Collider (LHC) at the European Center for Nuclear Research (CERN) in Switzerland are anticipated to be remarkably different than the last two decades. With large amounts of data expected, the focus of research transforms from probing novel particle interactions of LHC collisions at the highest energies towards unexplored precision measurements and searches that target physics processes with small interaction strengths and extensive background rates. As a result, additional rare and hidden processes within the Standard Model (SM) of particle physics, and potentially beyond the SM, are expected to emerge as the LHC's luminosity continues to increase. This research focuses on a robust physics program at the CMS (Compact Muon Solenoid) experiment to measure these smaller and inconspicuous processes by applying a new measurement technique that can identify light resonances that decay into quarks. This new technique, in conjunction with advanced Artificial Intelligence (AI) computational algorithms, can not only lead to further constraints on the production of dark matter but can also open up a wealth of unique measurements and searches, including precision measurements of fundamental properties of the Higgs boson and an extended exploration for dark matter. In addition to the proposed studies, the research will upgrade the current real-time data acquisition system for the CMS detector to provide enhanced capabilities that will enable AI-based real-time analyses of LHC collisions. The fully developed state-of-the-art system will empower new measurements of the Higgs boson, new searches for dark matter, and the analyses of a multitude of unexplored scientific phenomenon. Furthermore, a real-time AI system operating with the significant LHC data rates represents a unique blueprint for future low-latency applications within science.

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

Cryogenic Electron Microscopy and Spectroscopy for Topological Spin Textures in Two-Dimensional van der Waals Magnetic Materials

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Two-dimensional (2D) van der Waals (vdW) materials are one of the most promising quantum materials that could revolutionize information- and energy-related technologies because of two factors: (1) the exotic properties enabled by the quantum confinement and (2) the feasibility of integrating these properties into existing silicon technology to functionalize future devices. The unique atomically thin 2D vdW structures provide an ideal platform for competition between the spin, charge, orbital, and lattice degrees of freedom, giving rise to novel intrinsic magnetism and frustrated magnetism at the 2D atomic limit. The goal of this research project is to identify, understand, and manipulate the topological spin textures in 2D vdW magnetic materials and elucidate the underlying spin-orbit, spin-lattice, and spin-charge interactions using cryogenic electron microscopy and vibrational spectroscopy approaches. More specifically, the research will determine the topological charge and spin configuration of the topologically protected quasiparticles and clarify the underlying spin-lattice and spin-phonon coupling mechanisms. The findings will facilitate the desirable manipulation of topological spin excitation and spin transport dynamics via the control of external magnetic and electrical probes, providing practical implications and design principles for future spintronics and quantum information technologies. The development of cryogenic electron microscopy capabilities will also advance the nanoscale characterization of magnetic and electronic properties for a broad range of strongly correlated systems.

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

Domain-Decomposition Induced Parallelism for Scientific Deep Learning at Extreme Scale

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A scale gap exists in scientific machine learning, or the intersection of computational science and artificial intelligence. Current tractable computational science problems are orders of magnitude larger than those in machine learning. In this project we will bridge that gap by developing parallel computing frameworks that connect deep learning problems and algorithms to classical computational science problems, at extreme scale. We target both data-driven scientific machine learning problems, posed through deep neural networks, and physics-driven problems, posed jointly through neural networks and physical models, to advance capabilities in DOE science applications. Our approach focuses on exploiting domain decomposition to extract additional parallelism in deep neural network training and to enhance interaction with high-performance computational tools for physics simulations. One theme of this research focuses on accelerating neural networks with new distributed algorithms induced by domain decomposition. Another theme centers on identifying and exploiting optimal domain decompositions for highly heterogeneous neural networks. The final research theme aims to demonstrate the enhanced parallel efficiency and scalability on applied problems related to, for example, subsurface imaging and additive manufacturing on state-of-the-art supercomputers. Technology developed in this project will integrate with and enhance the DOE's extensive high-performance computing ecosystem.

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

Controlling Photochemical Reactions with Optical Cavities

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Photochemistry promises access to otherwise inaccessible reaction pathways and products through the absorption of light. The challenge to meeting this promise is controlling these photochemical reactions with enough specificity to be of practical value. Placing molecules in optical cavities enables strong interactions of molecules with light and has the potential to drive photochemical reactions in novel and unexpected directions. To fully realize the potential of optical cavities in the context of photochemistry, theoretical tools must be developed to simulate these processes. This is particularly challenging because the unusually strong light-molecule interactions in the cavity require the nuclei and electrons of the molecule and the photons composing the light to be treated simultaneously. While quantum electrodynamical (QED) methods capable of describing light-molecule interactions exist in the chemistry and physics communities, they have rarely been combined with techniques to simulate photochemical reaction dynamics. This research will develop a suite of simulation methods that combine state-of-the-art approaches for describing the quantum states of molecules with QED treatments of light in optical cavities. This research will explore the possibilities for controlling the yields and specificity of photochemical reactions by manipulating the light-molecule interactions occurring within the cavity.

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

Interacting Topological Electronic States in Group-V Network Materials

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The theory of topological phases and phase transitions, which is the seminal work of the 2016 Nobel Prize in Physics, has bridged particles in high energy physics and electrons in crystalline solids. Dirac, Weyl, and Majorana fermions predicted in the Standard Model have found their counterparts in solid-state topological materials. These emerging quantum materials have been leading to deeper knowledge of important topics in physics and display a kaleidoscope of novel electronic properties with great promise for technology applications. Thus far, the research in this young field has mainly focused on a non-interacting single particle scenario. On the other hand, the electron-electron correlations are ubiquitous in many processes and known to drive fascinating phenomena. Therefore, extending the topological physics to the regime of interacting electronic system is expected to produce new quantum states and exotic phenomena. With this vision, the overarching goal of this project is to study how electronic correlations entangle with topology to give rise to new states and properties. The approach will be based on Group-V network material platforms to establish interacting topological electronic states, study the technological useful colossal magnetoresistance and its connection with topology and electronic correlations, and design novel material systems that can be further functionalized. This research will advance our understanding of the interacting topological quantum materials, seed new areas for deeper inquiry, and generate critical momentum for the deployment of quantum materials in information storage, sensing, and quantum computing applications.

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

Understanding Local Coevolution at Semiconductor Photocatalysts Involving Coating Protection and Corrosion Mitigation

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A promising approach for generating solar fuels uses particulate photocatalysts, in which reductive and oxidative products are coevolved in close proximity. Previous photocatalysts use oxides or nitrides. Despite decades of study, often with trial and erorr improvements to rates and selectivity, the solar-to-fuel conversion efficiencies remain much lower than the theoretical limit. This project will develop oxide coatings to protect semiconductors, such as silicon and gallium indium phosphide, to achieve efficient and durable photocatalysis. The surface of coated photocatalysts will be functionalized with nanoparticle or molecular co-catalysts. Understanding the coevolution locally at reductive and oxidative sites will advance the photocatalyst design beyond trial and error. Since the coating may develop pinhole defects over time, such understanding also helps mitigate photo-corrosion and improve durability. The objectives of this research include: (1) elucidating the roles of nanoparticle co-catalysts, molecular co-catalysts, and corrosion pinholes for charge separation; (2) characterizing the multi-scale coupled processes at the liquid interface; and (3) tuning the local energetics and kinetics by adjusting the co-catalyst local environment. The studies will take advantage of a recently developed kinetic model for photocatalysis by combining local measurements with numerical simulations to quantify important processes at the photocatalyst/liquid interface. Thus, photocatalysts with coating protection and corrosion mitigation can be designed to utilize the various co-catalysts for producing fuels or chemicals by harvesting solar energy.

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

Parameterizing wet removal of aerosol-forming oxygenated gases and its regional and global impacts

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Particles suspended in the atmosphere ("aerosols") are responsible for a large fraction of global deaths and have a substantial impact on the Earth's energy balance, but their impacts remain uncertain and difficult to model. Much of this particle mass is formed when gases emitted by natural and man-made sources undergo sunlight-driven chemistry that produces soluble and condensable compounds, forming particles. While these "aerosol-forming gases" are being chemically transformed, they are also being removed from the atmosphere by precipitation and settling to the Earth's surface, which can have a significant effect on the formation, growth, and removal of aerosols. Unfortunately, the parameters that control removal of gases from the atmosphere are highly uncertain, and almost no real-world observations exist on the role of precipitation in this process. The goal of the proposed research is to use existing and new data to quantify the rates at which atmospheric gases and particles are removed by precipitation and to understand the role of precipitation in the formation of aerosols across several sites. Characteristics of precipitation and atmospheric gases and particles will be used to estimate removal of gases by precipitation at 12 globally distributed facilities in the DOE Atmospheric Radiation Measurement (ARM) network. These existing data will be combined with unique measurements collected in 2014 at the Manacapuru, Brazil ARM facility as part of the ARM GoAmazon campaign, and new measurements of precipitation and removal of gases in Blacksburg, Virginia. The major outcome of this research will be an improved understanding of the regional and global impacts of precipitation on the formation of aerosol that is informed by real-world measurements and representative of diverse geographical regions. Additional scientific advances expected from this research include new methods to calculate the removal of gases from widely available measurements, increased availability of these data, and advances in atmospheric chemistry models.

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

Node-to-Code Comparison-Centered Interactive Performance Visualization

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Large computational endeavors such as climate models, energy simulations, and analytics libraries require efficient use of vast and complex resources. Increasing the efficiency, or *performance*, of these programs necessitates understanding the interactions between the program itself, the data it operates on, the libraries it uses, and the hardware on which it runs. Poor performance can be due to previously unseen scenarios that therefore cannot be checked automatically. Some of the information needed to understand these scenarios may be known to developers but not available in machine-interpretable form. Furthermore, often one needs a mental model of how the program and resources behave before they can formulate performance optimization strategies.

Visualization encompasses a class of methods in exploratory data analysis that use the human visual system to aid reasoning and understanding. It can be particularly helpful in situations where too little is known to directly compute or estimate the desired answer. The performance analysis of supercomputing applications is one such case. However, current performance visualizations are not designed for the scale of the performance data that is presently collected nor the complexity of performance factors such as the source code, input data, libraries, and hardware. These problems are magnified when attempting to compare performance between multiple executions of the same program. This project focuses on developing and evaluating scalable, interactive visual approaches that allow performance analysts to connect factors in performance from the hardware nodes on which the programs run to their source code and compare across multiple executions, thereby enabling them to understand and ultimately improve the efficiency of their applications.

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

Quantum logic spectroscopy of radioactive molecules for probing fundamental symmetries

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The heavy elements at the bottom of the periodic hold much promise and unique opportunities for basic science and technology. But, the radioactivity of these elements presents challenges. This project aims to use one such element, radium, as the cornerstone for studying and controlling radioactive molecules made with bottom-row elements with both high efficiency and high precision. Trapped radium ions will be used to synthesize trapped radium-based molecules and study their properties with quantum logic spectroscopy, a quantum information technique that was originally developed for optical atomic clocks that has recently been applied to molecules. With radium-based molecules the project will also be able to study properties of the radium nucleus and set the stage for using radioactive molecules to address profound questions centered on time symmetry violation, such as why is the Universe filled with matter, but lacks antimatter? A few rare radionuclides have massive octupole shape deformations, e.g. radium-225 and protactinium-229, which makes them exceptionally sensitive to time symmetry violating or equivalently charge parity violating physics. When these special nuclei are incorporated into a molecule, they can gain a further thousand-fold sensitivity enhancement due to the molecule's intense electric field. The combined nuclear and molecular sensitivities may be exploited to search for a tiny time symmetry violation signal using just a single trapped molecule.

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

Tracking the Mechanisms of Catalytic Reactions on Ligand-Protected Gold Nanoclusters

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Catalysts enable the production of an enormous array of chemicals on which modern society relies, but reduction of the costs and environmental impacts of this production will necessitate the development of new generations of catalysts that function efficiently in mild conditions. Furthermore, understanding and quantifying the chemical mechanisms during catalytic reactions will be necessary to optimize catalyst performance. This project focuses on an emerging class of catalysts, atomically precise metal nanoclusters, which are small nanoparticles that can be produced with precisely known chemical formulas and structures. These nanoclusters combine many of the advantages of nanoparticle catalysts, particularly exposure of reactive metal surface sites, with those of molecular catalysts, namely tailorable atomic geometries and the ability to produce the exact same catalysts in bulk quantities. Fully harnessing these advantages could lead to catalysts that require less energy input, form fewer byproducts, or enable new chemical transformations. Despite these advantages, progress on nanocluster catalysts has been hampered by a lack of understanding, or even direct experimental probes, of the catalytic mechanisms underlying their reactivity. This project aims to determine the mechanisms underlying key elementary reactions involved in electrocatalytic reduction and oxidation reactions with nanocluster catalysts. Using the unique capabilities of gas phase cluster chemistry techniques, the team will form and isolate elusive catalytic nanocluster-reactant complexes and probe the extent to which they activate small molecules such as CO_2 and the structures of intermediates involved in the reaction. The extent of activation will be tracked as the composition of the nanocluster is varied, elucidating the specific form of the cluster and the cluster-molecule interactions driving reactivity. These insights will be used to guide new efforts to precisely engineer more active sites on model catalytic nanoclusters. These studies will advance the optimization and deployment of nanoclusters as effective catalysts by (1) yielding improved mechanistic models that can be used to develop more active nanocluster catalysts for a variety of reactions, (2) identifying potentially more active nanocluster compositions, and (3) providing clear examples of successful approaches to engineering active sites.

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

Ion Transport in Highly Charged Polymer Membranes with Subnanometer Free Volume Elements

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Charged polymer membranes are key components of several ion separation technologies (e.g., electrodialysis and diffusion dialysis) and energy generation technologies (e.g., reverse electrodialysis and fuel cells). Developing membranes with better selectivity and throughput would improve the efficiency of existing technologies and enable the realization of emerging environmental and energy applications such as redox flow batteries, microbial fuel cells, ion-exchange membrane bioreactors, and electrochemical CO_2 reduction. Rational design of new membranes with desired functionality and tailored selectivity would be accelerated by improved fundamental understanding of the connection between polymer structure and transport properties. The overarching goal of the proposed research is to establish fundamental understanding of ion transport in highly charged polymer membranes with subnanometer free volume elements (FVEs). The properties of this unique and largely unexplored class of membranes are situated in a transition region between those of gas separation membranes, in which polymer backbone dynamics influence small molecule transport, and highly swollen charged membranes, in which tortuosity and Coulombic interactions are most important. The discovery of new ion transport mechanisms in highly charged membranes with subnanometer FVEs and molecular-level understanding of such phenomena could enable the design of membranes with properties that are specifically tailored for a given application. To better understand the connection between polymer structure and transport properties in this class of membranes, the proposed research combines membrane synthesis, advanced morphological characterization, and characterization and modeling of membrane transport properties.

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

Drawing Electronic Structure on the Nanoscale using Switchable Molecular Interfaces

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Nanoscale morphological variations are an omnipresent problem in materials for advanced energy technologies. Depending on the degree of variation, and how it effects the electronic structure and properties of a material, the impact can range from a decrease in the efficiency of an electronic device to a complete misunderstanding of a catalytic mechanism and poor catalytic selectivity. Atomically thin, two-dimensional materials are particularly sensitive to this inhomogeneity problem due to the realities of their synthesis and preparation, yet also uniquely suited to tuning and healing at the nanoscale level due to their responsiveness to the external environment. The goals of this research program are to understand how particular structural motifs modify the electronic structure of 2D materials and to design an easy way to heal or modify these motifs for specific functionalities, such as charge transport or ferroelectricity. Time-resolved photoemission electron microscopy will be used to uncover how nanostructures and their modifications determine the electronic structure and functionality of two model 2D materials, black phosphorus and indium selenide. The project will interface black phosphorus with a photoswitchable molecule and determine the mechanism by which isomerization of the photoswitchable molecule changes the electronic structure and dynamics of the interfacial black phosphorus material layer. The research will demonstrate the generalizability of the interfacial modification mechanism for encoding functionality in indium selenide. Using light to apply specific patterns on the photoswitchable molecular interfaces, the project will then draw new electronic structure on the nanoscale and encode charge transport or ferroelectricity in both 2D materials. Beyond the discernible goal of elucidating how specific structure variations dictate material processes, the research will generate an electronic structure-informed platform to explore how molecular interfaces sensitive to light, heat, or force can be used to redraw the electronic structure landscape and achieve tailorable materials for solar cells, catalysis, quantum information, microelectronics, or energy storage.

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

Adaptive and Fault-Tolerant Algorithms for Data-Driven Optimization, Design, and Learning

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Many paramount applications for the U.S. Department of Energy are formulated as nonsmooth variational problems. For instance, variational inequalities describe critical subcomponents of climate models including ice sheets and sea ice, as well as the interaction between fuel pellets and their protective cladding in light-water nuclear reactors. In addition, training machine learning models, parameter estimation in seismology, energy network resource allocation, and radio frequency cavity design for particle accelerators are all formulated as optimization problems. To efficiently and reliably solve these problems on advanced computational architectures, we will develop algorithms for stochastic optimization-based simulation that exploit adaptive, inexact, and randomized computations to accelerate convergence. Existing methods for nonsmooth variational problems suffer from numerous deficiencies, including slow convergence rates near solutions and performance degradation as the problem size increases. To ensure scalability to extreme scales, we will develop efficient algorithms for nonsmooth problems that rigorously manage inexact computations and refine approximation quality as the algorithm converges—permitting inexpensive approximations during early iterations. We will augment these algorithms with novel online modeling approaches based on randomized linear algebra and adversarial learning to discover underlying problem structures. Our algorithms will not only transform optimization-based simulation by exploiting the extreme heterogeneity of modern computing environments with adaptive and asynchronous computations but will also safeguard against hardware faults and failures through tunable randomized compression.

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

Ultrafast Coherent X-ray Scattering Studies of Quantum Materials

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Quantum materials have emerged as potential candidates to realize energy-efficient computing for ever-increasing technological demands of the internet of things, big data, and cloud computing. Quantum materials display strong correlations between their spin, charge, orbital, and lattice degrees of freedom, which results in a rich variety of electronic and magnetic properties. Emergence of novel quantum states under non-equilibrium conditions in quantum materials challenges the limits of understanding at microscopic length scales and ultrafast time scales. However, fundamental understanding of the role of nanoscale disorder and fluctuations in quantum materials is impeded by the lack of experimental methods which can access both characteristic lengthscales and timescales. This project focuses on utilizing time-resolved coherent x-ray scattering studies to understand the role of electronic and magnetic fluctuations in quantum materials and their dynamical behavior under laser excitation. X-ray photon correlation spectroscopy (XPCS) at synchrotron sources and upcoming x-ray free electron sources (XFEL) will be utilized to access both nanoscale lengthscales and fundamental timescales to study thermal fluctuations of electronic and magnetic order across phase transitions. Sample ground states will be carefully tuned via structural parameters including epitaxial strain, anion stoichiometry, and cation doping to investigate their role on evolution of electronic and magnetic ordering. These studies will enable mapping of the domain dynamics and correlations as a function of emergent electronic and magnetic ordering. The proposed project will utilize recently developed and upcoming user facilities such as National Synchrotron Light Source II (NSLS II), Linac Coherent Light Source (LCLS), and LCLS II as well as existing facilities such as Advanced Photon Source (APS) and Advanced Light Source (ALS). These studies will lead to development of a complete overview of electronic, magnetic, and structural properties of quantum materials with time scales down to the ultrafast regime and atomic resolution, to unravel nanoscale disorder in quantum materials and its evolution upon optical excitation.

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

Characterizing Plant-Specific Features of Mitochondrial Respiratory Complexes

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Despite the centrality of respiration to plant biomass accumulation, carbon flux, and acclimation, the fundamental mechanisms plant mitochondrial complexes use to produce electrochemical proton gradients that are converted into chemical energy remain unknown. A detailed functional and structural understanding of plant respiratory mitochondrial electron transport chain (mETC) complexes is essential to understand the fundamental mechanisms of biological energy conversion. By applying expertise in mitochondrial-membrane-protein biochemistry and structure biology, the PI recently obtained cryoEM structures of the protein complexes CI*, $CIII_2$, CIV and SC III_2+IV from *Vigna radiata* (mung bean)—the first high-resolution structures for mitochondrial complexes and supercomplexes for any plant. The project will characterize the plant-specific features of these and other plant mitochondrial respiratory complexes and supercomplexes functionally and structurally, using biochemical and biophysical approaches including chromatographic purifications, single particle cryoEM and, enzyme-kinetic analyses.

A deep structural/functional understanding of the components of plant mETC will provide insights into bioenergy conversion. This research will test hypotheses generated by the PI's recent structures to answer longstanding mechanistic questions such as the catalytic function of CI's carbonic anhydrase domain and the interplay between $CIII_2$'s dual roles. The research will also test novel hypotheses triggered by the structures, such as the potential functional role of CI*. These studies may produce additional breakthrough structures that will enable new detailed hypotheses regarding the mechanisms of these plant complexes and supercomplexes. The project will shed light on the fundamental tenets of electron transport in plant mitochondria and will generate approaches, materials, and hypotheses for the continued mechanistic examination of energy-converting enzymes in plants, advancing the field of plant respiration and bioenergetics. The research can also further the understanding of other areas of plant biology such as photosynthesis, biomass accumulation, and stress response.

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

When Covalent Organic Frameworks Meet Cross-coupling Reactions: Directed Synthesis, Mechanistic Investigation, and Energy Application

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Assembling molecular subunits into well-ordered architectures enables the precision synthesis of materials and furnishes novel properties. It had been a formidable task to construct artificial crystalline organic polymers until the discovery of covalent organic frameworks (COFs) in 2005. COFs represent an emerging class of crystalline porous materials that permit the integration of organic units into periodic networks. COFs feature intriguing properties such as high crystallinity, permanent porosity, lightweight character, versatile synthesis, and adjustable structures, which underpin their use in energy relevant applications such as catalysis, supercapacitors, photovoltaics, rechargeable batteries, and radionuclide sequestration. The formation of COFs usually hinges on reversible reactions which impart defect-healing to yield the most thermodynamically stable crystalline materials. Notwithstanding, the reliance upon reversible reactions limits the chemical stability and structural complexity of COFs. Therefore, moving bulk COF synthesis beyond the common reliance on reversible reactions will create novel COFs with exceptional chemical robustness and optoelectronic properties inaccessible by conventional means. The current synthesis of COFs beyond reversible reactions is mainly limited to the growth of 2D COFs at confined interfaces, whereas the facile synthesis of bulk COFs via single-step irreversible reactions remains largely underexplored. Among numerous irreversible reactions, transition-metal-mediated cross-coupling reactions are recognized as the most versatile synthetic toolkits to access robust covalent bonds. The enormous functional group tolerance, mild reaction conditions, operational simplicity, and superb efficiency underpin their broad use in the synthesis of porous materials. However, the emergent materials are mostly amorphous. The objective of this research is to translate irreversible cross-coupling reactions into the realm of COFs through a feedback loop of directed synthesis, mechanistic investigation, and energy application. Thereby, freeing bulk COF synthesis from the 'tyranny' of reversible reactions. Specifically, self-directional monomers will be linked through cross-coupling reactions to afford as-yet-undiscovered robust COFs. To accelerate the COF formation, microwave-assisted synthesis will be applied. Further, pre-formed COF analogs will act as topology templates for the controlled synthesis of new COFs via cross-coupling reactions. These new COFs will be exploited in photocatalysis and explored in-depth to reveal the origins of catalytic properties. In addition to the directed synthesis, the formation mechanism of novel COFs will be unraveled by a combination of experimental and computational approaches including ex-situ kinetic studies, in-situ probes, and computational simulations. This research directly fits the Material Chemistry Program in Basic Energy Sciences (BES) since it will produce new COFs through mechanistic understandings and precise control of synthetic pathways.

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

Machine Learning-Augmented Multimodal Neutron Scattering for Emergent Topological Materials

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Topological materials are a class of quantum materials where the materials' electronic or functional properties are robustly protected against local perturbation. Such topological robustness enables a wide range of promising applications, such as next-generation electronics immune from energy dissipation, and fault-tolerant qubits for quantum computers. However, topology is seldom considered as directly measurable, and scientists understand topological materials by measuring manifestations of topology from complex experimental probes. Neutron scattering offers unique advantages in elucidating topological quantum materials, such as high penetrating power, sensitivity to magnetism across multiple spatial scales, and a direct link to elementary excitations. Yet there has been a lack of clear mapping between topology and neutron spectra. The goal of this project is to capture the hallmark spectra signatures of topology in neutron scattering spectra by using machine learning to analyze high-dimensional spectra data. The project will a) capture the induced magnetic effect in topological insulators for dissipationless spintronics applications, b) elucidate the formation criteria of topological magnetic defects for computer memory and logic applications, and c) search for topological elementary excitations with potential thermal management applications. The project will offer new insights by revealing the hidden topological manifestations, in addition to enabling more efficient and reliable neutron scattering data analysis.

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

Resolving the Structure and Dynamics of Advanced Materials with Unprecedented Resolution

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Quantum materials present a range of remarkable properties with enormous potential for future energy-relevant technologies. Fundamental research to comprehensively understand the interplay of collective modes with quasiparticle dynamics and the discovery/characterization of new electronic phases at the relevant length, time, and energy scales is critical for explaining their macroscopic physical-chemical properties, such as thermal transport, electrical conductivity, and magnetism. The objective of this research is to develop a neutron probe with unprecedented resolution, which will be used to obtain deeper insights into the basic organizing principles and their responses to external perturbations that are at play in quantum materials. The new scattering methods developed with this research will also form a basis for next generation neutron scattering instrumentation, which can be potentially utilized to unveil novel properties of quantum materials, such as entanglement and chirality. The success of this research is essential to ensure the world-leading performance of the high-resolution neutron scattering instruments in Oak Ridge National Laboratory for the study of advanced materials.

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

Detecting Particle Dark Matter

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It is well established that dark matter pervades our universe, based on its gravitational pull, but the constituents of this substance remains a leading scientific puzzle. This research will develop theories and strategies to detect particle dark matter and uncover its properties. One aim of this research is to develop new theoretical tools needed to predict dark matter signatures in low-threshold direct detection experiments. Direct detection experiments aim to observe non-gravitational interactions of dark matter, but a large class of dark matter candidates could have easily evaded detection in existing experiments. Lower energy experiments would be sensitive to such candidates but are theoretically more challenging because they involve understanding detailed material properties. The research will lead to precise predictions and novel directions for direct detection in these new kinematic regimes. A second goal is to investigate the imprints of particle dark matter within our cosmos and in astrophysical data. Dark matter that has non-gravitational interactions during the early years of our universe can leave characteristic patterns in the cosmic microwave background or clustering of matter. This research will explore the cosmic history of dark matter candidates and apply observational data to search for possible particle interactions. Overall, the outcome of this research will be to broaden our searchlight to cover a wider range of well-motivated theories and could lead to new observational clues pointing us towards the particle physics of dark matter.

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

Improving Coherence Times for Quantum Devices Beyond the Next Decade

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Emerging quantum information technologies have the potential to revolutionize many areas in science and computing. It has recently been demonstrated that ionizing radiation contributes to errors in superconducting qubits. If these devices continue their current rate of improvement, ordinary levels of background radiation could become the dominant source of errors within the next decade. The goal of this project is to develop methods to reduce radiation impacts on superconducting quantum devices. The project has three thrusts. First, the response of qubits to a variety of tailored radiation sources will be measured to better understand and model how radiation interacts in these devices at the microscopic level. With this knowledge, new devices may be developed with intrinsically reduced sensitivity to radiation. Second, new types of cryogenic radiation sensors will be developed to better measure the qubit's environment in real time, including a first-of-its-kind hybrid device combining superconducting qubits and microcalorimeter radiation sensors on a single chip. Finally, developing new methods in quantum computing to integrate classical sensor data and detect radiation-induced conditions will enable more accurate quantum calculations with the application of sensor-assisted quantum fault mitigation (Sensor-QFM) concepts. The results of this project will provide a crucial stepping-stone on the path to realizing the full potential of superconducting quantum technologies.

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

Innovative High-Frequency Structures for High-Gradient Wakefield Acceleration

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High energy particle accelerators are crucial to the next big discovery in particle physics. To reduce the size and cost of particle accelerators, increasing the accelerating gradient (energy gain per unit length for the particle beam) is a research topic of critical importance. Advanced accelerator concepts hold the promise of revolutionary future particle colliders with dramatically higher gradients than what conventional accelerator technologies allow. Structure wakefield acceleration (SWFA) is a very promising, emerging advanced accelerator concept, where the high-gradient accelerating field is excited by an electron beam passing through an optimized structure in vacuum. This research will pursue two key concepts for high-gradient structures for SWFA: (1) developing advanced structures with novel, greatly improved electromagnetic properties, such as metamaterial structures; (2) pushing up the operating frequency of SWFA into the sub-terahertz and terahertz range. The research will pave the way for a future collider based on these innovative SWFA concepts, and could also lead to new applications in high power microwave sources and in compact light sources for scientific and industrial applications. This research will capitalize on the unique beam lines equipped with the world's highest charge cathode at the Argonne Wakefield Accelerator at the Argonne National Laboratory.

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

Nanomaterials for use in Radionuclide Generator Systems for Alpha Emitting Radionuclides

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Radionuclide generators are devices used to provide short-lived radionuclides to researchers that are not located near a production facility. They work by using a long-lived parent radionuclide that decays to the short-lived radionuclide of interest, allowing for repeated separations of the daughter over the half-life of the parent. The most famous example of such a system is the ^{99}Mo/^{99m}Tc system where ^{99}Mo is strongly bound to a resin-based column and ^{99m}Tc is routinely eluted for nuclear medicine applications. Targeted alpha therapy (TAT) has grown significantly in recent years as a methodology of interest for cancer therapy. TAT utilizes alpha decay, a prominent decay mode of actinide elements, to induce cell death in cancer cells. Several alpha emitting radionuclides have short half-lives, requiring the use of a radionuclide generator system for use in research and clinical applications. Two such radionuclides are ^{213}Bi (45.6 m) and ^{226}Th (30.6 m), which are available via decay of their parent radionuclides ^{225}Ac (9.92 d) and ^{230}Pa/^{230}U (17.4 d/20.8 d), respectively. A major drawback in the development of radionuclide generator systems for alpha emitters is the deposition of their energy (4-9 MeV) in short µm path lengths. The same benefit we get from alpha decay for cancer treatment destroys traditional resin systems at activities required for clinical use (>100 mCi). As traditional radionuclide generator systems are ineffective for alpha emitting radionuclides, we must rethink how we develop these generators. Metals are more radioresistant than the organic materials used in resins and thus could be beneficial for use in alpha emitting radionuclide generator systems. Moreover, if we take advantage of the physical process of alpha decay for separation it could be possible to overcome some of the chemical limitations. During alpha decay the daughter radionuclide has significant recoil energy (~100 keV), which is high enough to break chemical bonds (eV) and travel significant nanometer distances in various materials. Nanomaterials have been used in a variety of applications including environmental, medical, and chemical. These materials have the potential to be a promising solution in the development of radionuclide generator systems for alpha emitting radionuclides, however to date have not been investigated for this purpose. Furthermore, harsh chemicals would not be required for the separation as it would rely on the physical processes in alpha decay. This would facilitate the delivery of short-lived radionuclides in a form that is amenable to immediate use in radiolabeling reactions minimizing synthesis time and therefore increasing radiochemical yield.

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

First Principles Measurements of Temperature and Transport Properties in Warm Dense Matter

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The realization of inertial fusion energy requires the development of novel diagnostics that allow model-independent first principles measurements of ion temperature and transport properties of high-density, high-temperature plasmas. Also important to understand is the behavior of matter as it passes through the warm dense matter regime on the way to these dense fusion plasma states. Warm dense matter (WDM), an intriguing state characterized by having near solid electron densities (i.e., $> 10^{21}$ cm^{-3}) and extreme pressures and temperatures (P > 1 Mbar, T > 1 eV; 11,605 K), lies in a region of phase space not well described by condensed matter or plasma physics, making experimental characterization essential. While this state of matter is ubiquitous throughout the universe, found in the cores of giant planets and stars, and in inertial fusion energy processes, it remains challenging to create and simultaneously diagnose experimentally. Such extreme states of matter are created in the laboratory by a variety of methods including shock compression using nanosecond lasers, or by isochoric heating via femtosecond lasers. The created states are therefore highly-transient, existing from a few picoseconds to a few nanoseconds, and have a large density of free electrons, making them challenging to probe using optical techniques. The advent of Free Electron Laser light sources such as the LCLS, SLAC, has revolutionized how WDM experiments are performed. The LCLS provides extremely bright X-rays, femtoseconds in duration, capable of penetrating and probing the highly-ionized and transient WDM state. While measurements of the structure of WDM using X-ray diffraction have become almost routine using these methods, the direct measurement of temperature, an essential thermodynamic parameter for understanding the phase diagram or equation of state, remains outstanding. This research project will develop high-resolution inelastic X-ray scattering techniques in the collective and non-collective scattering regimes at hard X-ray Free Electron Lasers to directly obtain first principles measurements of both temperature and transport properties i.e., viscosity and sound speed, from matter at extreme conditions. The techniques that will arise from this research proposal will provide unprecedented insight into WDM and inertial fusion energy process and will have significant impact on many additional and varied fields of physics including geophysics, astrophysics, shock and plasma physics, non-equilibrium thermodynamics, and the search for novel materials.

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

Building from Discrete Molecular Catalysts to Multidimensional Catalyst Architectures: The Effects of Charge Delocalization and Electronic Coupling on Electrocatalytic Activity

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The electrochemical reduction of carbon dioxide is an important strategy for storing renewable energy from intermittent sources like solar and wind in the form of chemical bonds. Molecular inorganic complexes show significant promise as electrocatalysts for the selective reduction of carbon dioxide to useful chemical feedstocks and solar fuels. An outstanding challenge is incorporating these molecular catalysts into heterogeneous, multidimensional structures that reduce carbon dioxide with high activity and stability, but also maintain the selectivity of discrete, molecular catalysts. The objective of this research is to determine how the complicated and interrelated effects of charge delocalization, intramolecular electrostatics, and electronic coupling influence catalytic activity and selectivity in extended multidimensional catalyst architectures. The specific research approach uses a combination of electroanalytical and spectroelectrochemical measurements to probe the relative influence of these effects on catalytic performance as the catalyst structures increase in complexity from discrete molecular catalysts, to multimetallic molecular assemblies, and finally to extended 1D and 2D catalyst structures. The results of this research will provide a template for the rational design of new multidimensional catalyst materials, comprised of molecular catalyst building units, for the efficient and selective electrochemical conversion of carbon dioxide to value-added products.

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

Epitaxial Stabilization of Novel Superconductors for Energy Generation, Storage and Distribution

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Superconducting materials hold great promise for applications in energy generation, storage, and distribution. However, known superconductors still lack the transition temperatures, critical fields, or pairing symmetry to be fully exploited for these applications. This has not only continued to motivate the optimization of known superconducting materials, but further driven efforts for the discovery of new families of superconductors. This Early Career program will exploit the characteristics of the copper oxide-based superconductors as design criteria in the search for additional new materials that could host high-temperature superconductivity. The plan is to design, synthesize, and probe with atomic-scale precision metastable nickelate and cobaltate thin films. This work will tackle two intertwined synthesis challenges: 1) how does one control the local oxygen coordination and environment in a complex oxide material during synthesis and 2) how does one monitor and manipulate changes to the oxygen coordination post-synthesis. In both thrusts, new synthetic techniques are proposed that will allow reaching previously unexplored compounds. While the main work will focus on developing specific techniques for the stabilization and exploration of hypothesized superconductors, it is notable that the ability to create novel oxygen coordination environments should have broader impacts for a variety of non-perovskite oxide materials.

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

What is the Matter Within Polaritons: Molecular Control of Collective Hybrid States

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When carbon-based organic semiconductors emit or absorb light, a discreet event occurs in which energy is exchanged between particles of light (a photon) and electrical current (an electron). Instead of such discreet jumps, it is possible to make devices in which the photons and electrons mix together, forming entirely new hybrid states called polaritons. This can be done by placing certain molecular materials between two very closely spaced mirrors in a microcavity. The mirrors act like miniature boxes and trap photons, allowing them to interact and combine with electrons in the semiconductor. The resulting states blend the character of the two parent particles, leading to entirely new behaviors ranging from enhanced conductivity and energy transport to altered chemical reactivity. This approach holds the promise to rewrite molecules' energy landscape and tune their functional properties at will, without recourse to laborious synthetic chemistry. Yet fundamental questions about this concept prevent its application: What properties does the polariton inherit from the parent molecules? How can we influence these behaviors with molecular structure? This research will tackle these questions and develop a detailed understanding of how the complexity of organic semiconductors can be harnessed to control polariton behavior. The effort calls for cutting-edge laser spectroscopies to record the ultrafast processes inside the microcavity, systematically correlated with the properties of the parent organic semiconductor. This work will lead to new, fundamental understanding of the nature of both molecular materials and light-matter interactions, paving the way to a future where we can non-synthetically rewrite molecules' properties. Moreover, the principles uncovered will spur new approaches to exploit polaritons for more energy-efficient light-emitting and light-harvesting systems and open new opportunities from photocatalysis and sensing to room-temperature quantum devices.

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

Probing Quantum Materials with Evanescent Waves
Using Advanced 4-Dimensional Scanning Near-Field Optical Microscopy

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When light strikes a host material, the inherent light-matter interactions that take place encode extremely valuable information about the material's properties under study. Of particular interest are the long-wavelength excitations at the infrared (IR) and terahertz (THz) frequencies, where critical low-energy physics can be explored noninvasively in most quantum materials. Currently, the performance of existing IR & THz microscopies is largely limited by their spatial resolution, which has severely hindered the ability to understand a wide array of exotic quantum effects that typically emerge from the nanometer length scales. This research will develop advanced scanning near-field optical microscopy capable of examining quantum materials under extreme conditions at cryogenic temperatures and high magnetic fields, while extending imaging to nanometer length scales, femtosecond time scales, and the IR and THz spectral range simultaneously. The result of this four-dimensional characterization will be a greater understanding of two-dimensional quantum materials that possess intriguing quantum phases of matter and novel properties, including superconductivity, metal to insulator transitions, and topological states. Harnessing strong light-matter interactions represents a unique way to explore the uncharted territory of quantum systems under extreme conditions, which is far beyond what is attainable with conventional optics and could lead to the development of new types of quantum devices on-demand. The nano-optics methodologies developed in this research will benefit the explorations of a broader class of quantum materials for both fundamental science and potential technological applications.

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

Simulation-based Inference for Cosmological Parameter Estimation and Discovery

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The earliest and latest epochs of the Universe are marked by periods of cosmic acceleration — an increasingly rapid expansion of space-time. While the exact cause remains a mystery, powerful clues are encoded in large corpuses of imaging data obtained by telescopes that scan the sky during multi-year observational surveys. The conventional computational tools used to decode cosmic clues rely primarily on hand-parameterized analytic mathematical models and relatively static, inflexible algorithms. However, next-generation surveys, like the Cosmic Microwave Background Stage 4 (CMB-S4) project and the Vera C. Rubin Observatory's Legacy Survey of Space and Time (LSST), both with significant DOE roles, have unprecedented instrumental sensitivity and will produce data of commensurate size and complexity. This necessitates new algorithms and modeling techniques that have appropriately extraordinary speed and adaptability, allowing us to achieve sufficient levels of detail in our descriptions of the data. Data-driven computational tools, like artificial intelligence (AI), have these characteristics, but they critically lack interpretability. In this project, we will use frameworks like simulation-based inference that combine AI with statistical methods to model cosmic probes, enable new measurements of cosmic acceleration, and discover new physics in cosmological data.

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

Novel Data-Processing Strategies for New Physics Searches and Precision Luminosity Measurements at the Large Hadron Collider

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The Standard Model (SM) of particle physics has been remarkably successful in explaining observed phenomena at the forefront of fundamental physics, yet experimental observations and theoretical considerations indicate that the model is still incomplete. Predictions from the SM continue to be stringently tested by experiments at the Large Hadron Collider (LHC), the world's highest energy particle accelerator, at the European Organization for Nuclear Research (CERN) in Switzerland. This research plans to develop and deploy innovative data-processing and event reconstruction algorithms that can greatly advance the physics discovery potential of the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC. New algorithms using next-generation machine learning techniques to reconstruct charged particles will be developed while also employing sophisticated data-processing methods, which will enable researchers to apply such algorithms "on-demand" only to the most relevant subset of the large dataset collected by the experiment. The tools in turn will identify physics processes involving two photons that get emitted by the colliding LHC beams to produce massive particles with unprecedented accuracy. Specifically, a measurement of the SM quartic coupling between photons and W bosons together with direct searches for new physics phenomena in high-energy photon-photon collisions will be performed. Complementing this program, design studies, prototype development, and performance measurements of a new state-of-the art addition for the ATLAS silicon detector will be pursued in order to advance precision measurements of, and extend the discovery potential for, several physics processes during the future High-Luminosity LHC running period.

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

Accurate calibration of SNS neutrino flux with a heavy-water detector for COHERENT

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Neutrinos are the lightest, most rarely interacting matter particles known to science. Through precise measurements of a newly observed type of neutrino interaction – coherent elastic neutrino-nucleus scattering (CEvNS) – the COHERENT collaboration, working at Oak Ridge National Laboratory's Spallation Neutron Source (SNS), aims to illuminate exciting possibilities beyond the Standard Model, while simultaneously benchmarking detection methods for both supernova neutrinos and hypothesized dark-matter particles. The largest uncertainty in these measurements is the flux of neutrinos created when 1-GeV protons strike the thick mercury target at the SNS. Based on physics simulations and worldwide measurements of similar processes, this rate can only be estimated to about 10% accuracy. This research program will support COHERENT's physics goals by completing a heavy-water neutrino detector that will make a dedicated, benchmark measurement of the electron-neutrino flux from the SNS, based on well-understood neutrino interactions in deuterium. The research team will build the second and final module of the planned heavy-water Cerenkov detector, allowing COHERENT to reach the necessary statistical precision. The flux measurement will significantly improve the accuracy of the neutrino-interaction results in every other COHERENT detector, and it will enable a better understanding of other, similar sources around the world.

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

From Atomic Nuclei to Infinite Nucleonic Matter within Chiral Dynamics

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The quest to describe classes of phenomena that occur in the atomic nucleus lies at the heart of nuclear physics. These quantum mechanical phenomena play a major role in the birth and evolution of the universe, in astrophysical environments, in energy production through fission and fusion reactions, and in industrial and medical applications via use of stable isotopes and radioisotopes. Understanding the structure and dynamics of nuclei and strongly interacting matter is, therefore, the primary focus of many nuclear experimental programs and theoretical efforts. The present research will aim to develop a clear and coherent picture in which microscopic models accurately describe atomic nuclei while simultaneously predicting properties of infinite matter, e.g., pure neutron matter, relevant to the structure and internal composition of neutron stars. It will make use of state-of-the-art computational techniques and high-performance computing to broaden the applicability of variational and Green's function Monte Carlo methods, currently limited to bound states with mass number $A \leq 12$. The results will directly address some of the fundamental questions at the frontier of nuclear science and will complement the US Department of Energy's major investments in supporting present and future nuclear physics experiments at low-, medium-, and high-energy.

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

Development of an Integrated Multiscale Methodology for Simulating Electrocatalysis at the Metal Oxide - Electrolyte Interface

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Electrocatalysis uses an electric current combined with a catalytically active surface to carry out chemical reactions that would otherwise not occur. Due to its ability to use electricity generated from renewable sources, electrocatalysis will play a vital role in the transition to a society based on sustainable energy. As examples, water electrolysis can be used to split water into hydrogen and oxygen gas, while CO_2 electrolysis can be used to convert carbon dioxide into valuable fuels and chemicals. Despite its utility, large scale adoption of many electrocatalytic technologies is hindered by lack of suitable catalysts that can efficiently carry out the reactions without wasting a significant fraction of the electrical energy. The key difficulty in developing more efficient electrocatalysts is the poor understanding of how the reactions occur at the atomic level. The overall goal of this project is to develop a multiscale method to simulate kinetics of electrocatalytic processes on metal oxide surfaces in the presence of a full atomistic description of the electrochemical interface. The project will also provide an open-source simulation code enabling researchers to perform realistic atomic level simulations of electrocatalysis with high accuracy and low cost. This, in turn, will equip computational researchers with a vital tool for understanding how to overcome the current limitations in important electrocatalytic processes such as oxygen evolution and CO_2 reduction.

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

First Principles Approach to Exciton Transport in Energy Materials

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The absorption of light by matter follows a universal mechanism that drives crucial reactions in both natural and engineered systems. Processes ranging from photosynthesis, to photocatalysis, to energy harvesting in photovoltaic cells all begin in the same way: the absorption of light creates an exciton—a correlated electron-hole pair that carries energy rather than charge. In photovoltaics, the relaxation of an initial high energy exciton into a lower energy state and its separation into individual charge carriers dictate how much current can be generated from the absorption of sunlight. In photosynthetic light-harvesting complexes, energy is transmitted by excitons with surprisingly long coherence times. In optoelectronics, excitonic interconnects have the potential to integrate the fast speeds of information carried by photons into modern semiconductor-based electronics. In quantum information and sensing, excitons allow for the optical preparation and transduction of quantum states with specific spin, polarization, energy, and momentum. Hence, a predictive understanding of exciton energies and coupling to light, as well as dynamical properties related to their decoherence, relaxation, transport, and diffusion, is essential for the engineering of materials' properties across all these fields, and more. This project aims to develop and apply a range of first-principles theories (i.e., theories built *ab initio* from the governing principles of quantum physics without any empirical parameters) based on the GW one-particle self-energy plus the Bethe-Salpeter equation approach for two-particle interactions within many-body perturbation theory to understand exciton dynamics in materials of interest for optoelectronics, energy harvesting, and energy transport. Targeted materials include layered transition metal dichalcogenides, hybrid metal-organic halide perovskites, and topological materials. The developed methods will allow for predictive simulations of exciton transport and dynamics in the ballistic, diffusive, and intermediate regimes.

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

Elucidating the Molecular Origins of Enhanced Carbon Mineralization Kinetics in Adsorbed Water Nanofilms

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In the earth's subsurface, abundant rocks rich in divalent metal silicates such as basalt formations have the theoretical capacity to mineralize CO_2 by an order of magnitude greater than the estimated emissions from burning all fossil fuel resources on Earth. The accessible capacity of these rocks depends in part on the composition of the injected fluid, which directly influences the mineralization products and their rate of formation. In a fluid dominated by CO_2, carbonation will be mediated by nanometer-thick water films coating mineral surfaces. Through advanced molecular simulations, theory, and experiment, this project aims to uncover underlying molecular mechanisms of carbonation reactions in thin water nanofilms. The work will provide an understanding of the factors governing the rates of carbonation reactions in water-poor systems. This basic understanding can ultimately pave the path toward envisioning carbon-neutral mining practices, designing advanced reactive fluids for the enhanced oil and gas recovery from unconventional reservoirs, and developing water-efficient carbon-negative concretes for the construction of sustainable energy infrastructures in arid climates.

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

Improving candidate gene discovery by combining multiple genetic mapping datasets

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Identifying the genes involved in the adaptation of plants to their local habitat and to environmental stresses are essential goals of plant scientists across a range of research fields. Knowledge of such genes helps plant breeders to introduce beneficial traits from wild relatives into high-yielding modern crop varieties. Plant biologists can also use that information to understand the role of genetic variation in plant development, evolution, and stress response. However, it is complicated to validate the function of genes at the molecular and physiological levels and determine the importance of the different variants of a gene responsible for a particular trait. Identifying gene function is further complicated when several genes are responsible for a trait of interest. Reducing the number of candidate genes and making an informed decision on which ones should be validated is particularly challenging. This project's goal is to understand the impact of phosphorus deficiency and cold stress on sorghum lipid metabolism and develop mathematical approaches that will integrate results from different genome-wide association studies and population genetics indexes of selection. With these approaches, metabolic profiling data from a large number of sorghum lines under phosphorous and cold stress will be combined with analyses of geolocated natural populations adapted to those stresses and measures of genetic differentiation. Combining multiple independent datasets will enable the identification and ranking of candidate genes and metabolic pathways involved in these stress responses. The methods developed as part of this project will be applicable to other potential bioenergy crops and different environmental stresses.

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

Advancing accelerator beam modeling via high-dimensional phase space diagnostics at a high-intensity injector test stand

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This research aims to improve performance of high-power accelerators and support order-of-magnitude increase in beam power. High-power accelerators deliver beam to targets, producing secondary beams for experiments in fundamental and applied science. In operation, unintentional loss of particles along the beamline must be minimized. Loss control is an important facet of accelerator operations because it limits performance, as radioactivation in the tunnels can prevent maintenance. Visions for future high-power facilities require losses at or below current levels while increasing power to target by an order-of-magnitude or more. The research will advance fundamental understanding and predictive power to model beam halo in megawatt-class accelerators. A source of losses, halo is an undesired feature of beams that consists of particles far outside the core beam distribution. A challenge in beam halo control is the lack of reliable models, which have not been shown to agree with halo observations. Limited information of the real system plays a role, particularly the 6D phase space distribution of the bunched beams. This work leverages unique diagnostic capability at the Spallation Neutron Source (SNS) Beam Test Facility (BTF) to advance predictive capabilities for beam and halo distributions. This includes full and direct measurement of the 6D beam distribution as well as complete halo imaging. The compact BTF replicates conditions in the SNS front-end and will be used to generate a large dataset containing both input for simulation parameters and output for validation of the front-end model. More accurate modeling will lead to better loss control and improved performance of existing accelerators. Neutron scattering facilities as well as other applications of multi-megawatt beams, including proton drivers for neutrino physics, will benefit from this research.

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

Advanced Numerics for Atomization and Multi-Physics Interface Dynamics

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The atomization of liquid into small droplets plays a key role in a diverse range of environmentally-sensitive and energy-intensive processes, including, e.g., automobile spray painting, bubble aeration systems, medical nebulizer devices, and biofuel combustion. To explore the underlying mechanisms, optimize device design, and reduce material waste, the numerical simulation of these processes is often required in order to model droplet formation and their multi-physics driven behavior. However, traditional techniques are challenged by the highly complex geometry at play and progress using these lower-order approaches is stalling. In this work, we aim to significantly advance the state of the art in atomization numerics and multi-physics interface dynamics. We will develop higher-order numerics which enable, and then harness, sub-grid resolution of complex interfacial geometry, and apply these methods across a spectrum of next-generation DOE-relevant applications. The immediate goals of this work form a crucial stepping stone in the longer-term vision of coupling the two worlds of (i) high-fidelity multi-physics interface dynamics and (ii) surrogate-based reduced order models in order to explore the vast parameter landscape typical of applications in manufacturing and industry. In tandem with high performance computing, the mathematical and algorithmic advances developed in this work will help to address a variety of DOE mission-critical challenges in multi-scale and multi-physics dynamics.

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

Neutron Yield Scaling with Current in Dense Plasma Focus (DPF) Discharges

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The objective of this work is to understand the most outstanding and unresolved question in the nuclear fusion science underlying the dense plasma focus (DPF) z-pinch concept—why does the scaling of neutron yield versus plasma current decline dramatically above currents of about 3 million amps? State-of-the-art DPF machines developed by DoE are addressing mission deliverables; this complementary basic research seeks to move beyond the state-of-the-art. This project combines world-class computer simulations with experiments on a newly commissioned megajoule-class DPF platform, the MegaJOuLe Neutron Imaging Radiography (MJOLNIR) experiment. The fundamental science program is heavily guided by the simulation efforts, and the experiments utilize new diagnostics to make the critical measurements hypothesized to be important in understanding the variance in performance and roll-off in yield that has been observed to date. The ultimate goal is to identify the barriers that prevent strong neutron yield scaling (current to the 4^{th} power, or I^4), as plasma current is increased up to the maximum capabilities of the new platform, 4 million amps. Understanding and mitigating the physical mechanism(s) controlling the observed yield roll-off at high current will have a strong impact in the scientific community and open the door to a number of exciting basic and applied science applications. Neutrons can be used to "look through" objects, analogous to x-rays, but they are more effective than x-rays at creating images of materials containing hydrogen, such as fuel or water. A bright enough neutron source of this type could enable high-speed (50 nanosecond, or 50 billionths of a second) neutron "photographs" for imaging engine fuel flow or the human body. This source could also be used for national security applications, such as identification of isotopes within a contaminated waste area. For basic science, an effective high-brightness source would also enable a low-cost high-rep-rate high-energy-density physics (HEDP) experimental platform, which could be used to study shock physics, opacity experiments, and warm dense matter, among other HEDP phenomena. Prepared by LLNL under Contract DE-AC52-07NA27344.

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

Reducing Top Systematic Uncertainties in Cosmological Analyses with Type Ia Supernovae and Contaminated Photometric Samples

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A critical mystery in physics and a key research pillar of the DOE High Energy Physics (HEP) Cosmic Frontier program is to understand the nature of dark energy that causes the universe to accelerate in its expansion. While cosmological observations constrain the amount of dark energy to make up roughly 70% of the universe, its nature remains unknown. Type Ia supernovae (SNe Ia) were used to discover the accelerating universe and today provide some of the tightest constraints on its nature. The research project will develop new advances in analysis techniques that can significantly reduce the top systematic uncertainties in the cosmological analysis of the supernova sample measured by the Dark Energy Survey (DES). Specifically, using the expertise of the research group, the project will use new techniques and the largest data samples to constrain models of the unexplained `intrinsic' scatter of SNe Ia and the relation between SNe Ia properties and host-galaxy properties. The particular challenge of this work is that samples will have a small fraction of core-collapse contamination and host-galaxy mis-association that can significantly bias constraints on SNe Ia physics. By tackling this challenge, this work will both increase the statistical precision of the sample and reduce the largest systematic in current analyses. Furthermore, the research group will apply advances from the DES analyses to the Vera Rubin Observatory Legacy Survey of Space and Time (LSST) survey both in terms of survey strategy optimization and image pipeline performance, thus enhancing the science return of both of these DOE and National Science Foundation partnerships. This work will be done at both the image and catalog level to perform pixel-to-cosmology analyses of simulations of the LSST SNe survey. This work will enable the analysis of the LSST-Year1 SNe Ia sample, which will be 15x larger than the DES 5-Year sample.

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

Quantum materials, lattice gauge theory and QCD

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The confluence of modern scientific ideas from Quantum Chromodynamics (QCD) - the fundamental theory of nuclear interactions, condensed matter physics and particle physics has enabled notable discoveries of exotic phenomena in extreme astrophysical environments as well as in materials in tabletop experiments. This project brings together seminal ideas from lattice quantum field theory (QFT), dense-QCD and topological superconductors and insulators, the interrelations of which in two and higher dimensions could reveal novel phase structures of QCD as well as lead to the discovery of new quantum materials. Of great current interest is the realization of anyonic excitations because of their resilience in fault tolerant quantum computing and their ability to exquisitely diagnose topological phases of quantum materials. Advancing our understanding of anyonic excitations in QFT could, in turn, address foundational questions in the study of the QCD phase diagram and nuclear matter.

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

Electrocatalytic Modification and Upcycling of Polyvinylchloride and Chloroparaffins

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This research program will develop new reaction technologies that enable selective modification of chlorinated plastics to create materials with altered physical properties, improved lifetimes, and new end-of-life applications. Post-synthetic functionalization of polymers is critically important for modifying the physical properties of plastics that are prepared with limited control over the molecular structure. Polyvinylchloride (PVC) is an example of such a polymer, which has narrow range of macromolecular properties. Altering these properties such that PVC can be utilized in a wide range of applications requires high loadings (up to 50%) of plasticizers, toxic stabilizers, and volatile impact modifiers. These formulations limit PVC recyclability, safety, and long-term stability. As examples, PVCs containing different plasticizers cannot be recycled together. Over time, the non-covalent additives leach from PVC. Leached plasticizers present an environmental hazard and leave the resulting plastic brittle with an increased susceptibility to forming microplastics. Finally, disposal of chlorinated polymers is energy intensive because conventional approaches of polyolefin pyrolysis create corrosive and acutely-toxic products. The program objective is to develop solutions to these challenges through the discovery and mechanistic understanding of new reaction chemistries using electrocatalysis for C–Cl bond functionalization that can be applied directly on polymer chains. Through this research, the performance of PVCs will for the first time be controlled at the molecular level, rather than through formulations chemistries that rely on non-covalent additives.

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

Quantitative Characterization of Emerging Quark-Gluon Plasma Properties with Dynamical Fluctuations and Small Systems

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High energy collisions of atomic nuclei create extreme conditions to study the collective property of nuclear matter. Experiments at the Relativistic Heavy Ion Collider (RHIC) in the U.S. and the Large Hadron Collider (LHC) in Europe create a novel state of matter Quark-Gluon Plasma (QGP), which exhibits quarks' and gluons' degrees of freedom at a temperature exceeding 2 trillion degrees Kelvin. The QGP behaves like a nearly perfect fluid from the many-body effects of Quantum Chromodynamics (QCD). This hot and dense soup of elementary particles filled our universe a few microseconds after the Big Bang as the primordial liquid. The emergence of QGP's strongly coupled nature is studied by varying collision energy and system size at RHIC and the LHC. The current Beam Energy Scan (BES) program at RHIC further probes the QCD matter's phase structure, searching for the existence and location of the first order (liquid-vapor) phase boundary between ordinary nuclear matter and QGP terminating at a critical point. This project aims at elucidating QGP properties by understanding the dynamical evolution of stochastic fluctuations in relativistic heavy-ion collisions from large to small systems. This research will provide a quantitative characterization of the QGP properties, how it ripples, flows, and its phase structure by interweaving theoretical many-body nuclear physics, high-performance computing, and advanced machine learning techniques. The QGP viscosity and charge diffusion coefficients control how fluctuations of energy, momentum, and charge density dissipate in the system. The presence of a QCD critical point in a heavy-ion collision should lead to enhanced fluctuations and strong correlations of conserved densities. The out-of-equilibrium dynamics of these small ripples under a realistic hydrodynamic flow background elucidate the thermal, critical, and transport properties of the QGP. A new open-source theoretical framework will be developed to decode this information from the measured multi-particle correlations. This framework integrates the state-of-the-art 3D event-by-event QGP dynamics and the evolution of generic fluctuations. By further combining the theoretical framework with advanced statistical analysis, reliable phenomenological constraints on the QGP properties will be delivered when confronting the precision measurements from the RHIC BES program. This research will benefit the current Beam Energy Scan phase II and upcoming SPHENIX programs at RHIC, high luminosity runs at LHC, and the future Electron-Ion Collider (EIC) and Facility for Antiproton and Ion Research (FAIR).

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

Precision Science and Control of Pellet Fueling for Optimizing Tokamak Plasma Scenarios

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Pellet fueling is an essential requirement for burning plasmas, where deep particle delivery is required for fueling the fusion reaction occurring in the core. This change in primary fueling technology is required as fusion experiments enter the burning plasma regime, where conventional fueling techniques based on gas puffing are limited to the plasma edge, and will be replaced instead by cryogenic pellet injection for central fueling. However, this change in fueling source also yields qualitative differences in plasma behavior, with impacts on macroscopic stability and transport that affect other important aspects of burning plasma control. A detailed understanding of these interactions is critical for the successful integration of fueling needs with those of overall plasma performance. The goal of this proposal is to develop and optimize pellet-fueling processes for controlling and sustaining the high-performance plasma states required for ITER and other future burning plasma devices. This proposal will address several outstanding issues for the successful integration of pellet fueling within the ITER research plan, including magnetohydrodynamic stability and Edge-Localized Mode (ELM) control, and compatibility with divertor plasma detachment. This experimental research will be carried out at the DIII-D National Fusion Facility, and will be enabled by a number of significant upgrades to the DIII-D pellet injection system. Collectively, this proposal provides capabilities for precisely controlling and quantifying pellet particle sources in the plasma, as well as providing further increases to the available core particle source from pellets relative to other sources such as neutral recycling. These will be utilized in precision experiments to probe the impacts of pellet fueling on the desired plasma states, which must simultaneously exhibit high-confinement, ELM control, and integration with an acceptable boundary plasma state. These experiments will be coupled with theoretical modeling of the edge and boundary plasma under pellet-fueled conditions to elucidate the interplay between particle sources, stability and transport, and the fueling process. This understanding will be essential to the achievement of high-performance core-edge compatible regimes that are required for ITER operations as well as for the mission of a US Fusion Pilot Plant.

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

Discovery in the 4th Dimension: Shining Light on the Dark Sector

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The astrophysical evidence for dark matter and the profound questions in particle physics that were highlighted by the discovery of the Higgs boson suggests that new fundamental particles and interactions are awaiting discovery. The Large Hadron Collider (LHC), the world's most energetic particle accelerator at the European Organization for Nuclear Research (CERN) in Switzerland, will provide a wealth of high energy collision data that will make it possible to search for evidence of new physics. A hidden "dark sector" of particles that interacts very weakly with the Standard Model (SM) of particle physics may be key to understanding the characteristics of the Higgs boson and the nature of dark matter. Light dark sector particles that decay to known SM particles are predicted to be long-lived in many theoretical scenarios of physics beyond the SM. This research program plans to utilize the data acquired by the CMS (Compact Muon Solenoid) experiment at the LHC to search for long-lived particles by exploiting the capabilities of sensitive muon detectors and using artificial intelligence to develop novel computational tools and methods to advance the studies. The research will investigate two possible scenarios containing exotic physics signatures: (1) searches for low-mass, long-lived particles decaying into muons and (2) hadronic showers involving decays of the Higgs boson that are identified in the CMS detector's muon system. Such searches will be complemented by designing and developing next-generation electronics and firmware for a new CMS precision timing detector capable of ultra-fast timing information to measure the trajectories of charged particles traversing the CMS detector. Ultimately, the proposed program will enhance the physics capabilities during the future high-luminosity era of the LHC and will be crucial in the detection of delayed signals from long-lived particles that can shed light on the dark sector.

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

Orchestration for Distributed & Data-Intensive Scientific Exploration

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Scientific exploration and hypothesis generation is increasingly dependent on the convergence of scientific modeling, data analytics, and machine learning. The result is data-intensive workflows that are composed of multiple stages of computation and communication between distributed and heterogeneous computing resources. Data movement is frequently the most significant bottleneck, which is compounded by increasingly large data volumes. Our research objective is to enable workflows, written in a variety of languages, that have production-like performance in massively distributed environments with multiple computing paradigms. Our approach will develop techniques to orchestrate data and tasks within distributed workflows. Our tools will generate workflow-specific execution templates, based on data-centric execution analysis and modeling, that select data locations and layouts for storage and memory that improve locality, reduce data movement overhead, and better use the fastest data resources. The impact will be increased scientific capability due to improved workflow performance.

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

AutoNeurify: Automatic Infusion of Learning in HPC Applications

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High-performance computing (HPC) applications have become essential for scientific progress. Computational methods for data collection and simulation are critical in making foundational discoveries in nearly all scientific disciplines. HPC applications are also essential for addressing humanity's big problems, such as understanding and mitigating climate change, the energy crisis, and for drug discovery. Consequently, scientific discovery can be accelerated by improving scientific software by speeding up their execution, and lowering the expertise required by scientists to deploy and maintain software. Recent research has shown the benefit of using machine learning to speed up HPC applications. However, there is a significant burden on scientists to use machine learning. The project develops AutoNeurify, an end-to-end system to automatically infuse learning in HPC applications. AutoNeurify will enable scientists to improve the performance of HPC applications by using machine learning in their problem-solving process while lowering expertise required for maintenance and deployment, and avoiding hidden technical debt often found in real-world machine-learning systems.

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

Designing Molecular Interactions at the Electrode-Electrolyte Interface in Nitrogen Reduction

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Nitrogen-containing compounds are industrially important species and are commonly used in fertilizers, pharmaceuticals, and polymeric resins. The Haber-Bosch process is the dominant method for converting dinitrogen gas to ammonia, which is the primary feedstock for other nitrogen-containing chemicals. However, the Haber-Bosch process is highly energy-intensive and requires both high temperature and pressures. Electrochemical synthesis is an attractive approach for ambient dinitrogen conversion. A robust electrocatalyst is typically needed to break the strong bond of dinitrogen, but fundamental understanding on factors that promote high product selectivity and conversion is limited. This research program will fill this knowledge gap by developing chemical strategies to catalyze the conversion of dinitrogen to ammonia and other related chemicals. The objectives of this program are focused on 1) tackling the poor selectivity, 2) improving the catalytic rate, and 3) generating valuable commercial chemicals such as urea and acetamide. More broadly, strategies developed from this program will facilitate the design of efficient electrocatalytic systems for the synthesis of chemical commodities and alternative fuel sources.

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

Electron Beam Magnetic Field Mapping Technology for Undulators and Magnets

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This work will investigate an innovative magnetic field probe especially suitable but not limited to the characterization of insertion devices for light sources such as undulators and wigglers. Examples of such systems include the undulators planned for the Advanced Light Source Upgrade (ALS-U), where a complete magnetic characterization of the device is an integral part of its construction and certification. Current magnetic field measurement technologies for such hardware include Hall Effect probes, wire-based systems, and sensing coils. Hall Effect sensors are widely utilized for local field mapping and are the technology of choice for most magnetic characterizations. Nevertheless, these sensors have limitations such as direct current offset, nonlinearity, temperature drift, sensor aging, and the planar Hall effect. Their long-term gain and output can change with time and temperature, requiring frequent recalibration. This research proposes a paradigm shift, aiming to develop a novel sensing technology based on a micro–Cathode Ray Tube (mCRT) integrated with an image sensor. This technology utilizes an electron beam that emulates the actual beam traversing the undulator or magnet when in operation but with lower energy. The mCRT shoots a stream of electrons at the imager, which is mounted perpendicularly to the beam and located at the opposite end of the tube. Electrostatic lenses continually manipulate the electric field and project a pattern onto the image sensor. This pattern is dependent on the magnetic environment present at the beam path and can be translated into field measurements. With this unique approach, all limitations inherent to Hall probes are eliminated and important advantages such as radiation hardness and cryogenic operation are gained, thus resulting in a state-of-the-art magnetometer that will improve magnetic metrology in the future.

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

HED magnetized plasma turbulence - Simulations, Experiments, and Theory

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Magnetized turbulence is a key process in astrophysical phenomenology, and small-scale, fluctuation dynamo action – the stretching, twisting, and folding of magnetic fields due to turbulent motions – is currently our best working hypothesis to account for cosmic magnetic fields. Despite the broad consensus among astrophysicists that magnetic field amplification via fluctuation dynamo is behind the observed cosmic magnetism, the specifics of the process are still poorly understood and vigorously debated. The reasons behind this state of affairs are that the mechanism eluded experimental demonstration for decades, while theoretical and numerical studies have largely resorted to simplified models that make the description of the process tractable. The advent of high-power laser systems and the scaling of the equations of magneto-hydrodynamics (MHD) have enabled a new field of high energy density (HED) research in which astrophysical phenomenology is investigated through laser-driven experiments. One such effort by the TDYNO (turbulent dynamo) Collaboration recently demonstrated fluctuation dynamo for the first time in the laboratory, using the OMEGA laser at the Laboratory for Laser Energetics (LLE) and guided by high-fidelity simulations performed with the FLASH code. Building on this success, this research effort will holistically study HED magnetized turbulence in regimes where plasma physics processes are important and go beyond the simplified approximations used in current theoretical models and numerical simulations. This effort engages with the problem of HED magnetized turbulence in a novel, two-pronged way: (1) High-performance computing (HPC) resources at the LLE and at Lawrence Berkeley National Laboratory will be leveraged to perform three-dimensional FLASH simulations of driven, compressible, radiative magnetized turbulence and explore the properties of magnetized turbulence and dynamo for realistic HED full-physics plasmas. (2) Then, building on the experimental achievements of the TDYNO Collaboration, validated high-fidelity FLASH simulations will be used to design, execute, and interpret laser-driven experiments that will experimentally demonstrate the properties of fluctuation dynamo and magnetized turbulence in the plasma regimes charted by the driven-turbulence simulations. This concerted effort combines theory, HPC simulations with FLASH, and experiments on our nation's laser facilities to establish a basis for laboratory astrophysics investigations on the nature of magnetized HED turbulence and fluctuation dynamo.

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

Probing New Physics with Precision in the Higgs Sector at the Large Hadron Collider

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The Standard Model (SM) of particle physics summarizes our current understanding of the elementary constituents of matter and their interactions. Although most of its predictions have been tested successfully to a high level of accuracy in a variety of scientific experiments, the model falls short of being a complete theory of the fundamental interactions in the universe. The Higgs boson, discovered at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland, is the first fundamental scalar ever observed and thereby plays a unique role to probe the SM and search for any direct experimental evidence for new particles and forces beyond the SM. This research program plans to use data from the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC to advance the understanding of the Higgs sector that in turn will be distinct and complementary to proposed future lepton colliders. The research aims to determine the Higgs boson self-coupling through a simultaneous analysis of several Higgs measurements within the formalism of the Standard Model Effective Field Theory, a model-independent interpretation of deviations that might appear in a wide range of models beyond the SM. By applying modern machine learning computational techniques, the studies will also address key measurements targeting double Higgs production at low di-Higgs invariant mass as well as single Higgs production at large transverse momentum, both of which are crucial pillars of the Higgs self-coupling and the broader LHC physics programs. Complementing these studies, future high-luminosity runs at the LHC (HL-LHC) will critically depend on the performance of the ATLAS inner tracking detector, and therefore, the program also involves developing a new silicon pixel tracker for the experiment to exploit increased forward tracking acceptance that can enhance the phase-space for precision Higgs boson measurements. The efforts will develop modular assembly procedures to ensure that high-quality silicon-based devices are implemented in the new pixel tracker, while simultaneously provide optimizations for the reconstruction of charged particles traversing the tracker's forward region. Such advances are expected to have deep impacts in the design of ultra-sensitive particle instrumentation and technologies for use in future high radiation and dense collision environments anticipated during the HL-LHC era.

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

Probing and Understanding the Spatial and Energy Distributions of Plasmonic Hot Carriers via Single-Molecule Quantum Transport

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The generation of non-equilibrium hot carriers in photoexcited plasmonic nanostructures leads to unique light-matter interactions at the nanoscale and offers new transformative opportunities for a range of applications, including photochemistry, solar energy harvesting, and optical sensing. Key to making real use of these hot carriers lies in probing and understanding how 'hot' they are and where they are spatially distributed on the surface of a plasmonic nanostructure. The goal of this research program is to develop an experimental approach that enables systematic study of hot carrier distributions in a variety of plasmonic nanostructures. This approach leverages quantum transport through single molecules to access and probe plasmonic hot carriers. Specific objectives of this research include: (1) to probe the steady-state spatial and energy distribution of hot carriers on noble metal nanostructures; (2) to gain mechanistic insights into the geometric effect and material dependence of plasmonic nanostructures; (3) to investigate local thermal effect associated with plasmonic excitation. This research will create foundational knowledge that paves a path towards designing and engineering plasmonic nanodevices for efficient and tunable hot carrier generation. The advances that emerge from this program also hold promise for improving the efficiencies of many energy-related processes, including catalysis, solar cells, and light detection.

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

Realizing the constraining power of galaxy clusters on cosmic acceleration: from DES to LSST

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Why is the Universe accelerating? Is it caused by a cosmological constant, dynamic dark energy, or modification of general relativity? For the first time in human history, we have telescopes powerful enough to answer these questions. However, in recent years early- and late-Universe experiments tend to disagree with each other. In particular, early-Universe experiments indicate larger density fluctuations than late-Universe experiments if we assume general relativity is true. Does this difference come from unknown physics or errors in our experiments?

This research will use galaxy clusters to address these issues. The number density vs. mass of galaxy clusters reflects how cosmic density fluctuations evolve under the influence of cosmic acceleration. This work will use gravitational lensing to accurately infer the mass of galaxy clusters and cosmological parameters. In particular, this work aims to realize the enormous constraining power of galaxy clusters from the upcoming Rubin Observatory Legacy Survey of Space and Time (LSST). The research team first plans to comprehensively understand the systematic errors in the current Dark Energy Survey (DES) galaxy cluster data. The team will then apply the lessons learned from DES to developing data analysis methods for LSST, both of which are DOE and National Science Foundation partnerships. The proposed research will synergize with the galaxy cluster studies using NASA's Roman Space Telescope, paving the way for realizing the constraining power of current and next-generation cosmology experiments.

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

New Synthetic Approaches Towards Atomically Precise π–d Conjugated Materials

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The discovery of carbon nanomaterials has led to transformative advances in a variety of sectors, from energy storage and conversion to nanoscale electronics. Inspired by the exciting functional versatility and fundamental physics observed in carbon-based conjugated materials, synthetic chemists have sought to replicate these structural motifs in other material types. In particular, π–d conjugated metal–organic frameworks, which are reminiscent of graphene, have attracted significant recent attention. However, unlike carbon-based materials, which boast an incredible diversity of 0D, 1D, and 2D nanoallotropes, the structural space of π–d conjugated frameworks remains relatively unexplored. This research aims to address the nanoscale materials gap by developing bottom-up syntheses of atomically precise, dimensionally reduced π–d conjugated materials. A complementary research thrust aimed at understanding the formation mechanisms of π–d conjugated frameworks will take place alongside these endeavors, guiding future efforts towards precise crystal size and morphology control. Together, this multifaceted research program will address critical structure–property knowledge gaps and expand the functional and structural scope of this exciting new class of conjugated nanomaterials.

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

Building a Framework to Understand Transition Metals' Behavior in Euxinic Conditions

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Euxinia (anoxic and sulfidic aqueous conditions) has played a critical role in sequestering transition metals (TMs), from relatively abundant iron and manganese to strategically scarce cobalt and vanadium, through geological time. A central question for illuminating TM transport and sequestration mechanisms in euxinia is – how do the TMs react with aqueous sulfide produced by sulfate-reducing bacteria in complex low-temperature geochemical settings? The goal of this project is to address the existing gap between our understanding of the structure, bonding, and speciation in transition metal sulfide species and field observations of transition metal distributions. We approach this problem through laboratory experiments using multiple analytical tools to reveal the underlying reaction mechanisms of TM-sulfide systems and to connect the TM-sulfide interactions with the electronic states observed in TMs under different solution conditions. The basic information to be obtained through this study will be critical for understanding the evolution of euxinic geochemical environments and for developing relevant strategies in resource recovery and environmental remediation. Additionally, the proposed study resonates strongly with two emergent and high-impact research themes in geochemistry from incipient hypoxia in oceans and local water bodies to the biogeochemical cycling of vanadium which has been increasingly added to the atmosphere because of switching to the use of heavy oils, tar sands, and bitumen as combustion sources worldwide.

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

Using ARM Data and Multiscale Models to Advance the Understanding of Liquid-Phase Cloud Response to Aerosol Perturbation over Ocean and Land

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Aerosol particles in the atmosphere can affect the Earth's climate directly by scattering or absorbing radiation or indirectly by changing the properties of clouds (such as cloud particle size or cloud lifetime). This "aerosol indirect effect" on liquid-phase clouds remains highly uncertain in present and future climate scenarios. Qualifying the aerosol indirect effect in observations is challenging because changes in cloud properties due to meteorological variations often mask out the cloud responses to aerosol perturbations. In current climate models, the aerosol indirect effect tends to be overestimated because the oversimplified physical representations of aerosol and cloud processes required to efficiently simulate global climate in numerical models misrepresent the net effect of aerosol-cloud interactions occurring at scales much finer than the model resolution. This project will use DOE's long-term Atmospheric Radiation Measurement (ARM) observations, complemented by satellite retrievals and numerical simulations, to study the aerosol indirect effect on liquid-phase clouds. This project will untangle the aerosol-cloud interactions from the meteorological controlling factors by simultaneously constraining multiple key large-scale conditions through matching and clustering, which will better detect the aerosol indirect effect in observations. Furthermore, this project will conduct observationally constrained large eddy simulations to identify how the cloud responses at small scales generate a net aerosol indirect effect at scales that are relevant to the effective resolution of current and future climate models. This project will bridge the gap between ARM observations and the DOE Energy Exascale Earth System Model (E3SM) via an emphasis on the process-level understanding and the causal discovery. Overall, this work will advance our understanding of liquid-phase cloud processes crucial to aerosol-cloud interactions in both observations and numerical models.

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Data-driven Discovery of Inorganic Electrides for Energy Applications

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Electrides represent a unique class of materials where excess electrons trapped inside crystal cavities behave as anions. The trapped electrons are loosely bound near the Fermi energy level and can be used to design new materials with low work functions or minimum thermodynamic work to remove electrons from the solid, high electron mobility, and nontrivial band topology. However, despite the rapidly growing interest in electrides by physicists, chemists, and materials scientists, electride research has been hindered due to a lack of candidate materials. This research aims to accelerate the discovery of electrides through developing an advanced materials screening method that combines group theory, crystal structure prediction, machine learning, and high-throughput screening. Specific objectives of this research include: (1) incorporating symmetry relations into materials structure screening, (2) developing physics-informed machine learning models that can perform quick evaluations of materials' structural and electronic properties; and 3) constructing an electride database by screening promising material structures within a large chemical space. The simulation results and database will provide the materials science community with a large number of potential electrides, allowing the experimental community to test these predictions and probe potential technological applications. These computational approaches will be transferable across all classes of inorganic materials and may be utilized for a wide range of energy research activities.

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