Towards Facile Synthesis of High-Entropy-Alloy and Complex Concentrated Alloy Nanoparticles

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This research will develop a facile synthesis strategy for complex concentrated alloy (CCA) nanoparticles using the solid-state self-assembly of nanoparticles from thin films of oxide precursor materials. Complex concentrated alloy (CCA) nanoparticles, including high-entropy alloys (HEA), have unique physical and chemical properties for many applications, such as catalysis, sensing, hydrogen storage, and energy-related applications. The synergy between the electronic interactions of the metals is advantageous for various electro- and thermo- catalytic reactions where the nanoparticles display superior stability, selectivity, and activity compared to conventional alloys. Despite their unique properties, the synthesis of these materials is complex, which limits their use beyond laboratory demonstrations. The objectives of this project will employ in situ X-ray absorption spectroscopy and in situ microscopy techniques to track the nanoparticle's bulk diffusion, nucleation, and growth as a function of thin film oxide properties. The project outcomes will be transformative, as the study will couple fundamental understanding from the characterization of thin films to develop a new synthesis strategy for laboratory-scale development of supported CCA and HEA nanoparticles.

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

Probing Nuclear Dipole Responses

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The way that nuclei respond to electromagnetic radiation has profound implications for neutron stars, f or the synthesis of heavy elements, for nuclear medicine, and even industrial applications such as the design of nuclear reactors. Of particular importance is the dipole response of nuclei which causes protons and neutrons to oscillate in opposite directions. This response causes one side of the nucleus to have more positive charge than the other. Many contributions to the nuclear dipole response overlap and are hard to isolate. Additionally, isolating the contributions is made more difficult due to deficiencies in past measurements. The present research uses sensitive experimental probes of the nuclear dipole response to resolve these different contributions. This research will also develop independent calibration standards for dipole response measurements to validate modern experimental studies and investigate historical experimental discrepancies. Experiments will be performed at three laboratories with different capabilities: the Texas A&M University Cyclotron Institute, γELBE at Helmholtz-Zentrum Dresden-Rossendorf in Germany, the iThemba Laboratory for Accelerator-Based Science in Cape Town, South Africa. The results from each type of experiment will probe different aspects of the nuclear dipole response.

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

Tuning Bulk and Interfacial Electrolyte Solvation to Control Electrochemical Transformations

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Electrochemical energy technologies such as batteries, water electrolysis, and carbon dioxide/carbon monoxide reduction (CO_2RR/COR) are required for clean energy and to transform manufacturing. Across all these technologies, water is essential and can be a reactant and solvent. Carbon monoxide reduction (COR) to C_{2+} products such as ethylene (C_2H_4) exposes water's undesirable dilemma: How might we enhance high selectivity for hydrogenated products such as C_2H_4 while suppressing undesired water breakdown to yield hydrogen? The challenges facing electrochemical devices could be solved if we improved our fundamental understanding of interfacial phenomena at solid/liquid interfaces that then allows us to optimally control electrochemical transformations under applied potentials. Here, we propose to control water's availability and solvation to control its reactivity in electrochemical transformations such as COR. To tune water's behavior, we will remove its duality and confine it as solely a reactant. Coupling electrolyte solvation control with novel catalyst design that enhances carbon coupling will allow for selective and efficient COR to hydrogenated products. Fundamental insights generated from this work will enhance our understanding of bulk solvation effects and interfacial molecular sciences at the catalyst/electrolyte interface and provide a pathway for clean energy deployment and transformative future manufacturing.

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

Developing Techniques to Enable Intelligent Dynamic Reconfigurable Computing for Sparse Scientific Problems

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To efficiently scale the performance of scientific computing in the post-Moore's Law era, this research proposes techniques for developing intelligent, dynamically reconfigurable systems to allow diverse workloads to reach their peak performance without sacrificing performance for common cases. For years, scientific computing has relied on commodity computing platforms equipped with general-purpose programmable processors. Even though such platforms have been able to deliver the required computational throughput (i.e., FLOPS), their scalability and energy/cost efficiency are concerning in the post-Moore's Law era. One reason for this is the inherent contradiction that scientific computing workloads are typically sparse, while computing platforms have been designed for dense data. As a result, even high-end supercomputers like Frontier and Fugaku achieve no more than 0.8% and 3% of their peak FLOPS, respectively, when running the sparse HPCG benchmark. To improve computation efficiency and resource utilization, hardware specialization can be employed, but it is not practical since it is a slow and costly process, and one specialized solution cannot fit the diverse requirements of scientific computing workloads. To address this challenge, this research develops techniques for intelligent dynamic reconfigurability, unifying hardware and software in a holistic manner, adapting them together to run a program or multiple programs efficiently. As proof of concept, we prototype our techniques using available FPGA technologies, providing insights for further improvement. This research covers various levels of the computing stack, from user interface and algorithm optimizations to computer architecture and hardware, and explores both traditional and modern techniques, such as integrating machine learning into the configuration environment. Ultimately, the goal of this research is to democratize efficient high-performance computing for scientists across diverse fields, from physics and medical sciences to various engineering domains.

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

Extending the Reach of Light Source Facilities with Precision Laser Plasma Injectors

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Particle accelerator-driven light source facilities provide an invaluable tool to a robust community of scientific users. In particular, the x-ray free electron laser (XFEL) stands out as it allows scientists unparalleled access to spatial and temporal scales at the angstrom and femtosecond scale, respectively. Advances in FEL physics and improvements in the constituent accelerator components are now needed to make new research paradigms accessible. With this in mind, a radical new approach to the generation and acceleration of electron beams is gaining widespread attention for its potential to produce ultra-high brightness electron beams, which in turn promises a major breakthrough in XFEL performance both for current facility upgrades and new facilities. With regards to the stringent stability and reliability requirements of light source facilities, however, plasma-based accelerators have thus far remained notably deficient. The primary goal of this research is to demonstrate the production of ultra-high brightness electron beams generated by a laser plasma accelerator (LPA) with a level of stability, precision control and reliability comparable to the rigorous requirements of light source facilities. This work will provide a blueprint for the development of a plasma-based modality of electron beam injectors which can revolutionize light source facilities in a number of ways, including, but not limited to, i) injector upgrades for large scale facilities like the Linac Coherent Light Source and ii) driving complementary plasma-based light sources at existing facilities or at future compact facilities with unique capabilities.

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

Shining New Light on the Dark Sector

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Most of our universe is dark. It is dark literally---visible mater makes up only 5% of the total energy content---and conceptually, as known particles populate just a few of 60 orders of magnitude in mass between the lightest (Hubble) and the highest (Planck) known particle physics scales. Within this vast range, we believe outstanding theoretical questions are answered at scales far more energetic than those we can access directly. This includes theories that address puzzles of low-scale symmetries as well as frameworks such as string theory that seek to solve quantum gravity. Both generically predict new ultralight, feebly interacting particles known as axions that are also excellent dark mater candidates. The discovery of the axion, or one of its ultralight particle cousins, would shed light on our dark universe and throw open a window on the highest energy scales.

This project will develop the theoretical foundation for novel axion and ultralight particle searches in the sky and in the lab, following a three-pronged approach. The first direction is investigation of experimental approaches in the search for axion and ultralight particle dark mater, specifically new photonic structure designs which can enable dark mater to convert to visible light. Second, ultralight particles that are a smaller component of the energy content of the universe may explain discrepant measurements of the expansion rate of the universe at early and late times; this project will advance cosmological tests of these ultralight particles and connect them to laboratory probes. Finally, new particles may exist but not be present as dark mater. The extreme environments of black holes and neutron stars can create ultralight particles in their vicinity and this project will study these unusual dynamics and develop precise observational strategies for their detection. These three approaches will cast a wide net for axions and ultralight particles to reveal the dark constituents of our universe and of the theoretical framework which underlies it.

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

Accurate and Precise Weak Lensing Analyses for Cosmological Surveys

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The acceleration of the expansion of the Universe is one of the biggest mysteries in cosmology today. The scientific community and the Department of Energy (DOE) have embarked upon a series of grand cosmological experiments to solve this enigma. These experiments will make multiwavelength observations of the night sky at an unprecedented scale in data volume and quality. The largest DOE cosmological experiment that will observe optical wavelengths of light is the Vera C. Rubin Observatory. This observatory, once completed, will execute the ten-year Legacy Survey of Space and Time (LSST) of the entire Southern Hemisphere night sky, producing some of the largest volume catalogs of distant galaxies to date. By carefully studying the statistical properties of the shapes of these galaxies, scientists can learn about the properties of accelerated cosmic expansion. These studies, called weak gravitational lensing studies, are challenging to perform in cosmological surveys due to multiple experimental and theoretical uncertainties. The research funded by this Early Career Award will develop a new measurement technique for weak gravitational lensing called deep-field metadetection and apply it to the LSST. Deep-field metadetection will extract weak gravitational lensing signals from LSST with approximately 15% less noise than previous-generation measurement techniques while remaining unbiased. The commensurate gains in constraints on the degree of cosmic acceleration from weak gravitational lensing will be equivalent to nearly doubling the number of observations taken during the LSST. This research program will make fundamental contributions to the Rubin Observatory LSST and our understanding of cosmic acceleration.

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

Enhanced Fine-Scale Statistical Modeling of Environmental Extreme Events in Complex Systems from Multiple Sources

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The overarching goal of this research program is to develop novel general statistical models, combining classic methods with deep learning, to advance the understanding and modeling of extreme events arising in complex systems, which are characterized by multimodal (multisource) and multiscale outputs. We are motivated by the drastic impacts of environmental extreme events on human systems or other natural systems. Simulations from physics-based models tend to underestimate extreme intensities or misrepresent trajectories or spreads of extremes, and would hence benefit from observation-driven statistical correction (potentially online) or post-treatment. The misrepresentation of extremes leads to misevaluated risks for systems and living populations suffering from extreme environmental stressors. In turns, this results in inadequate responses and increased exposure or costs, such as the 2021 Texas power crisis and the recent Hurricane Ian demonstrated. This highlights the need to understand and mitigate environmental extremes, especially in a world of changing climates and extremes. Our working hypothesis relies on the fine-scale observation-based statistical enhancement of low-frequency and dynamical content summary statistics from physics-based model simulations to improve the representation of extreme events i.e. their intensity, spatiotemporal extent and associated uncertainties. Our research objective is to augment traditional statistical models with flexible neural network techniques in the development of (1) summary statistics of extremes from multiple large-scale numerical model outputs; (2) coupling derived large-scale summaries with fine-scale statistics of observational extremes; (3) accounting for temporal dynamics between normal and extreme conditions as well as long- term changes observed on measurements and projected model outputs; and (4) developing statistical metrics adequate to extremes to validate the proposed strategy and generally assess extremes from various datasets. These statistical models will serve as a post-treatment of numerical model outputs with enhanced representations of extremes or will be used online to provide corrections and more accurate simulations.

The significance of this program resides in advancing the understanding and predictability of observed and simulated complex systems, which is a central mission of DOE that covers many application domains such as climate and weather models, power grid systems, or building science. These systems have experienced the impact of changing extreme events and environmental stressors. Hence, it is critical to advance the understanding and predictability of extremes to adapt preparedness and emergency management responses.

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

Towards a quantum-enhanced multi-cavity haloscope for high-mass QCD axion detection

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The nature of dark mater is one of the most perplexing open questions in physics today. The axion is a compelling hypothetical particle that could account for the dark mater in our universe, while simultaneously explaining why quark interactions within the neutron do not appear to give rise to an electric dipole moment. Current approaches to detect dark mater axions rely on resonant microwave cavities. The most sensitive detection technique in the 1–10 GHz frequency range—a range motivated by numerous theoretical predictions—makes use of the axion-photon coupling and is called the "axion haloscope". Axions are resonantly converted into detectable microwave photons in a tunable, high-Q cavity permeated by a strong magnetic field. Existing direct-detection axion dark mater experiments are expected to explore the 1–4 GHz range of the well-motivated frequency decade. Future detectors designed to leverage traditional haloscope techniques to search above 4 GHz will face significant challenges. Decreased detector volume and an increase in quantum noise conspire to make axion detection nearly impossible without new strategies to boost signal and reduce noise at these higher frequencies. The implementation of multi-cavity systems and readout based on quantum sensing are promising approaches to address the loss in sensitivity. However, these approaches must be synthesized into a mutually compatible experiment concept to reach target sensitivity. Furthermore, solutions to improve detector sensitivity come at the cost of increased complexity—a complexity that may not be tractable without advanced automated detector controls at high frequencies. Taking a broad view and treating the solution-compatibility and experiment-complexity problems as a single entangled challenge, this research will address both with the help of a new multi-cavity research and development platform. The project will start from a systems engineering perspective and stress test promising techniques together under realistic data-taking conditions. Specifically, two interconnected haloscope scalability tasks will be undertaken: 1) the union of the multi-cavity approach with a readout based on quantum sensing and 2) the adaptation of machine learning techniques for detector controls to combat the trend towards increasing complexity. The result will point toward a synthesized strategy for detecting the elusive axion above 4 GHz.

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

Epitaxially Imposed Control of Chiral Transport Phenomena

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Many novel quantum and topological phenomena in materials are derived from or exhibit chirality, a lack of mirror symmetry. These phenomena range from novel forms of superconductivity to unusual one-dimensional (1D) states that are bound to the edge of a material. Both quantum and topological phenomena are critical elements for new classes of quantum devices and sensors, called *chiraltronics*. The overarching goal of this project is to create new chiral material paradigms for which symmetry and dimensionality can be directly controlled by tailoring atomically precise interfaces. These new material platforms can be tailored to elucidate how lattice, electronic, and magnetic characters determine and affect chiral phenomena. This understanding is a critical step toward new applications. To achieve this goal, this project will be subdivided into two tasks: (1) deploying new atomic-scale structures that can be used to stabilize and understand unusual, low-dimension chiral states and (2) understanding how materials with chiral structures and unusual coupling of the spin and momentum (altermagnets) can interface with superconductors to attain desired functionalities. Achieving the objectives of this project requires a strong synergy between thin-film synthesis using molecular beam epitaxy and advanced characterization of quantum and topological phenomena in the materials. This feat will lead to the ability to control and fingerprint chiral phenomena and will ultimately reveal fundamental design principles for a new generation of quantum materials with transformative possibilities.

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

Nuclear Tomography through Entanglement-Enabled Spin Interference

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Protons and Neutrons are the basic building blocks of almost all visible mater in the Universe. Astonishingly, the rules that govern these basic building blocks dictate the mater formed over 18 orders of magnitude in scale – from tiny atomic nuclei to massive astronomical objects like neutron stars. However, protons and neutrons are not fundamental, but are themselves dynamical quantum objects built from quarks that are 'glued' together by gluon particles which mediates the strong nuclear force. A fundamental goal of nuclear physics over the last several decades has been to understand the internal structure of protons, neutrons, and nuclei. To this end, one of the primary goals of the future Electron Ion Collider is to construct multi-dimensional maps of the quarks and gluons within large nuclear objects. This project utilizes a recently discovered quantum effect in which entanglement enables wavefunction interference between distinguishable particles. Hidden in these interference patterns is information about the distribution of gluons within protons, neutrons, and large nuclei – enabling a new approach to nuclear tomography. This project undertakes the development of this newfound quantum effect to explore the dynamic properties of gluons within large nuclei and to investigate the details of their quantum spin structure. By developing this novel entanglement-driven technique, this project also aims at providing new opportunities to impact searches for physics beyond the Standard Model and for investigating nuclei as entangled quantum objects.

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

Engineering Continuous Trait Variation in Bioenergy Feedstocks to Optimize Growth on Marginal Lands

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Bioenergy crops constitute an important renewable source of raw material to produce fuels and chemicals. To be economically viable without competing with food and feed crops, these crops must be able to grow in soils with low water and nutrient contents. Sorghum has great potential as a bioenergy crop due to its high biomass yield and drought tolerance. However, new varieties are needed to tolerate increasing water, nutrient, and temperature stresses caused by climate change. A commonly used approach to generate improved yield and stress tolerance in sorghum relies on genetic analysis of large sorghum populations, which takes a long time. Furthermore, relatively little is known about the traits involved in abiotic stress tolerance, hindering crop improvement through breeding and genetic engineering. This research will develop a novel approach to understanding and optimizing root architecture traits. Synthetic biology strategies will be used in sorghum and a model grass to generate a series of plants with increasing root depth or branch density. Engineered plants will be studied to understand the roles of root features in stress resilience. With these tools, this project will accelerate the development of optimal bioenergy crop varieties and contribute to the establishment of a vigorous bioeconomy, ensuring energy stability in the face of a changing climate.

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

Shining Light on the Higgs Self-Interaction

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The discovery of the Higgs boson in 2012 was a strong confirmation of the Standard Model (SM) of particle physics. Nevertheless, a decade later, many outstanding questions about this new boson remain, including its relation to electroweak symmetry breaking and how new physics might shape its properties. Over the last decade, many properties of the Higgs have been measured with great precision, while crucial other properties, such as the Higgs self-interaction, remain experimentally unconstrained. Measuring the Higgs self-interaction and understanding its role in electroweak symmetry breaking is a major goal of the physics program at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN), located near Geneva, Switzerland. The measurement can be performed directly in extremely rare, high-energy collisions resulting in pairs of Higgs bosons. Innovative analysis techniques and data collection methods will be required to observe such a rare process. This research program therefore searches for effects of new physics on Higgs pair production using data collected by the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC. A measurement of the Higgs self-interaction at the LHC will either reaffirm the SM nature of the Higgs or point to new physics beyond the SM. Finally, to ensure that ATLAS can make the best use of the data produced during the high luminosity running period of the LHC, scheduled to begin later this decade, this research will develop novel techniques to select interesting collision data in real time using machine learning algorithms in Field Programmable Gate Array (FPGA)-based technology. The deployment of such sophisticated algorithms will enhance the search sensitivity to Higgs pair production as well as other rare processes at the LHC. The analysis and data-collection techniques developed through this project will advance our understanding of the Higgs boson at unprecedented scales and shed light on the outstanding questions in particle physics, not only at the LHC but also at the proposed future colliders.

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

Fixed-Field Superconducting Magnets for Rapid, High Power Acceleration of Muons and Protons

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Future experiments in High Energy Physics require new particle accelerators with unprecedented need for rapid, high-power acceleration. A promising paradigm to meet these demands is fixed-field acceleration, in which alternating gradient magnet structures are employed to transport beams of different energy without magnetic field change. Application of superconducting magnet technology to these unique accelerator designs allows for higher bending fields and gradients, enabling more compact layouts with larger accelerating energy range (reducing cost and improving performance). Yet, superconducting magnet technology optimized for this application remains largely undemonstrated. The objective of this research program is to address this gap in technology through optimization and test of a novel superconducting magnet design tailored for fixed-field acceleration.

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

Assessing Climate Impacts on Coastal-urban Flooding Through High-resolution Barotropic and Baroclinic Ocean Coupling

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The primary objective of this project is to bridge the divergent scales between the global climate drivers of sea level rise and the local coastal impacts of extreme events in the Energy Exascale Earth System Model (E3SM). This objective will be accomplished by unifying two classes of models: Earth system models (ESMs) and barotropic coastal flooding models. ESMs incorporate interactions between separate geophysical systems. Because of their complexity, however, the 3D ocean model components of these ESMs operate at a resolution far coarser than what is needed to resolve complex coastal regions. On the other hand, while 2D barotropic coastal flood models efficiently describe tidal and storm surge processes at high resolution, they neglect density effects and lack connections to the climate drivers associated with sea level rise.

Our project extends the mode-splitting approaches that ESM ocean models currently use to separate fast, barotropic free-surface waves from slower, density-driven baroclinic flow. Such approaches typically work by evolving the baroclinic mode at a larger time step than the barotropic mode. In contrast, we will employ mode splitting in space as well as time, such that the barotropic and baroclinic modes are two-way coupled between different resolution meshes. This coupling will enable an increase in the horizontal resolution of the 2D barotropic mode, allowing the model to resolve tides and storm surge in estuaries and rivers without the expense of refining the 3D baroclinic mode to coastal scales. With this new capability, E3SM will be able to resolve coastal-urban flooding processes due to sea level rise, tides, and storm surge in long-term climate simulations, enabling comprehensive studies of the effects of climate change on extreme water levels in coastal-urban systems. The project will focus on the major urban centers of the United States Mid-Atlantic region, with a particular emphasis on Baltimore, Philadelphia, and New York City. The coastal-urban regions in this area experience exposure to extreme flooding and associated risks related to the combination of tropical cyclones, tides, and sea level rise under climate change. This project seeks to provide local stakeholders with a fully integrated assessment of future flooding risks in these communities.

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

Expanding the Fundamental Understanding of At-211 Chemistry: Towards Improving Binding and Complexation

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Astatine-211 (At-211) shows promise for cancer treatments when connected to a targeting agent like a monoclonal antibody, especially for non-localized cancers. The challenges to utilizing At-211 in patients are the availability of production, the relatively unknown chemistry of astatine, and the development of appropriate targeting agents. Because of At-211's short (7.2 h) half-life, this means that the number of laboratories where development of radiotherapies and studies of the fundamental astatine chemistry has been performed is limited.

The increasing demand for isotopes utilized in Targeted Alpha Therapy (TAT) has indicated the need to develop systems and technologies to facilitate high yields, while minimizing the process time of recovery for the radionuclide. Our overarching goal is to expand the fundamental chemistry of At-211 binding and complexation, so insights gained can be applied to developments in separations, purifications, and chelating agents for this interesting and important element. Ultimately, an improved understanding of At-211 could significantly decrease the time required for the recovery and use of this TAT isotope, leading to an overall increase in the availability of At-211 for treatment as well as research purposes.

To achieve the goal the following Specific Aims are proposed:
Specific Aim 1: Investigate the nature of AtO+ interactions with ketone ligands.
Specific Aim 2: Study the effects of other ligand types on the AtO+ extraction.
Specific Aim 3: Examine AtO+ behavior with zirconium phosphate nano-platelets.
Specific Aim 4: Enhance student and trainee recruitment, engagement, and involvement.

Ultimately, success in all four of these specific aims will influence the technologic development of not only the At-211 recovery—as shown by our previous success with the 3-octanone system—but will also provide a foundation to transform this TAT isotope into a usable form, leading to an overall increase in the availability of At-211 for treatment, as well as research purposes.

This research was selected for funding by the Office of Isotope R&D and Production and the DOE Established Program to Stimulate Competitive Research.

Elucidation and Validation of Genes Associated with Biological Nitrification Inhibition in Populus

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To provide crops with the nitrogen they require for robust growth, nitrogen fertilizer is added to the soil to increase yields. However, nitrogen use efficiency (NUE) in bioenergy crops such as poplar is low, which may result in pollution of waterways by nitrate runoff, emissions of the potent greenhouse gas nitrous oxide, and reduced carbon dioxide sequestration in soils. One of the main reasons for this low NUE is the activity of microbes that convert soil nitrogen into nitrate and nitrous oxide in a process called nitrification. Plant roots exudate chemicals (biological nitrification inhibitors or BNIs) that reduce microbial nitrification. Thus, controlling the production of BNIs by roots can help mitigate nitrogen loss and improve NUE in bioenergy crops. Despite substantial research in this area, little is known about the genes and pathways involved in root BNI production. Furthermore, the current methodologies used to analyze BNI-related traits in plant populations are inefficient. This project will use genome-wide association analysis of a large poplar population to discover and characterize genes involved in the production of BNIs and, therefore, understand their role affecting NUE. A high-throughput mass spectrometry approach will be developed to analyze nitrification and mineralization in samples from the soil surrounding poplar roots at an unprecedented scale, while metabolomics and soil nitrification studies of root exudates will help identify BNI-associated genes. This knowledge will provide avenues to increase NUE in bioenergy crops with the concomitant increase in carbon sequestration, given the tight connection between the carbon and nitrogen cycles. Furthermore, the outcomes of this project will contribute to our understanding of ecosystem function and to inform the design and engineering of more efficient bioenergy crops.

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

Deciphering the Spatiotemporal Evolution of Driven Phenomena in Quantum Materials

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Quantum materials host intriguing properties such as magnetism and superconductivity, because of the cooperative behavior of the electrons (electronic order). The materials can provide the foundation for next-generation quantum information science (QIS) systems and energy-efficient microelectronics if their fundamental behavior is understood. A challenge is that the electronic order varies across the material (i.e., it is spatially heterogeneous) because of the presence of different types and densities of defects (e.g., point defects and stacking faults) and of elastic strain. Harnessing the full potential of these materials thus requires a fundamental understanding of how the heterogeneous electronic order responds to external electromagnetic fields and controls macroscopic material properties, as well as of how the defect landscape shapes the way that the electronic order evolves as a function of time.

This program seeks to develop fundamental knowledge of the relationships among spatial heterogeneity, materials response to external stimuli, and the defect landscape in quantum materials, here specifically in van der Waals (vdW) materials. To achieve this goal, this program will take advantage of the unprecedented X-ray coherence from new and upgraded synchrotrons and free electron laser facilities. We will probe how electronic order evolves on multiple length and time scales in a series of vdW materials in response to external electric and optical excitations. The insights gained will enable rational design and control of materials behavior by tuning the defect landscape. This will be relevant to applications in QIS, clean energy, and microelectronics.

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

Viability of a Molten Salt Liquid Immersion Breeder Blanket System for Heat Removal and Power Extraction in Fusion Devices

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Currently, the maturity of the magnetically confined fusion devices with molten salt based blanket systems, referred to as liquid immersion blanket systems, is not as mature or well researched as liquid metal or solid blanket systems. As a result, enabling Research & Development (R&D) necessary for liquid immersion blankets and associated balance of plant (power conversion) technologies is needed for a fusion power pilot plant. Specifically, this is to address the ability to do 1st wall and blanket heat exhaust and power extraction with molten salts. This Fusion Energy Science (FES) career project will advance the FES's mission by focusing on enabling R&D for liquid immersion blanket concepts to support fusion power pilot plant development. The aim of this research is to assess the ability to do heat exhaust and power extraction needed by a fusion device within the megawatt range using a liquid immersion blanket system and the molten salt, FLiBe. Crucially, these foundational studies will establish a baseline of system and component-level performance requirements during steady-state and transient operations expected of a fusion pilot plant.

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

Design of Molecular Spin Qubits Featuring Clock Transitions via Encapsulation of f-Elements in Polyoxometalates

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Quantum information science (QIS) represents an emerging paradigm with the potential to revolutionize a diverse range of scientific fields. To advance efforts within QIS, actinide polyoxometalate (POM) complexes will be synthesized and tuned so that they can serve as quantum bits (qubits) for quantum information processing applications. Multiple pathways have been explored for the physical realization of qubits, which are at the core of any QIS system; however, electron spin-based qubits offer unmatched promise if long coherence times can be realized. This is a multifaceted challenge as electron spin superpositions are very sensitive to magnetic and environmental noise, which can result in decoherence via multiple pathways. This project will focus on f-element complexes that feature atomic clock transitions as this is a known route to protect electron spin qubits from external magnetic noise, thereby prolonging the duration of coherence times within molecules. Atomic clock transitions originate from tunnel splitting gaps that are a result of crystal field wavefunction mixing; however, there is limited knowledge on how to consistently access these transitions within f-element complexes. The first stage of this project involves the investigation of POM complexes with uranium, neptunium, and plutonium to identify species that demonstrate desired values for coherence times and tunneling gaps. Using this knowledge, POM complexes will then be synthetically tuned so that clock transitions can be accessed more systematically in f-element complexes, and these efforts will be paired with extensive materials characterization, including SQUID magnetometry, synchrotron, electron paramagnetic resonance, and magneto-infrared spectroscopies, to elucidate a comprehensive understanding of how to harness the potential of atomic clock transitions for QIS applications.

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

Understanding Implosion Physics Degradations to Advance IFE-Relevant Targets

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For half a century, researchers across the globe have worked to harness the potential for fusion energy to provide clean electrical power for the indefinite future. Inertial Fusion Energy (IFE) is one of two major approaches and the recent achievement of ignition and gain >1 in inertial confinement fusion (ICF) at the National Ignition Facility (NIF) has increased interest in IFE as a practical fusion energy solution. Demonstrating ignition in the laboratory was a grand scientific challenge and yet harnessing that fusion energy will be yet another grand engineering challenge on the road to fusion power production. One of the central questions facing an IFE reactor system is whether inertial fusion targets can produce significant energy gain, reliably, cheaply, and rapidly when integrated with the full reactor system. Ignition experiments have shown a significant sensitivity to enhanced radiation losses induced by impurities from the capsule shell mixing into the burning fusion fuel (mix) and implosion asymmetries because both effects compete with fusion heating. The maximum target gain in ICF depends on a competition between fusion heating and losses (from expansion, radiation, and conduction). It is therefore plausible that asymmetry in the system or a sudden increase in losses due to impurities (say from mix, introduction of wetted-foam, or high-Z cone material) could negatively affect the total gain by harming the fusion power balance. This work will assess the impacts of asymmetry and mix, establish the role of asymmetry and mix in limiting gain or preventing ignition for IFE systems, set IFE system requirements for managing these issues, and forecast impacts for several IFE concepts. This work will compliment ongoing efforts in ICF while pivoting to understand how these degradations impact IFE reactor systems by advancing the understanding of hydrodynamic instabilities and asymmetries into the realm of IFE target design. Success in this research will advance our capabilities in understanding the cost and performance needed for future IFE reactors.

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

A Planetary-Scale Data–Model Integration Framework to Resolve Urban Impacts Across Scales and Examine Weather Extremes over Coastal U.S. Cities

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Urbanization leads to widespread modifications to the Earth's land surface and directly impacts more than half of the total global population by influencing weather and climate. These impacts are expected to magnify in the future due to increased urbanization and greater rural-to-urban migration. Current-generation Earth System Models (ESMs) inadequately represent urban areas and processes. They either ignore urban land completely or treat cities like biologically inactive surfaces with discrete and crudely specified properties. These simplified representations are insufficient for capturing variability in urban impacts on weather and climate across global cities. The limited number of ESMs that do represent urban areas do not account for temporal changes due to urban evolution, which is the combined result of urban expansion and varying surface properties over time. This urban evolution will become increasingly important in the future as the world keeps urbanizing. These issues are particularly relevant for complex coastal–urban environments, characterized by strong land-to-water spatial gradients in both surface and atmospheric variables. Current-generation ESMs cannot sufficiently resolve interactions between urbanization and coastal processes, which can have potentially critical impacts on weather and climate, especially during extreme events.

To address these model deficiencies, the proposed research aims to develop a globally consistent data–model integration framework for the Department of Energy's Energy Exascale Earth System Model (E3SM) to resolve urbanization and its feedbacks to the atmosphere across multiple spatial and temporal scales with a focus on coastal U.S. cities. To accomplish this, the E3SM Land Model will be improved to incorporate more accurate urban characteristics and processes derived from planetary-scale satellite imagery and satellite-derived datasets, other gridded products, and machine learning (ML) techniques for recent past, present, and potential future scenarios. A range of urban-scale measurements from various sources will also be compiled to create a model testbed for quantifying uncertainties throughout the model development process. Beyond the importance of this testbed for this project, it will be an essential resource for the wider urban climate community. Finally, a hierarchy of E3SM simulations, both coupled and uncoupled, across scales constrained by ML algorithms will be run to examine km-scale urban climate variability and generate groundbreaking insights regarding coastal–urban interactions.
Overall, this work will not only develop an advanced urban parameterization for the next generation of ESMs but will also generate tools and datasets that can better assess and advise climate adaptation and mitigation strategies as we prepare for a warmer and more urban future.

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

Interpretable Deep Learning for Advancing Field-Enhanced Catalysis

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Electric fields can modify the adsorption of polarized species and enhance the reaction rates and selectivity by a few orders of magnitude. These field-enhanced chemical processes provide a sustainable, energy-efficient, modular setup to store renewable electricity chemically. However, the high-cost of computations for field-dipole interactions on energetics has resulted in a trial-and-error approach for field-driven experimental processes. It is important to develop an interpretable deep learning approach to advance an in-depth understanding of field-dipole effects and promote electrostatic catalysis.

In this research, we focus on a case study of carbon-neutral hydrogen production and utilization, e.g., ammonia cracking and synthesis, over earth-abundant metal catalysts. In particular, we will (1) probe the local fields of nanoparticles under working conditions, (2) predict field-driven adsorption energetics with an interpretable deep learning approach, and (3) discover the optimal field-dipole effects on catalysis.

Interpretable deep learning of field-dipole interaction represents a new paradigm for designing high performance catalysis where large local field exists for renewable-energy related technologies, such as electrostatic catalysis, electrocatalysis, and fuel cells. The fundamental science of how field-dipole interactions has the potential to alter the energetics of ammonia cracking. In addition, synthesis of earth-abundant-based nanoparticle catalysts with low-coordinated sites will improve the energy efficiency of carbon-free hydrogen production, utilization, and storage.

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

Harnessing Quantum Geometry of Correlated Electrons for Next-Generation Photovoltaics

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Understanding how light interacts with mater is foundational to tailoring optical properties and designing next-generation photovoltaics for solar energy harvesting. To exceed the limitations of conventional semiconductors, a key new frontier concerns harnessing the collective quantum-mechanical behavior of electrons in correlated quantum materials, to convert light into electric current. Such materials are governed by a fascinating but delicate interplay of spin, charge, and orbital degrees of freedom arising from strong electronic interactions. However, they pose a profound theoretical challenge in understanding their optical properties. This project will develop a novel theoretical and computational foundation for emergent photogalvanic responses in strongly correlated quantum materials, deeply tied to the interplay between strong electronic interactions and the quantum-geometrical structure of the electronic wave functions which couple to light. A central goal is the development of generic design principles for a new class of Mot bulk photovoltaics, materials that are insulators due to strong repulsion between electrons but can efficiently rectify light into electrical current. To this end, key objectives include predicting many- electron photovoltaic responses for paradigmatic low-dimensional polar Mot insulators, devising quantum-geometrical guiding principles for photogalvanic responses in correlated and topological van der Waals heterostructures, and developing new computational tools which combine first principles modelling with many-electron simulations to drive the discovery of new correlated photovoltaic materials. Insights gained from this project will establish strongly correlated electron systems as a transformative new platform for photovoltaic applications, with broader theoretical ramifications for other photon-based spectroscopies, optical driving, and control of correlated and topological quantum materials.

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

Functionalization of Methane and Carbon Dioxide Using Earth Abundant Metal Frustrated Lewis Pair Catalysts

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The valorization of methane, a major component of fossil fuels, and carbon dioxide, the thermodynamically favored product of fossil fuel combustion, is a challenge of global proportions. These two potent greenhouse gases are often considered waste due to their thermodynamic stability and kinetically inert bonds which are an obstacle to their conversion into commodity chemicals. To incentivize the capture and use of these gases as an abundant and sustainable source of chemical feedstock, pathways that easily break their bonds and convert them into value-added products are needed. The goal of this research is to use so-called sterically frustrated Lewis pairs (FLPs), which are Lewis acid-base pairs that have unquenched acidity and basicity when combined, to develop catalytic cycles that functionalize methane and carbon dioxide to yield industrially important commodity chemicals.

Over the course of this project, complexes containing earth abundant metals of Groups 8-13 will be paired with bulky bases to generate FLPs that activate methane and/or carbon dioxide. This FLP reactivity will be coupled with the inherent reactivity of the metal to generate industrially viable and environmentally benign catalytic routes to a variety of chemicals. Specifically, catalytic cycles that convert methane to methanol, acetic acid, and acetaldehyde, as well as those that convert CO_2 into acrylic acid or acrylate will be designed using four different ligand platforms. These systems will be optimized through parameterization of steric and electronic factors that affect catalyst activity. Thermodynamic studies that measure the hydricity and bond dissociation energies, in addition to kinetics experiments and computational analyses, will be conducted to provide mechanistic insights about these systems that may be extrapolated to design additional processes that commoditize other challenging small molecule targets. Furthermore, these systems will be heterogenized to create economical, industrially viable, and sustainable catalysts from earth abundant metals.

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

Symmetry in Quantum Field Theory

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Symmetry is a powerful mathematical tool for organizing the diverse physical phenomena described by quantum field theory. The unifying theme that gives symmetry its essential power is its invariance under continuous deformations of a physical system including changes in characteristic energy scales. This invariance provides a deep conceptual bridge between symmetry in quantum physics and topology in mathematics. Recently, there has been explosive progress in this foundational discipline driven by the discovery of new concepts of symmetry. These higher symmetries act on extended dynamical objects such as strings or membranes, which often emerge as collective excitations of quantum fields. A paradigmatic example is a tube of flux and energy connecting confined quarks.

The main aims of this project are to harness these new notions of symmetry and understand their implications. First, this research project will explore and generalize new notions of symmetry across myriad examples of gauge theories. This includes developing the necessary mathematical framework which is described by topological quantum field theory. Second, the project will explore the constraints of these novel symmetries on phases of quantum systems and strong coupling dynamics. Finally, the reserach will apply these new symmetries to potential physics beyond the Standard Model. In this arena the research program will investigate whether new notions of naturalness suggested by these symmetries lead to new phenomenological models of particle physics.

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

Forecasting Thermoelectric Performance in 2D Metal-Organic Frameworks Through Ab Initio Atomistic Modeling

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Thermoelectrics are a class of materials and devices that convert a temperature difference into electricity (i.e., generate electricity), and vice-versa. To realize maximum efficiency, thermoelectrics must be excellent electrical conductors but poor thermal conductors, two properties that are interconnected and difficult to disentangle. Metal–organic frameworks (MOFs) are highly porous coordination networks with exceptionally large surface area and modularity. Through different combinations of property-correlated building blocks and topology, MOFs can be tailored to myriad applications such as gas storage, sensing, catalysis, and energy storage. Due to their porosity MOFs have extremely low thermal conductivities, a principal requirement for thermoelectric applications. By the same token, however, in addition to being thermal insulators, MOFs tend to be electrical insulators as well. Applications requiring electrical conductivity, such as thermoelectrics, have thus been largely overlooked. Devices have become increasingly efficient, thereby requiring much less power to function, and dependent on other properties such as flexibility and added functionality. MOFs, which exhibit flexibility and additional functionality, are ideal candidates for energy efficient thermoelectric devices. The objective of this research is to develop the fundamental knowledge to predict how molecular structure controls electrical (and to a lesser extent thermal) conductivity in MOFs to inform the rational design of thermoelectric MOFs. The insight gained from the work will help guide the development of smart materials (e.g., wearable devices, biomedical implants, portable electronics) and give rise to novel applications and devices (e.g., heat powered sensors or catalysts).

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

Unraveling the Heavy Side of Radiochemistry: A Macromolecular Approach to Unlock Novel Actinide Chemistry

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While radioisotopes such as actinides and radiolanthanides have unique physicochemical properties that make them the cornerstones of strategic sectors—including, energy, medicine, space exploration, defense, and research—only a modest number of their compounds have been characterized to date. Such knowledge gaps preclude comprehensive understanding of their coordination chemistry, spectroscopic, magnetic, and electronic properties. The synthesis and characterization of metal-ligand complexes typically provide invaluable information on the coordination chemistry and physicochemical properties of elements across the periodic table. Problematically, studying complexes of radioelements is inherently challenging due to radiation-related constraints and limited access to compatible research facilities. Further compounding these challenges is a lesser-considered aspect of radiochemistry: the high cost and low availability of the isotopes severely restrict the experimental space and chemical systems investigated. In fact, most synthetic approaches and spectroscopic tools available today are not compatible with highly radioactive and/or rare isotopes, in part, because these approaches and tools require large amounts of materials, a factor that correspondingly raises costs, increases workers' exposure, consumes precious isotope resources, and hinders such discoveries as the resolution of the *f*-electron challenge. This research will use a macromolecular approach—leveraging a class of ligands called polyoxometalates—to (a) overcome the limitations inherent to classic radiochemical techniques, (b) unravel novel coordination chemistry for actinides, (c) leverage these novel compounds to decipher the electronic, spectroscopic, and magnetic properties of the most critical and elusive heavy elements, and (d) develop polyoxometalate- driven radiochemical separations. This project's pragmatic and efficient approach should significantly expand understandings of the chemistry of actinides as well as other difficult-to-study radioisotopes and could open a frontier in radiochemistry impacting the isotope supply chain—from the basic science of *f*-elements to isotope processing and separation, to novel actinide materials.

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

Optimization of the nEXO detector for enhanced sensitivity to neutrinoless double beta decay of ^{136}Xe

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The experimental observation of neutrinoless double beta decay would have revolutionary implications for neutrino physics, theories beyond the standard model, and cosmology. This work will enhance the prospects of the next Enriched Xenon Observatory (nEXO) experiment by addressing a critical challenge in all experimental searches for neutrinoless double beta decay: material radioactive backgrounds. The project has three objectives. First, this research will improve the nEXO projected sensitivity on the neutrinoless double beta decay half-life of ^{136}Xe by *ca.* 20% by mitigating the most prevalent backgrounds predicted for nEXO: impurities of ^{222}Rn and its progeny in the detector. Second, enhanced control of exposure-based backgrounds will be tackled through improved assay methods, with a focus on radioactivity from dust particulate fallout on detector materials. Finally, this work will develop high-purity Cu-based alloys with yield strength significantly larger than pure Cu. In the context of the nEXO detector, increased strength translates into reduced production time, increased performance, and potentially further reduced backgrounds. The nEXO experiment is a major investment in the understanding of neutrinos. While targeted to nEXO, this work will inform the extent to which low-background experiments can reach the greatest sensitivity through mitigation of backgrounds in materials and in the environment into which these experiments are built.

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

A Captivating New Spin on Energy Storage

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Trapping, storage, and transport of fuels are central themes of current energy research, with significant emphasis placed on improving safety, efficiency, and sustainability. Towards the goal of divestment from petrochemicals, much research continues to focus on small gaseous molecules—mainly H_2 and CH_4—to serve as alternative fuel sources. For practical applications of these alternative fuels to supplement or even replace gasoline and diesel fuels, safe and effective on-board vehicular storage methods must be realized. A promising strategy for hydrogen storage is to use adsorbent materials—like metal-organic frameworks (MOFs)—upon which gaseous molecules can be efficiently captured due to the material's high porosity. Even though significant progress has been made towards the development of advanced materials with high-efficiency storage, the U.S. Department of Energy (DOE) target storage goals have not been met. Several challenges remain, most notably those related to the requisite storage pressure and temperature falling outside of DOE target parameters. Many of these challenges are rooted in an incomplete understanding of the fundamental chemical physics of the small gaseous molecules themselves. For example, recent advancements show that molecules in their lowest-energy nuclear-spin state have higher storage capacities in MOFs in scale cryogenic applications, but methods of selective enrichment of such quantum states are currently unavailable for molecules other than H_2. If gaseous fuels could be selectively enriched in their lowest-energy form, then combining enriched fuels and MOFs would be a viable path toward energy storage and transport efficiency. Our new research program will produce laboratory-scale samples of alternative fuels that have been prepared in specific nuclear-spin quantum states via a novel method using paramagnetic MOF materials at cryogenic temperatures. Using advanced spectroscopic methods, this research program will investigate the fundamental gas/surface interactions to realize optimal conditions for nuclear-spin enrichment. Our research towards the precise control and artificial enrichment of nuclear-spin isomers will reveal new underlying physics related to nuclear spins. Achieving a fundamental understanding of the mechanisms for artificial enrichment is a key step towards optimal storage devices for alternative fuels, enabling their use for a more sustainable and green energy future.

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

Understanding the Relationship between Surface Lattice Rigidity and Single Photon Emission Dynamics in Strongly Confined Cesium Lead Bromide Perovskite Quantum Dots

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Cyberattacks and hacks are growing threats to the United States' national security. Such persistent risks demand quantum information sciences that offer the possibility of ultra-secure communications. Photonic quantum networks are promising quantum communication technologies, since photons can be transmitted with minimal loss. To build photonic networks, single photon emitters (SPEs) are required. Colloidal lead halide perovskite quantum dots (QDs) with high luminescence efficiency at room temperature are ideal SPE materials. Moreover, strongly confined perovskite QDs (SCPQDs), whose physical sizes are smaller than the Bohr diameters of their excitons, are predicted to have high single photon emission purity—the most important characteristic of SPEs—due to their fast biexciton Auger recombination processes. Unfortunately, current SPEs based on individual perovskite QDs exhibit severe stochastic emission intermittencies and unexpectedly low single-photon purity. A fundamental understanding of the insufficient single-photon emission performance is still lacking. With a focus on cesium lead bromide SCPQDs, this project aims to understand the relationship between surface lattice rigidity of perovskite QDs and their single photon emission dynamics. Recent advances have shown that the surface latices of perovskite QDs are soft and can substantially affect their excitonic behaviors. This research will apply supramolecular matrices to tune the surface lattice rigidity of SCPQDs embedded in them and explore the single photon emission properties of these SCPQDs, including emission rates, single photon purity, and photon coherence. The knowledge gained in this project will advance the development of scalable, on-demand SPEs for compact photonic devices and quantum photonic networks operating at room temperature.

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

Reconnection-Driven Turbulent Cascade in Magnetized Collisional and Collisionless Plasmas

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Understanding the transfer of energy across scales in magnetohydrodynamic (MHD) and kinetic plasma turbulence is crucial for tackling many outstanding space and astrophysical problems, such as solar and stellar coronal heating, star formation, and cosmic-ray transport. For more than half a century, it has been widely accepted that the energy cascade in turbulent plasmas such as the Sun's atmosphere is controlled by magnetohydrodynamic wave interactions. However, one essential feature of plasma turbulence is the ubiquitous presence of sheets of intense electric current (known as current sheets), which are preferential locations for rapid breaking and reconnection of magnetic field lines, a fundamental physical process in magnetized plasmas whereby stored magnetic energy is converted into heat and kinetic energy of charged particles. Recent analytic and numerical studies suggest that magnetic reconnection may facilitate the turbulent energy cascade from large to small scales when the magnetic reconnection process becomes fast enough compared with the nonlinear eddy turnover time scale. It is yet an open question whether magnetic reconnection can significantly change the transfer of energy in both MHD and kinetic scales in a wide variety of plasma systems. This project aims to investigate the interplay between magnetic reconnection and turbulence, and the associated heating and particle acceleration in both resistive MHD and collisionless kinetic regimes. The proposed research combines state-of-the-art numerical simulations and theoretical analysis to explore the frontier of the interplay between turbulence and magnetic reconnection in the regime where the tearing instability plays an important role. This new regime could have profound implications on how energy at large-scale cascades down to small-scale and eventually converts into thermal and nonthermal energy of particles.

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

Sustainable Ironmaking: Using Photons to Understand and Drive the Mechanism of H_2-Based Direct Iron Reduction

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Steel is a pillar of modern society and our sustainable energy future, as it is the go-to alloy for robust, reliable, and customizable conditions. However, steelmaking accounts for 8% of global CO_2 emissions. Over half those emissions occur as Fe is separated from O in iron ores: hematite (Fe_2O_3) to iron (Fe). Established blast-furnaces use coal as a reductant producing 1.5 molecules of CO_2 per Fe. Hydrogen direct reduction (HyDR) of iron ores generates H_2O byproduct at lower reaction temperatures. While promising, scaling HyDR's endothermic kinetics and mass-transport limited solid-gas mechanism has been slow due to poorly understood fundamental science. Longstanding questions as to how to understand and control competing mechanisms and thermochemically limited mass transport in the defected and impure minerals still hinder commercial viability for the >100 megaton/yr throughput required to match blast furnaces. Iron ore "fines" produced industrially are nanoparticles that react differently from bulk materials due to their larger surface-to-volume ratios. This project explores how the nanograins native to iron ore fines dictate the chemistry that has previously been overlooked. Using advanced spectroscopy and imaging techniques, this work studies how distortions in the energy landscape caused by the nanoconfinement offer opportunities for enhanced mechanistic control. The fundamental science from our project will provide key insights into strategies to efficiently drive Fe—O separations in iron oxide ores to help decarbonize this critical technology.

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

Phase-space engineering of supra-thermal particle distribution for optimizing burning plasma scenarios

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This five-year project aims to design, validate and optimize the multiscale physics of self-consistent and numerically efficient reduced models of fast ion transport within whole device modeling with simultaneous radio frequency and neutral beam injection heating. Research activities include comprehensive exploration studies to engineer ways of minimizing energetic particle transport in order to maximize core fusion performance, using tools that build on recent developments in fundamental nonlinear kinetic theory and their associated numerical implementations. This proposal aims at leveraging those recent advances into practical macro-stability ramifications in NSTX-U and DIII-D, and high-fidelity transport projections to burning plasma conditions, such as those expected in ITER. The control and avoidance of energetic particle-driven magnetohydrodynamic instabilities are essential ingredients for achieving burning plasmas relevant to economical, high gain fusion reactors. Although ITER will employ comparable amounts of radio frequency and neutral beam injected heating power, the energetic particle transport under such a combined scenario still remains poorly understood. The overarching goal of this project is to deliver and exploit a validated, fully predictive and integrated fast ion transport workflow, accounting for both radio frequency and neutral beam injection heating sources, collisions and Alfvénic eigenmodes in different regimes of instability excitation. This project aims at delivering concrete solutions for integrated scenarios currently being studied in preparation for burning plasmas. Physical insights will be actively pursued to divert and mitigate deleterious fast ion phase space flows in NSTX-U, DIII-D, and ITER while simultaneously ensuring compatibility with macroscopic performance constraints. The successful demonstration of the proposed quantitative prediction of fast ion transport and combined neutral beam injection and radio frequency scenario development will potentially help to close the energetic particle gap for ITER burning plasmas.

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

Hierarchical Assembly of Biomimetic Active Mater Driven by Non-Equilibrium Actin Turnover

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Living organisms display many enticing features that, if embedded within synthetic materials, would have transformative applications in the fields of material science and energy. Cells are composed of molecular machines and energy-consuming polymers that produce mechanical work at the protein scale, leading to spectacular emergent behaviors at the macroscopic scale, such as spontaneous motility, replication, self-healing, and morphogenesis. However, the rational design and control of programmable materials that robustly mimic these features are still in their infancy. This proposal's goal is to elucidate how energy-consuming proteins work coherently over multiple length scales to generate complex, yet organized, structures and motion. Specifically, we will establish a new in vitro model system where coupling between reaction/diffusion-mediated pattern formation and polymerization of actin filaments mimics fundamental features of morphogenesis. This work will set the fundamental design rules for building low-energy multiscale materials that can autonomously accomplish tasks greater than the sum of their parts. The resulting machines will be less prone to catastrophic failure due to the distributed and hierarchical mechanisms that drive their motion.

We propose a synergistic experimental/modeling approach that combines biochemistry, soft mater physics, mathematics, and machine learning. Micron-scale beads covered with an actin nucleating protein self-propel when immersed in a solution of actin monomers and actin-binding proteins, mimicking the motility of small parasites such as listeria. One overarching goal is to investigate how emergent behaviors propagate across multiple length scales. A variety of emergent behaviors will be investigated at the single bead length scale, between pairs of beads, in dense colloidal suspensions, and in three dimensional polymeric materials composed of treadmilling actin filaments.

With our growing demand for alternative energy sources, efficient low-energy materials that harness chemical energy from their environment to produce programmable and controllable flow patterns are a highly sought-after goal in soft robotics, bioengineering, and materials sciences. This project will establish fundamental design rules for creating multiscale materials endowed with life-like properties. The resulting machines will be less prone to catastrophic failure due to the distributed and hierarchical mechanisms that drive their motion.

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

Multi-Linear Representations for Quantum Characterization, Control, and Computation

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What quantum mechanical problems can be solved efficiently with future generations of classical computers? What are the fundamental scaling limits of characterizing and controlling quantum devices and their computing architectures? Current approaches to answering these intertwined questions are limited by either oversimplified noise models or unsustainable classical compute requirements. This research program simultaneously addresses both these challenges by developing memory-efficient algorithms based on the multi-linear representation (MLRep) theory of low-rank linear operators for quantum characterization, control, and computation. To maximize the scale at which realistic semi-coherent quantum device dynamics can be modeled with classical computational resources, we first develop scalable MLRep algorithms factorizing a low-rank quantum state's coherent *and* incoherent correlations. The developed MLRep algorithms will subsequently be integrated into a characterization workflow scaling the construction of empirical error bounds with respect to select quantum processes. The characterization framework will assess the quantum processes' quality as well as demonstrate the feasibility of MLRep-mediated quantum control. Finally, with the goal of accelerating computational science, the project's MLRep algorithms will be compiled into a new linear algebra package gauging classical high-performance computing resources' ultimate potential in quantum control and computation.

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

Mapping the space-time evolution of quarks and gluons at RHIC

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Fundamental building blocks of the observable universe, quarks and gluons, can be studied in relativistic collider experiments as energetic interactions liberate and produce particles which are observed by state-of-the-art particle detectors. One of the biggest unsolved mysteries in nature is in quantifying the mechanism by which quarks/gluons metamorphosize into stable particles such as protons and other
hadrons that make up what we see all around us. Such a transition encodes critical features of the theory of strong interaction i.e., quantum chromodynamics (QCD), one of the four fundamental forces. Our group will study relativistic collisions at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) with the new sPHENIX detector that has just started taking data for the first time in 2023. Heavy ion collisions are a perfect laboratory to study the properties of the early universe as they recreate conditions, high temperature and energy densities, supposed to have existed a few micro- seconds after the big bang. Jets, collections of particles resulting from the fragmentation of highly energetic quarks/gluons, have the right time-scale for probing these conditions.
Our results will enable an extraction of the dynamics of quarks/gluons for the first time in high energy nuclear physics. These results satisfy the mission critical need and success of a central goal of BNL and RHIC's nuclear physics program – studying the production, evolution and eventual demise of the emergent Quark-Gluon Plasma (QGP) and its microscopic transport properties.

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

Generating and diagnosing extreme beams for next-generation high energy physics and fundamental science experiments

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Particle accelerators have been the leading tool for fundamental discovery science and high energy physics for more than a century. Progress in society's understanding of the fundamental interactions of Nature has been predicated by advances in accelerator technology and associated improvements in the particle beams they generate. To continue probing the natural world with greater precision, the next generation of accelerators will need to produce higher intensity particle beams with extreme properties beyond the current state of the art. The research carried out in this project will produce the extremely bright and intense electron beams needed to serve the next generation of high energy physics and fundamental science experiments. These beams will enable us to conduct experiments that will shed light on open questions in fundamental quantum physics, astrophysics, and the design of future particle colliders. Concurrently, these beams will broadly benefit society by enabling the study of important ultra-fast chemical and biological processes through the generation of bright bursts of X-rays. This research program outlines a multi-faceted effort towards designing, optimizing, and measuring the electron beams required to drive these future experiments, leveraging the expertise across SLAC National Accelerator Laboratory, and taking advantage of a suitable user facility, the Facility for Advanced Accelerator Experimental Tests (FACET-II), which can both host the experiments and whose scientific program can profit from their outcome.

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

Demonstrating enabling technologies for a spectroscopy instrument for the next cosmic survey

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Understanding the physical processes responsible for the accelerated expansion of the universe is one of the most important questions in physics. In the last decades, there has been tremendous progress in our understanding of how dark energy dominates its expansion in later times. However, the mechanisms driving the expansion in its earliest moments have been less explored. Those marks from the early universe are imprinted in the distribution of mater at large scales in current times. To observe those features, extensive surveys mapping the three-dimensional distribution of the galaxies in the universe should be conducted. The scientific community is pursuing the construction of the next-generation spectroscopic facility for that purpose, which should provide at least an order of magnitude increase in observational power compared to the current experiments. This project aims to demonstrate the technology for constructing such a large spectroscopy instrument. The program will be centered on increasing the survey speed and science reach over existing equipment. It will be focused on the development and characterization of miniaturized robotic fiber positioners to increase the number of accessible targets per telescope light-collecting area and the development of sensor technologies that maximize the detection efficiency of the distinctive features in the photon spectrum needed to map galaxy motion. Very sensitive optical silicon imagers, which provide single photon counting capability, will be used for the later. In the final stage of the project, the construction of a small-scale instrument for a sky demonstration will be evaluated based on the readiness of these technologies.

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

Probing Water Cycle Processes and Extremes in Coastal and Urban Environments Using Water Isotope Ratio Tracers and Numerical Tags

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Coasts represent some of the most dynamic and complex natural systems on Earth and are of outsized importance, relative to their area, for national and global economies. Nearly half of the global population lives within 100km of a coast and up to 90% of the world's international trade passes through coastal infrastructure. Coastal zones sit at the nexus of societal and environmental challenges: urbanization of coastal regions is expected to continue while risks from extreme events, sea level rise, ground water salinization, and coastal erosion are increasing due to climate change. These intersecting challenges motivate a need for Earth system models (ESMs) that can represent coastal systems in detail to better understand risk to and resilience of coastal cities arising from climate change and increased urbanization.

Recent advancements in computational capability have enabled new ways of representing coastal systems in ESMs, such as the Department of Energy's Energy Exascale Earth System Model (E3SM). While improvements have been made to parameterization and representation of coastal processes, the impacts of these changes can be hard to assess at a process level. Furthermore, urban systems remain at the sub-grid scale for all but the highest resolution configurations of ESMs and therefore are highly parameterized. These limitations prevent a detailed understanding of coastal processes, their interactions with coastal cities, and the individual hydrologic processes that drive responses to extreme events or determine the success or failure of proposed mitigation and adaptation interventions.

This project will address these limitations by developing a comprehensive water tracking system throughout E3SM. This tracking system will also provide capability to simulate water isotope ratios, which are a commonly used tracer of hydrological processes. Existing water isotope ratio observations will be compiled to validate the E3SM water isotope and tracer capability. Next the new water tracer capability will be used to investigate the representation of coasts and their response to urbanization and extreme events in E3SM. The new water tracer capability will provide new ways to compare model simulations with tracer observations and enhance confidence in coastal and urban process representation in E3SM. The proposed research activities would enhance the E3SM's capability to track water sources, sinks, and transport throughout the hydrological cycle and across model components, ultimately improving our understanding of urban-coastal system interactions. By connecting this new tracking system to the existing capabilities, the enhanced E3SM can be utilized to study coastal change, extreme event susceptibility, and urbanization impacts on precipitation and flooding, and potential solutions for increasing coastal city resilience. E3SM simulations will be conducted in both in idealized coastal-urban settings, as well as a case study of Houston, TX using data from the TRACER ARM campaign. The new framework has enormous potential to advance our understanding of the hydrological cycle in both natural and urbanized coastal systems and enable E3SM to answer a broad set of coastal-urban questions.

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

The Development of a Real-Time Accountancy Open Framework for Fusion Energy

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Fusion Energy, generated by atoms fusing together versus splitting apart, is what powers our sun and the stars. It is widely considered the commercial energy source of the future for its potential to produce immense power, while generating no long-lived radioactive waste or greenhouse gas emissions. Commercializing Fusion Energy has become increasingly attractive in recent years, with national laboratories and universities partnering with private companies to make it a reality. Deuterium and tritium (DT), isotopes of hydrogen, are the most promising fuels for commercial production of energy from fusion. In this process, DT must be continuously supplied to the fusion reaction, ensuring that the power output is consistent. DT is supplied to the fusion reaction by the fusion fuel cycle, a series of components that clean-up reaction chamber exhaust and recycle DT to be re-fed as fuel. However, tritium is a radioactive material that requires special treatment and, therefore, a commercial fusion fuel cycle must have complex systems for extracting, moving, processing, and collecting this isotope. Because it is a critical material in the system and because it is radioactive, tritium needs to be accurately accounted for inside the fuel cycle to monitor inventory in different parts of the system as well as transport into and out of the plant. The amount of tritium in the system can be monitored using a method known as batch processing, but this requires outages or planned interruptions to fusion operations. Fusion energy plants must operate the complex fuel cycle continuously but, to date, there is no known method of monitoring tritium levels within an acceptable accuracy range of less than 1% under continuous operating conditions. Furthermore, accountancy techniques need to consider losses of tritium from burn-up and permeation into and through materials involved in the process; tritium gains through the production of tritium using fusion neutrons (breeding); and measurement noise that accumulates in sensors during operation. This research will couple machine learning methods currently used in self-driving cars and radar tracking with physical measurements of tritium in the fuel cycle to develop a framework for real-time accountancy of tritium gain and loss. The machine learning algorithms, known as Bayesian prediction algorithms, take information from a virtual computational model of the fusion test system, and data from the tritium measurement sensors, to provide an integrated visualization of tritium inventory with incredible accuracy. The successful development of real-time accounting of tritium levels (an “accountancy open framework”) during fusion operation is critical to the success and efficient operation of commercial Fusion Energy.

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

Probing Correlated Phenomena in Graphene Constrictions

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Understanding the quantum electronic properties of charge carriers in nanostructures can have significant implications for the advancement of future quantum technologies. This research focuses on designing and engineering clean and tunable graphene-based nano constrictions and probing correlated phases in these artificial potential landscapes. This is an underexplored area in two-dimensional material research, primarily due to technical difficulties related to disorder and the lack of control over the confinement potentials. These challenges will be addressed by integrating clean van der Waals heterostructures having gate tunable electronic phases with scanning probe microscopy (SPM)-based nanolithography techniques. This will enable nanoscale electrostatic control with contaminant-free interfaces, thereby creating high quality and tunable constrictions. The quantum electronic properties of these structures will be investigated by employing different measurement techniques, including transport and advanced SPM, and tuning experimental knobs such as temperature, electric and magnetic fields. These studies aim to understand the interaction effects in the transport of Dirac electrons through narrow 1D channels and explore the quantized supercurrent in superconducting quantum point contacts formed within graphene-based moiré systems, where distinct quantum phases can be switched on and off electrostatically in a single material. Furthermore, this investigation will characterize the charge and statistics of emergent quasiparticles of fractional quantum Hall states and examine their potential manipulation and braiding by local probes. The outcomes of this project will have important implications for the development of novel quantum devices and the advancement of quantum information technologies.

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

Unraveling Ultrafast Electron-Nuclear Dynamics in Molecules

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Photoinduced molecular processes play a key role in physics, chemistry, and biology. In nature, light triggers a large variety of chemical reactions such as photosynthesis, vision, and the formation of vitamin D, but also can cause undesirable radiation damage. Furthermore, the interaction of light with mater forms the basis of important technological applications such as solar cells in which photoinduced charge transfer and light harvesting are essential. What all these processes have in common is capturing the energy of light and its transformation into other forms of energy like heat, electricity, or chemical energy. On a microscopic level, the energy conversion processes result from correlated motion of electrons and nuclei after photoexcitation or photoionization of a molecule. Although much has been achieved in the understanding of fundamental physics underlying the electron-nuclear interactions and dynamics, the accurate numerical simulation of light-induced processes taking place in realistic polyatomic molecules remains an unsolved problem. The objective of this research is to develop both exact and approximate computationally efficient quantum dynamics methods capable of simulating the light-driven electron-nuclear dynamics in polyatomic molecules that account for non-adiabatic effects and include multiple electronic states. While the main focus is method development, all new methods are applied to describe properties and behavior of systems of physical, chemical, and biological interest, interpret recent experimental measurements, and guide future experimental efforts.

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

Using Ancient Enzymes for Modern Photosynthesis

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Nature's CO_2-fixing enzyme Ribulose-1,5-carboxylase/oxygenase (Rubisco) has a slow catalytic rate and exhibits poor substrate specificity, such that Rubisco catalysis often limits the rate of photosynthetic carbon assimilation and thus the growth and yield of crop species. Rubisco's catalytic limitations are exacerbated under high temperature, which is especially concerning because the average global temperature is projected to increase roughly 5.7°C by the year 2100. A previous study used a computational "time machine" to reconstruct ancestral Rubisco sequences that operated under higher CO_2 and temperatures approximately 25 million years ago. Each of these reconstructed enzymes have several amino acid substitutions relative to modern day tobacco Rubisco, and some of them exhibit improved catalysis and thermostability. To understand the mechanism by which these substitutions influence Rubisco activity and thermal stability, new Rubisco mutants will be created containing different combinations of the amino acid substitutions found in the top performing reconstructed Rubiscos. These new Rubisco variants will be produced in an *E. coli* synthetic biology expression system, and their kinetic profile thoroughly probed to pinpoint which aspect(s) of the CO_2- reduction chemistry are modified at different temperatures by the amino acid substitutions. How these mutations confer enhanced thermostability to Rubisco will also be computationally predicted and experimentally validated. To demonstrate that these ancestral Rubiscos improve plant growth under different, including projected future, CO_2 concentrations and temperatures, the performance of reconstructed and new Rubisco variants inside plants will be mathematically modeled across different CO_2 pressures and temperatures. Top performing variants from the modelling will be expressed in tobacco plants and their growth, photosynthetic efficiency, and Rubisco kinetics evaluated under different environmental conditions. This research will provide fundamental insights into how changing the enzymatic environment can enhance the efficiency of biological carbon capture.

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

Nature-Derived Materials for Redox Flow Batteries

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Redox flow batteries are a promising technology in the search to find efficient large-scale storage options for the electricity generated by intermittent renewable energy sources such as solar, wind, or hydropower. The battery consists of negative (i.e., anolyte) and positive (i.e., catholyte) electrolytes separated by an ionically-conducting membrane. The charging/discharging efficiency and the amount of energy stored in a redox flow battery depends on the properties of the electrolytes. Wide-scale utilization of this technology has been limited by the availability and cost of electrolyte materials as well as loss of capacity over time, particularly those focused on metal-based redox species. Organic redox flow batteries are promising alternatives due to their high structural diversity and synthetic tunability. In this project, we take inspiration from Nature by utilizing fungal or plant perylenequinones (PQs) that can be biosynthesized via fermentation or *in vitro* cultures in our energy storage research to improve the efficiency and storage capacity of redox flow batteries.

Using the redox active PQs to create new electrolyte materials enables reactions with a higher number of electrons (i.e., higher charge) as anolyte, catholyte, or both in a symmetric flow battery. In addition to being more efficient, environmentally friendly, and sustainable, the same electrolyte material can be used in both positive and negative components of the battery avoiding cross-contamination and offering promising features for large-scale stationary energy storage applications such as low cost, an easy manufacturing process, greater stability, and simple recycling post-process. Pushing the boundaries of what can be accomplished with these Nature-optimized molecules, we will determine their performance in a membrane-free setup with two immiscible redox electrolytes. This approach will present the first example of a true symmetric biphasic redox flow battery.

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

Room Temperature Stabilization of Ordered 2D Charge Density Waves in Atomically Thin Materials

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In crystals, charge density waves are a spontaneous rearrangement of electrons that mediate metal-insulator transitions, compete with superconductivity, and demonstrate ultrafast non-volatile switching. Room temperature access to ordered two-dimensional charge density waves would provide next generation computing that is a paradigm shift toward energy efficient computing, low-voltage logic, and quantum-based devices. This research will investigate novel quantum phase of mater, where low-temperature charge density waves are stabilized at room temperature through out-of-plane charge twinning in confined atomic layers. Moreover, at higher temperatures, ordered states emerge, suggesting fragile quantum states can be enhanced. Discovery and synthesis of novel charge density waves requires high-resolution scanning / transmission electron microscopy (S/TEM) where the picoscale, nanoscale, and microscale structure can be measured directly. This research will control emergent charge ordered phases and unveil the mechanics of transformation using in-situ S/TEM with electrical and temperature measurement on nanostructured devices.

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

Fourier and Fractional Neural Operators to Unveil Topological Textures in 3D Magnetism

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The ever-increasing demand for data storage and computation has spawned the search for unconventional computing schemes. To achieve the needed paradigm shift in technology, functional materials hosting information-carrying objects must be identified. Three-dimensional (3D) magnetic textures are promising candidates as information-carrying objects because of their expected robustness to perturbations, quantified by a topological index, and manipulation by electrical means. However, interesting 3D topological textures have not been possible to create or manipulate on demand. The objective of this research is to discover magnetic materials where 3D topological magnetic textures can be created and manipulated by implementing novel machine-learning algorithms. For this, it is fundamental to define new models of magnetism that can describe both atomic-scale interactions that resolve topological defects, and long-range interactions that resolve the object's profile and coupling to the environment. In other words, a new description of the fundamental physics and manipulation by electrical means on equal footing utilizing analytical and computational methods is needed. Two models based on Fourier transform and fractional calculus will be introduced. These models will set a physics-informed basis for novel machine learning algorithms and provide a physical definition of the prediction error to inform their plausibility. This research aligns with DOE's mission by introducing new theories and computational methods for the discovery of materials with tailored and remarkable properties, specifically for energy- efficient manipulation of information.

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

Quasi-Tretiz methods for problems governed by vector-valued Partial Differential equation

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This project is concerned with the development of high-performance, efficient and robust techniques for the numerical simulation of complex physical phenomena governed by vector-valued variable-coefficient equations in three dimensions. On the one hand it includes advanced computational methods for problems in strongly inhomogeneous and anisotropic media. On the other hand it includes applications to plasma physics and aeroacoustics. For instance, in the field of waves in plasmas, inhomogeneity comes into play in a non-uniform plasma – when its density is not constant – while anisotropy comes into play in a magnetized plasma – in the presence of an equilibrium magnetic field causing the plasma properties to vary depending on the direction considered.

The computational methods under consideration are called quasi-Tretiz methods. Tretiz methods are seeing a renewed interest in the scientific community as various techniques have recently been explored to tame an important issue of numerical methods based on wave-like basis functions, the well-documented issue of conditioning. Like them, quasi-Tretiz methods rely on local problem- dependent basis functions. However, unlike Tretiz basis functions, their basis functions are not exact solutions of the governing equation. They were precisely introduced to leverage the benefits of Tretiz methods while tackling problems governed by variable-coefficient equations, since exact Tretiz basis functions do not exist in general for such problems. This project will develop quasi- Tretiz methods for vector-valued equations in three spatial dimensions, both from the theoretical point of view and from the practical point of view.

The expected outcome of the project is improved simulation capabilities for electromagnetic wave propagation, in terms of

- performance of numerical methods, including high-order accuracy, scalability, and efficiency,
- robustness in regimes including high contrast, high anisotropy, and high frequency,
- complexity of mathematical models.

Beyond wave-propagation, the development and implementation of high performance quasi-Tretiz methods also represents a significant step towards broadening the domain of application of Tretiz methods in general, as (1) they do not require the knowledge of explicit solutions to the governing equations, and (2) they allow for more flexibility in the choice of basis functions.

In addition, the proposed work will lead to new scientific contributions at the interface between the fields of mathematics and plasma physics.

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

Generalized Electronic Coarse-Graining for the Hierarchical Design of Organic Neuromorphics

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Neuromorphic computing devices that mimic the neuronal and synaptic functionality of biological organisms have the potential to transform modern computing by overcoming the energy intensive von Neumann computing paradigm. A leading materials class for neuromorphic computing devices is organic materials capable of sustaining simultaneous electron and ion transport, but structure-function relationships for these materials are absent due to the hierarchical couplings between length scales that dictate performance. While molecular modeling approaches to neuromorphic materials design hold the potential to elucidate materials design rules, such approaches are inhibited by the prohibitive computational cost necessary to perform quantum mechanical calculations at the required length scales (~10-100 nm). This work will introduce a coarse-graining method that leverages machine learning to enable chemically transferable quantum mechanical predictions at ~10-100 nm, facilitating the systematic and hierarchical design of organic neuromorphic computing materials capable of transforming the modern computing infrastructure.

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

Towards Intelligent Scheduling for Adaptive Scientific Computing with Heterogeneity

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In order to keep up with trends in computer architecture and software, high-performance computing (HPC) must adapt to heterogeneity, extreme scale, and dynamism. The complexity of HPC systems is increasing as hardware vendors strive to improve computing capability while managing power consumption. To achieve high performance and throughput, scientific computing applications must be able to fully leverage these large-scale and heterogeneous resources. Meanwhile, scientific simulation and analysis workflows are also becoming more complex and dynamic, incorporating components with varying execution times and resource requirements. Traditional bulk-synchronous execution models are no longer sufficient to capture these patterns. Manual resource allocation decisions require significant time and effort from application developers in order to understand their workload and computing resources. Even with a good understanding, deciding how to allocate resources remains highly challenging. Manual and heuristic-based decisions often result in the under-utilization of resources and inadequate performance. This project aims to develop an intelligent scheduling framework that can automate resource allocation and deliver better performance for adaptive scientific workflows on HPC systems. Specifically, we will design a tree-search-based approach to find high-quality resource allocations for specific workflows and distill the knowledge in the trees into a policy. We will devise deep learning-based surrogate models for fast evaluation of the quality of allocations sampled by the trees, without actually executing the scientific workflows on HPC systems for each and every allocation. To further enhance the accuracy of the surrogate model and the performance of the distilled policy, we will adopt active learning strategies to guide the acquisition and usage of additional real execution data. The developed techniques in this project will have a direct impact on HPC systems, improving resource efficiency, reducing energy consumption, and lowering overall operating costs.

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

Selective Photochemical Reactions for the Discovery of Triplet Photosensitizers

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The evolving demands of the modern world call for new materials with advanced performance and minimal environmental footprint. However, the prevailing one-at-a-time approach to synthesis and testing creates a significant bottleneck for experimental validation and discovery, even when automated. Triplet photosensitizers, light-harvesting molecules with long-lived excited states, can couple photoexcitation to chemical reactivity for solar energy conversion. It is challenging to design triplet photosensitizers composed solely of light elements, and many of the techniques used to measure key properties are not amenable to high-throughput experimentation. The objective of this project is to bypass design by directly identifying photosensitizer candidates from libraries of chromophores on the basis of their light-induced reactivity. Selective photochemical reactions that "tag" triplet photosensitizers will be combined with high-throughput techniques to isolate and analyze the resulting products. This experimental platform will be guided by data science and has the potential to reveal non-intuitive structure-property relationships. The resulting photosensitizers will be applied to the solar-fueled deconstruction and upcycling of commodity plastic waste.

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

REASON-3D: Randomized, Entropic, Adaptive, and Scalable Optimization for Non-Intrusive Data-Driven Design

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Global transitions in energy, economy, and national security have accelerated the need for a new state-of-the-art in robust and efficient optimal design and decision-making technology. The randomized, entropic, adaptive, and scalable optimization for non-intrusive data-driven design (REASON-3D) project aims to deliver on this requisite advancement in an intensive, multi-faceted, five-year research initiative targeting, among others, adaptive, adjoint-free PDE-constrained optimization with provably mesh- independent, high-order, risk-averse optimal design, and optimization of long-time quantities of interest from chaotic systems. The cross-cutting theme is to harness new paradigms in variational and probabilistic analysis to propel research and innovation into critical mission areas.

The overall goal of REASON-3D is to reach a new pinnacle in extreme-scale computational science and engineering through entropic, randomized, adaptive, adjoint-free, and massively-scalable algorithms for design, prediction, and decision-making. Moreover, the project aims to deliver new adaptive algorithms for scalable, risk-averse, data-driven engineering design applications, contribute to established software libraries, and enable extensible next-generation workflows to maximize impact and facilitate broad adoption at domestic research institutions.

REASON-3D will advance multiple new synergistic optimization and simulation paradigms to achieve its overall goal.
1. The project will leverage a new non-intrusive randomized differentiable programming (RDP) paradigm to enable the solution of mission-critical scientific computing problems where traditional differentiable programming methods are impractical or unstable. The key idea here is to compute non-local stochastic gradients instead of local deterministic gradients.
2. The project will exploit a state-of-the-art advancement in entropy regularization methods to geometrically mollify non-smooth objective functions and pointwise bound constraints in Sobolev spaces. In turn, REASON-3D will deliver not only new optimization algorithms but also a new finite element methodology that we intend to use to target invariant domain-preserving hyperbolic flow simulations.
3. The project will deliver scalable, adaptive sampling strategies for randomized differentiable programming and entropy regularization that leverage existing DOE software infrastructure, e.g., the rapid optimization library (ROL) and the modular finite element methods (MFEM) library.

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

Advanced Additive Manufacturing of Silicon Carbide for Fusion Applications

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Enabling future fusion power plants requires manufacturing advanced materials for high-performance components and structures. Rapidly evolving additive manufacturing (AM) technology provides flexibilities in geometries, unique material microstructures, and quality control to satisfy fusion application needs. Silicon carbide (SiC) shows significant promise for fusion applications because of its ability to operate at high-temperature and with a range of coolants, opening the way for high-energy conversion efficiency. A current scientific challenge is that the fusion operating environment necessitates demanding performance requirements for resistance to high-energy, fusion neutron irradiation. The aim of this research is to develop a mechanistic framework for AM of highly radiation resistant SiC. This research uses binder jet printing of SiC powders in combination with chemical vapor infiltration of SiC, a novel process developed at Oak Ridge National Laboratory (ORNL). The neutron irradiation experiments of traditionally fabricated SiC materials relevant to AM processing will identify radiation tolerant microstructures. Tailoring microstructure of AM SiC will be explored based on machine learning-based analysis on the relationship between the AM processing parameters and the resultant microstructure. This research leverages the ORNL unique capabilities for irradiation experiments, characterizing neutron-irradiated materials, and AM processing equipment dedicated to SiC materials. This research will support prototyping and component testing under a future fusion technology program essential for enabling fusion energy systems.

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

Selective Nucleation of Rare Earth Element Phases on Mineral Surfaces

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Mineral surfaces can exert profound control over the geological distribution of elements, thanks in large part to their ability to catalyze precipitation processes such as crystal nucleation and growth. There is a growing body of evidence that common mineral surfaces can bias precipitation pathways toward non-classical processes and stabilize novel surface-specific phases that would not be predicted from bulk equilibrium. This project will elucidate the molecular-scale factors that influence precipitation pathways on mineral surfaces, in order to better understand how they influence the geological distribution of critical elements. The study will focus specifically on the rare earth elements (REEs), which are critical materials for clean energy technology.

A key aim of this project is to understand how factors such as surface charge, ion correlations, and interfacial solution structure influence the mechanisms of mineral surface precipitation. The REEs will provide an ideal case study for understanding these processes, because they display systematic variations in key parameters such as ionic radius, solubility, hydrolysis, and points of zero charge, that can be leveraged to elucidate the underlying physical controls. By comparing the precipitation pathways for representative 'light' and 'heavy' REE phases, this research will reveal how couplings between the physical properties of the mineral surface and the precipitate (such as electrostatic charge and epitaxial lattice match) can select between precipitation pathways. This will be achieved by using a combination of advanced experimental and theoretical tools. The precipitation of REE surface phases will be tracked with atomic resolution by applying in-situ atomic force microscopy (AFM) and scanning transmission electron microscopy, and the precipitate composition will be characterized using surface sensitive infrared spectroscopy and synchrotron x-ray adsorption methods. Complementarily three-dimensional AFM tools will be applied to map the local electrostatic fields and solution structure of the interface, to determine their stabilizing influence. The surface phases will be modeled using a combination of charge frustrated lattice gas simulations and molecular dynamics simulations. The results will reveal whether common mineral surfaces such as aluminum oxyhydroxide and phyllosilicate surfaces can drive distinct precipitation outcomes, and test whether the resulting precipitates show element-specific selectivity that can be leveraged to drive the separation or enrichment of REEs. This research will produce fundamental knowledge on the molecular-scale mechanisms of REE precipitation, and mineral precipitation in general. This knowledge will help to better describe the geochemical behavior of REEs and facilitate the identification of novel REE ores and the development of improved recovery schemes with lower environmental impact.

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

Model Reduction by Deep Learning: Interpretability and Mathematical Advances

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Many real-world applications in science and engineering involve large-scale, complex, and expensive data simulations and inversions of physical processes. Model reduction plays a significant role in these applications, which allows one to reduce the data dimension and the size of the problem. Classical projection-based linear model reduction methods have demonstrated great success when the underlying model is linear and low-dimensional. However, a large number of objects in applications exhibit low- dimensional nonlinear structures, and many physical processes are nonlinear. The success of model reduction crucially depends on a good discovery of the latent structures in nonlinear models.

In the past decade, deep learning has revolutionized several fields, and neural networks have been introduced to data simulations and inverse problems. When deep learning is used for model reduction, many works focus on designing network architectures and proposing training techniques to obtain successful predictions for specific problems. The mathematical and statistical understandings of these techniques are limited. The widely open and challenging questions are: 1) How can one interpret the success or failure of model reduction by deep neural networks? 2) How can one improve model reduction by ensuring mathematical interpretability, adaptivity, and robustness?

This project aims to answer these fundamental questions to advance the mathematical and statistical understandings of deep learning. This project has three thrusts. Thrust A aims to develop interpretable deep learning-based nonlinear model reduction methods, analyze the generalization error, and explore various network architectures. Thrust B studies the benefits of neural networks in discovering intrinsic data structures and adapting to function regularity at different scales and locations. Thrust C focuses on computational improvements and science applications of model reduction techniques. This project has a potential to drive significant advances in scientific machine learning. The proposed model-reduction methods can be used to analyze large datasets and simulate complex phenomena in physics, biology, and engineering. The investigation on interpretability, generalization error, adaptivity, and adversarial robustness will advance the mathematics of deep learning and model reduction.

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

Analog-Digital Hybrid Simulation of Quantum Field Theories with Advanced Ion Traps

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Quantum field theory (QFT) is a powerful theoretical framework that underpins much of modern physics, helping us understand subatomic particles and their interactions. However, computing the dynamics of QFT models can be an immensely challenging task. Quantum computers promise to efficiently simulate such models using qubits, which are computational bits that take advantage of quantum phenomena like entanglement and superpositions to create powerful quantum algorithms. But encoding physical interactions involving photons and other bosonic particles is difficult even for these advanced systems due to the infinite-dimensional state spaces involved. To overcome this challenge, we are developing an analog-digital hybrid quantum simulator based on trapped ions. Linear chains of atomic ions trapped in free space with electric fields offer exceptional qubit properties and are a leading platform for quantum computing. In our scheme, the ion qubits are combined with multiple sets of vibrational modes, represented by the motion of the ion chain in the trap. These modes are a quantum version of the overtones on a guitar-string and provide additional quantum resources. They can not only facilitate discrete, or digital, quantum computational gates by coupling different ions together but also act as bosonic degrees of freedom directly. This follows the idea of analog quantum simulation, where a quantum system is engineered to evolve like another system of interest. Using both digital and analog elements allows for more efficient encoding and simulation of QFT problems. We are constructing a new type of ion trap based on micro-fabrication of 3-dimensional glass structures to create the ideal experimental platform for analog-digital hybrid quantum simulations.

Probing the Emergent Hadron Mass through Pion Structure Measurement at the AMBER Experiment

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Understanding the origin of the hadron mass, which constitutes 99% of our visible universe, is one of the central goals of nuclear physics. The Higgs mechanism, although provides mass for the fundamental building blocks of the mater, can only contribute a very small fraction (~1%) of the nucleon mass by itself. The vast majority of the mass is believed to come from the strong force that tightly binds quarks and gluons together. Therefore, measurement of the quark and gluon structure of the hadron is of utmost importance in understanding how the hadron mass emerges through the strong interaction. Any successful theory needs to reconcile both the heavy proton mass and the very light pion mass simultaneously. In contrast to the abundant experimental measurements of the proton structure, the data on the pion structure is very scarce and outdated. The goal of this research is to provide a comprehensive study of the internal structure of the pion by colliding high-energy pions with a carbon target at the AMBER experiment at CERN. The primary R&D of this study involves the development of a silicon-strip-based vertex detector, which will significantly improve the reconstruction precision of the AMBER spectrometer and consequently leads to the best measurement of the pion structure to date. The result yielded from this study will provide the needed sensitivity to understand and constrain the mechanisms responsible for the emergence of the hadron mass.

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

Resurgence of Markov Random Fields for Scientific Machine Learning: New Mathematics for an Old Framework

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Markov Random Fields (MRFs) is a general class of probability distributions related to Boltzmann distribution in physics, Gibbs measure in mathematics, undirected graphical models in computer science, or energy-based models in machine learning. MRFs have been used for modeling of natural systems at equilibrium since the creation of statistical physics, and hence serve as a natural and interpretable modeling foundation for many scientific applications. Yet, unknown training algorithms, as well as the lack of tools for generating predictions from these models present the main barriers to the widespread use of MRFs in Scientific Machine Learning. This project aims at eliminating these known barriers by advancing the mathematics behind machine learning methods for MRFs. We address the challenge of designing a suite of efficient learning algorithms that incorporate physical symmetries, deal with heterogeneous and noisy data sets, construct MRFs in a form which allows for generation of predictions and sampling, and have a robust implementation. As a demonstration of a wide applicability of the developed methods, this project focuses on open problems in several distinct scientific areas that require rigorous learning of interpretable and physics-informed probabilistic network models from distributed data: many-body quantum physics, power grids, turbulence, and field theories.

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

Integrating Machine Learning Models into E3SM for Understanding Coastal Compound Flooding

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Coastal-urban regions in the United States are home to 40% of the nation's total population, produce more than $9.5 trillion in goods and services, and employ 58.3 million people. They have a high concentration of infrastructure, are often economic centers, and are crucial in water and nutrient cycling. But unfortunately, these regions suffer from severe flooding, and backwater effects caused by pluvial, fluvial, and coastal processes that greatly exacerbate the flood risks. Therefore, there is an urgent need to improve understanding and simulation of backwater effects and mitigate the induced floods, and this urgency is escalating with increasing coastal development, population growth, and vulnerability of infrastructure to the floods. However, coastal backwater effects are difficult to simulate because of their multiple interactive drivers and complex, interrelated land-river-ocean processes. The effects have not been well represented in the Energy Exascale Earth System Model (E3SM) partly because of insufficiency of incorporating data and deficiency in model grid configuration. Coastal-urban regions usually have many sensors, observatories, and radars that collect vast amounts of in situ and remote sensing data. These data contain critical information about drivers, processes, and their influences on coastal flooding. To address knowledge and modeling gaps in coastal-urban regions, this project will extract information from multi-source, multi-type data; develop mesh-free, data-informed, and physics- embedded river models using machine learning methods; and couple the river model with E3SM land and ocean models to advance predictive understanding of coastal compound flooding under climate change. The project will focus on two Mid-Atlantic River Basins, Susquehanna River Basin and Delaware River Basin, which include significant urban areas, have more than 4 million residents, and suffer from severe coastal flooding.

This research will advance understanding of feedbacks and interactions of extreme events at coastal- urban systems, enhance E3SM capabilities in simulating coastal compound floods with uncertainty quantification, and inform urban planning to mitigate the impact of climate change on communities, infrastructures, and economy.

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

Data-Driven Discovery of Dynamic Models to Characterize Energy Systems

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Rapid characterization of the generation, extraction, and storage of energy is an intrinsic problem across application areas, including material and biological systems. Physical modeling has traditionally been a powerful technique to gain human-interpretable insight into energy system's behavior. Recently, model selection methods using sparse optimization have provided means of data-driven, semi-automatic model generation and parametrization. However, methodological gaps limit the computational feasibility of model selection for systems with unmeasured variables and identifiability issues and from complex data sets with multiple underlying systems behaviors. This research will accelerate the rate at which we can characterize energy systems from complex data by developing new methods for sparse model discovery and experimental design for mechanistically-interpretable ordinary differential equations (ODEs).

A semi-automated method for discovering mechanistic ODE models would revolutionize our ability to rapidly understand energy systems. By combining state-of-the-art nonlinear parameter estimation with sparse penalization, our framework will expand the practical and computational limits of data-driven model construction from complex, real-world datasets. We will advance sparse-experimental design by integrating identifiability analysis with sparse optimization to inform the quantity and quality of data required and set guidelines for when model selection is feasible and robust. Finally, we will connect automated model discovery to perturbation theory to characterize complex data sets where multiple asymptotic limits (simplified models) are required to characterize distinct mechanistic behaviors across
time and variation in control parameters. While we will develop the method in the context of target biological and materials systems, such methods will be extendable to any system where nonlinear dynamics terms determine the behavior of a dynamical system (biochemistry, environmental systems, device physics, materials chemistry, catalysis science, etc.).

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

A multi-experiment common framework for neutrino cross section uncertainties

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What are the uncertainties on neutrino-nucleus interaction cross sections? This question faces all neutrino oscillation experiments, and sounds very simple but is actually extremely complicated. Experiments use ``event generators'' to simulate neutrino interactions, which rely on largely empirical models that are tuned to external measurements. However, large uncertainties remain, and a huge amount of effort goes into understanding how wrong these models might be, and in what ways. This becomes even more important as our experiments get more and more precise.

The Deep Underground Neutrino Experiment (DUNE) is the next generation long-baseline oscillation experiment. Scheduled to start physics in 2028, DUNE will measure oscillations using liquid argon time projection chambers as both Near and Far Detectors. The Short Baseline Program (SBN) at Fermilab has essentially the same setup but a much shorter baseline, and will start its two-detector physics run next year. These two experiments both need a robust framework for tuning the interaction model and describing its uncertainty. Furthermore, measurements made in SBN will be crucial inputs to eventual analysis in DUNE. The aim of this research is to develop a common tool for neutrino cross section uncertainties, and to integrate this tool into the analysis frameworks of both DUNE and SBN. The goal is for the huge effort of understanding neutrino-argon interactions and implementing uncertainties to be largely shared, and to make it straightforward to connect cross section measurements at SBN to oscillation sensitivities at DUNE.

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

Building a Scientific Foundation for a New Generation of Low Energy Adsorptive Separations: Probing the Role of Responsive Structural Flexibility using Synthetic Porous Frameworks

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We are elucidating fundamental insights into the relationship of cooperative flexibility in porous adsorbents and low-energy adsorptive separations. Our objective is to use hypothesis-driven empirical and computational efforts to understand the key structural and energetic variables of cooperative flexibility that influence selectivity and kinetics of adsorption, and thus separations from relevant mixtures. Metal–organic frameworks, both rigid and flexible, serve as the model platform for these studies, owing to their diversity, intuitive synthesis, high crystallinity, and computational feasibility. Specifically, we are using a series of established frameworks with previously characterized structures and observed flexibility, alongside the corresponding rigid structural analogs serving as control materials. These efforts will significantly advance the atomic- to meso-scale understanding of responsive cooperative flexibility in porous adsorbents. They will build a scientific foundation that promotes the intuitive design and application of cooperative flexibility in the pursuit of low-energy adsorptive separations for societally critical separations, such as purification of commodity chemicals, removal of pollutants from the environment, and isolation of critical minerals and elements.

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

Ultrafast Control of Topological Transport in Quantum Materials

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Topological quantum materials host large, anomalous, and often dissipationless electrical and magnetic transport responses arising from the non-trivial geometric nature of their electronic wavefunctions. Discovering pathways to actively induce and manipulate these responses using external stimuli is a central goal of the physical sciences because it could lead to functionalities based on the dissipationless energy transfer for applications in energy-efficient sensing and quantum information science.

This research program will engineer new forms of on-demand topological charge transport in quantum materials using femtosecond pulses of light. The electrical transport dynamics of light-induced topological states will be directly captured using a chip-scale ultrafast optoelectronic device architecture. The proposed strategy is to use ultrafast light-mater interaction to manipulate the topological character of materials by coherently breaking or imposing specific electronic symmetries, the nature of which can be controlled by adjusting the wavelength, intensity and polarization of the optical pulse. Mechanisms based on this strategy include the formation of photon-dressed Floquet states and the transient distortion of materials' crystal structure via the generation of coherent lattice vibrations. These mechanisms are predicted to lead to novel topological transport responses with no equilibrium counterpart. The results will further our fundamental understanding of topological phenomena out of equilibrium, establish new paradigms for optically manipulating quantum materials, and lay the groundwork for next-generation, energy efficient technologies.

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

Pushing the Boundaries of Precision: N3LO Predictions for the LHC

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High energy scattering experiments like the Large Hadron Collider (LHC) are crucial tools to deepen our understanding of fundamental interactions at high energy. In the absence of the discovery of new particles searching for deviations of measurements from our expectation and stringently probing our current understanding of interactions take the highest priority. Consequently, realizing the full potential of LHC phenomenology critically relies on our ability to predict the outcome of LHC measurements. The rapid advance of LHC experiments towards a high-precision era of probing the electroweak energy regime and the Higgs boson calls for the development of a new and improved level of precision predictions, which is the explicit goal of this research. Specifically, the goal is to establish so-called N^3LO (next-to-next-to-next-to-leading order) Quantum Chromodynamics computations as a standard for precision LHC phenomenology. This requires developing innovative ideas and algorithms for both analytical and numerical calculations of scattering cross sections, as well as refining our understanding of scattering theory. The outcome of this research will provide the wider scientific community with the knowledge and tools needed to tackle the challenges of the upcoming high-precision era at the LHC. Additionally, this research will generate cutting-edge predictions for key LHC measurements, offering valuable insights into the behavior of particles at the electroweak energy regime and the Higgs boson. By pushing the boundaries of precision in our predictions and contributing to the advancement of particle physics, this research brings us closer to unraveling the mysteries of the universe and deepening our understanding of the fundamental laws that govern it.

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

Physically Motivated Linking of Resolutions in Multiscale Models to Predict Thermal and Charge Transport in Self-Assembling Soft Materials

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Multiscale materials composed of hierarchical structures are common in nature. To take inspiration from nature and engineer our own multiscale soft materials, such as those based on proteins or polymers, we require a better understanding of how material properties arise from close couplings of structures and interactions across a range of length scales. Simulations that explicitly represent every atom in every molecule, as well as the interactions between them, are crucial for gaining insight into the molecular-level origins of thermodynamic and transport properties of materials. However, such simulations are computationally expensive and thus limited to small length and time scales. As a result, coarser models are also necessary, for describing mesoscale structures that also impact a material's properties. Unfortunately, mesoscale structures themselves subtly depend on atomic-level behavior, meaning that material properties typically arise from a complex interplay across length scales. Controlling this interplay is currently a grand challenge in polymeric materials used in flexible electronics, where material performance depends on both atomic-level details and mesoscale structure. Understanding these connections will help to design more robust, lightweight, ecofriendly electronics, as well as wearable sensors.

Rather than consider simulations at different resolutions as separate information sources, our innovative approach connects coarse and fine simulations within a single framework. To do this, we synthesize knowledge of physics with machine learning to build models that capture the information that is lost or gained in switching between resolutions. Our methodology is called variational autoencoder-based Monte Carlo (VAE-based MC), which provides a way to switch from an atomistic to a coarse-grained model, enhance sampling of configurations in the coarse model, and switch back to a finer resolution. In this way, we benefit from the larger length and time scales accessible to the coarse-grained model but recover the atomistic details necessary for building understanding on a molecular level. Excitingly, applying this methodology naturally identifies how models at different resolutions relate to each other and provides insight into how we can improve our multiscale modeling efforts by adjusting the way information flows between simulations at different scales. Our goal is to apply these techniques to better understand the connections between mesoscale structure and charge transport in electrically conductive polymeric materials. Our efforts will clarify the fundamental information that needs to be transmitted between atomistic and coarse-grained models of soft materials, generally advancing the state of the art in multiscale modeling.

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

Disentangling Nonlinear Spectroscopy to Control Nonequilibrium Energy Transport

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Recent advances in multidimensional spectroscopy provide unprecedented resolution in time, energy, and space, offering exciting new opportunities to reveal how molecules in solution and in extended molecular frameworks absorb, share, transport, and lose energy. These insights have the potential to guide the design of materials with technologically important properties such as the ability to direct transport for optimal energy conversion, manipulate charge flow for enhanced catalytic activity and selectivity, or suppress decoherence for robust quantum technologies (qubits, sensors, and memories). Unfortunately, this requires the ability to predict, interpret, and assign the spectral responses of condensed phase systems, which remains a formidable open challenge. This is especially difficult when the likelihood that molecules absorb light changes dynamically with nuclear motions (non-Condon effects) and when the molecular interactions prevent the application of simplified harmonic theories. To address this gap, we will develop and apply methods to predict nonlinear spectra of chromophores beyond the Condon limit, capture the signatures of nonadiabatic energy transfer in nonlinear spectra, and leverage physics-based machine learning to diagnose and manipulate energy transfer mechanisms. We will initially apply our techniques to predict and elucidate the energy transfer processes revealed by the multidimensional optical spectra of photosynthetic and chlorophyll-carotenoid complexes that are crucial in photoprotection, and porphyrin-based systems, as these are highly tunable and critical ingredients in natural and artificial energy conversion and electrocatalysis. We will then leverage the resulting insights to develop design principles for directed energy transport and tunable optoelectronic properties in porphyrin systems for applications in energy conversion and catalysis. Our proposed advances will be broadly applicable and offer a promising tool to interrogate and manipulate the optical and transport properties of systems ranging from biological dyes, to disordered organic semiconductors, and perovskites.

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

Improving Predictability of Aqueous Coastal Biogeochemistry During Floods, Storms and a Warming Climate

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Major human health and water quality issues are caused by flooding of coastal urban infrastructure, such as sewer systems, wastewater treatment plants, and nuclear power reactors. Floods in these coastal urban regions may directly impact local waterways by delivering bacterial and/or radioactive contaminants into local rivers and estuaries. In addition, the delivery of excess levels of nutrients can stimulate potentially harmful algal blooms, reduce oxygen levels and reduce water clarity, all of which impact biogeochemical budgets and local ecosystems and communities. Yet, these facilities, i.e. sewer systems, wastewater treatment plants and nuclear power reactors, are particularly prone to flooding because of engineering constraints that require proximity to shorelines for effluent discharge and large supplies of water. As climate changes, floods of coastal urban areas are likely to become more frequent and extreme due to rising sea levels, changes in precipitation extremes, and slower storms. Climate- change-driven alterations in flood characteristics will also impact how precipitation events affect biogeochemistry in coastal waterways, including estuaries where many urban centers are located.
Additionally, in urban settings, warmer temperatures and changes in land use may impact the delivery of contaminated water and excess nutrients, as well as the rates of biogeochemical processes. Advances in process-based modeling and machine learning have improved our understanding of floods and their impact on biogeochemistry in coastal urban waterways. Yet, a predictive understanding of coastal urban biogeochemistry remains difficult during extreme events.

This project will combine process-based and statistical machine learning modeling to address the Grand Challenge of modeling hydro-biogeochemistry during extreme events in coastal urban waterways. Specifically, the objective of this project is to analyze how floods of coastal infrastructure impact pollutant and nutrient fluxes to local waterways, and their impact on estuarine biogeochemical processes, on subseasonal timescales (days to a couple months) in modern-day and future climates. The city of Baltimore will be used as a case study to build on and contribute to ongoing DOE and local efforts, including the Baltimore Social-Environmental Collaborative (BSEC) Urban Integrated Field Laboratory (Urban IFL). Model results from the Energy Exascale Earth System Model (E3SM) climate model, as well as the implementation and analysis of a local Baltimore hydrodynamic-biogeochemistry model, will be used to better understand how coastal urban flooding impacts local estuarine biogeochemistry in different climate scenarios. Additionally, a combination of machine learning and sensitivity tests of the process-based model will be used to explore upscaling local observations and models from the Baltimore case study to coastal-urban system to worldwide.

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

Enabling Multiscale Laminography for *Operando* 3D Microscopy without Geometric Restrictions

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The objective of this research is to enable multiscale computed laminography for micron and nanometer resolution 3D imaging of extended samples such as standard pouch cell batteries. Standard computed tomography techniques do not work well for samples with flat geometries resulting in reconstructed volumes with imaging artifacts and poor contrast. Yet this battery geometry is commercially relevant and compatible with most other X-ray characterization. The research will study the 3D morphological and chemical changes occurring in operating batteries at both the hundreds-of-particles and single-particle level. The nanometer scale 3D imaging will provide information on how individual particles and interfaces are behaving, and micron scale will illuminate the heterogenous behavior of many particles to provide the statistical performance at the electrode level and any "crosstalk" between the cathode and anode. The development of 3D imaging of extended, flat samples will fill a significant characterization gap and is widely applicable to other important energy systems such as hydrogen fuel cells, flow batteries, and microelectronic devices.

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

Understanding Irradiation-Assisted Plasticity in Complex Concentrated Alloys

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This proposal addresses the strength-toughness trade-off challenge in structural metals under irradiation at intermediate temperatures (<0.4 melting point). In these conditions, irradiation and mechanical stress result in hardening and embrittlement via significant strain localization at dislocation channels, which is a critical contributor to irradiation-assisted stress corrosion cracking. Leveraging recent advancements in complex-concentrated alloys (CCAs – metallic alloys with multiple principal elements in high concentrations), this project will investigate the effects of microstructure on irradiation-assisted plasticity in CCAs and identify scientific principles for enhanced irradiation embrittlement resistance. Our focus is on the reduction in strain localization through tailoring deformation mechanisms, a process called planar-defect mediated delocalized plasticity (PMDP). PDMP has been shown to strongly influence mechanical behavior in unirradiated CCAs. To achieve this goal, we will systematically design and fabricate model CCAs and employ a range of advanced characterization methods, such as synchrotron-based analyses, high-resolution transmission electron microscopy, and atom-probe tomography, to examine the structural factors of CCAs before and after irradiation. We intend to utilize heavy ion irradiation, electron channeling contrast imaging, and nanoindentation to facilitate the investigation of a vast number of samples in a high-throughput manner. Subsequently, we will analyze the plasticity mechanisms of selected samples using proton irradiation and *in-situ* tensile tests within a scanning electron microscope. This project will enhance understanding of the complex structural response of CCAs to coupled radiation and mechanical stress. The principles developed through this work will guide the development of new CCAs and can be applied to other structural metals, thus improving irradiation embrittlement resistance in advanced nuclear energy systems.

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

Multimessenger tomography of ultrarelativistic nuclear collisions

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The protons and neutrons that form atomic nuclei are themselves made of smaller constituents known as quarks and gluons. When heavy nuclei are accelerated close to the speed of light and made to collide, a hot plasma of these elementary quarks and gluons is produced at the point of impact. The composition and temperature of this plasma are comparable to the state of the Universe microseconds after the Big Bang. The plasma radiates light at different wavelengths in the gamma-ray energy range, which has been measured in experiments at the Relativistic Heavy Ion Collider (RHIC) and the Large Hadron Collider (LHC). The light's energy spectrum and its direction of emission provide a unique window into the properties of the hottest regions of the plasma. In this research project, this electromagnetic radiation will be used to probe the viscosity of the quark-gluon plasma and, critically, study how it changes with the plasma's temperature. This will offer valuable insights into the plasma's transition from a liquid to a gas phase as its temperature increases. Measurements of electromagnetic radiation will be combined with other data sets to obtain state-of-the-art constraints on the plasma's viscosity. Machine learning techniques will be used to accelerate simulations of nuclear collisions and assist the statistical analysis of the data.

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

Modeling fast ion-mode interactions toward a stellarator fusion power plant

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One of the primary requirements for an effective fusion power plant (FPP) is the sufficient confinement of the fusion products, the energetic alpha particles produced in the deuterium-tritium reaction. These energetic particles must be confined sufficiently long such that they can deposit their energy in the thermal bulk and maintain the fusion burn. Furthermore, rapid losses must be avoided to mitigate destruction of the material walls of the fusion device. Energetic particles have historically been challenging to confine in stellarator magnetic confinement devices due to the possibility of unconfined orbits in the three- dimensional magnetic field. With recent advances in the numerical optimization of stellarator magnetic fields, new configurations have been obtained with excellent confinement of fusion-born alpha particles in the absence of perturbations. This breakthrough demonstrates that a stellarator may serve as an effective fusion power plant. There is, however, the potential for enhanced alpha losses due to interactions with perturbations in the background plasma. In particular, experimental measurements on magnetic confinement devices indicate that the resonant interactions between energetic particles (EPs) and shear Alfven waves drive substantial transport. Alfvenic activity is considered one of the major limitations to alpha particle confinement in a burning plasma.

Given the potential impact of fast ion instabilities in a stellarator FPP, we are motivated to advance the 3D modeling capabilities to efficiently and faithfully understand the nonlinear dynamics of mode-particle interactions and control them through 3D shaping. Looking forward to the many calculations required for scenario development and optimization of the magnetic field, we focus on applying reduced models and advanced computational techniques. The proposed work takes advantage of advances made in the related fields of condensed mater theory and dynamical systems in order to efficiently calculate the structure of the shear Alfven continuum and the impact of Alfven modes on the phase-space structure. Reduced quasilinear models will be developed and validated in order to more effectively interpret present day experiments and predict future FPPs. These models will be used to design new stellarator FPP concepts with enhanced EP confinement using numerical optimization techniques.

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

Understanding Nucleation and Film Growth Processes of Solution-Processable Renewable Energy Materials Printed from Confined Volumes

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Solution-processable semiconductors have shown great promise for next-generation energy technologies including, but not limited to, photovoltaics, supercapacitors, and batteries. However, the current scalable printing techniques for these materials result in reduced performance and stability of these layers, because the quality of films generated by these processes is poorer than in lab-scale fabrication techniques with greater process control such as spin-coating. Printing from confined volumes is a promising new approach that enables direct environmental control over the ink as it is being deposited onto the substrate—e.g., temperature, confinement gap (the distance between the substrate and superstrate), surface interactions, etc. The objective of this project is to answer the following three interrelated questions: (1) How does the high surface area-to-volume ratio of the substrate/superstrate and ink influence the nucleation and growth in solution-processed thin films? (2) Can a model for thin film growth from solution be developed that is analogous to the Structure Zone Model for thin film growth from vacuum deposition? and (3) How do the surface energies and chemistries of confining surfaces influence crystal nucleation and growth as well as the resultant film morphology?

These questions will be answered by correlating experimental spectroscopy and microscopy measurements with molecular dynamics simulations and computational fluid dynamics/phase-field modeling. The outcomes of this project will be the development of fundamental understanding and modeling of the molecular-scale nucleation and film growth processes of solution-processed thin films deposited from confined volumes. These efforts will be a significant step toward film-growth control analogous to that developed for vacuum deposition processes, leading to scalable meniscus-guided deposition processes that result in high-quality energy conversion and storage materials with lower cost, higher performance, and longer operating lifetimes than the current state-of-the-art.

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

From Molecules to Continuum: Exploring a Universal, Transferable, and Physics-Based Understanding of Chemical Dynamics from ab-initio

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Chemical dynamics – the coordinated symphony of photons, electrons, protons, and atoms – dominate the efficacy of energy harvesting in numerous renewable energy applications across a diverse portfolio of DOE Basic Energy Sciences priorities, from Direct Air Capture to Liquid Solar Fuel. The need for electronic structure theory guided predictions and interpretations of spectroscopic information is surging, driven by significant recent progress in multimodal experimental spectroscopies that probe chemical dynamics across a multitude of spatial, temporal, and energy scales. Due to its high accuracy-to-cost ratio, DFT, generally referring to the mathematically proven Kohn-Sham DFT (KS-DFT) formulism, has been the method-of-choice connecting theory and experiment. Yet, key distinctions persist among dominant DFT practitioners: quantum chemists favor orbital-like basis sets (e.g., gaussian type orbitals) and tend to focus their efforts on isolated molecular systems; in contrast, solid-state physicists leverage plane-wave basis sets (usually coupled with periodic boundary conditions) and tend to focus on descriptions of infinitely extended systems. The most important renewable energy solutions, however, are complex, heterogenous systems that are neither purely molecular nor crystalline. For example, gas phase molecules (such as CO_2 and H_2O) in nanoconfined environments encounter unique forces that transform their reaction outcomes. These confinement effects can have profound implications for the future of energy supply and climate change. As another example, noble metal nanoclusters efficiently capture light through plasmonic resonances. The plasmon modes subsequently dephase into hot electrons and holes that can be harvested to drive chemical reactions or transferred across nanoparticle-semiconductor interfaces for promising photocatalytic and photovoltaic applications. Real-space KS-DFT is one of the most promising theoretical methods for achieving electronic structure level insight into chemical dynamics in realistically large and complex systems with up to >10,000 atoms. We will exploit the power of this method to unveil a fundamentally new set of chemistry-structure-property relationships in heterogeneous systems at the nanoscale, where geometry, confinement, and atomic interactions interplay. The computational findings will be validated with multimodal spectroscopy experiments.

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

Toward a microscopic picture of hadronization and multi-parton processes

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Quarks and gluons are the fundamental building blocks of hadrons that make up a large fraction of the visible mater in our universe. Their unique properties and interactions can be studied in detail at collider experiments where they are produced at high energies. Quarks and gluons carry a color charge, described by the theory of quantum chromodynamics (QCD), that leads to their confinement into colorless hadrons shortly after their creation in collider experiments. This transition, which leads to the neutralization of color and the emergence of hadrons, is called hadronization. Despite extensive research, a microscopic picture of the QCD hadronization process has remained elusive due to its nonperturbative nature. Addressing this challenging question is one of the main frontiers of the US nuclear physics program, and our limited understanding of the associated multi-parton processes has become a bottleneck in various areas of high-energy nuclear and particle physics. To tackle this question, this project will develop a multi-pronged approach by leveraging three distinct but related methods: 1.
Perturbative QCD calculations of observables sensitive to multi-parton dynamics, 2. Quantum simulations of real-time dependent correlation functions that are relevant to understand the complex dynamics of hadronization, and 3. A.I. / Machine learning techniques that will provide new insights into the microscopic picture of hadronization by identifying patterns in collider data. The confluence of these different computational techniques will facilitate a novel and comprehensive approach to studying the QCD hadronization process from multiple perspectives. The research of this project is of direct relevance to the nuclear physics facilities in the US including the ongoing experiments at the Thomas Jefferson National Accelerator Facility and Brookhaven National Laboratory, as well as the future Electron-Ion Collider.

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

Investigating Microbial Extracellular Electron Uptake from Redox Active Solid Substrates: Mechanisms for Gaining Electrons from Minerals, Electrodes, or Other Microbes

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The ability of microbes to perform extracellular electron transfer—the exchange of electrons with the cells internal redox active metabolic components, with external redox active compounds such as conductive materials—has provided new insight into the diverse respiratory capacities of microbes and fueled the potential for microbe-electrode biotechnologies. Our understanding of the mechanisms of extracellular electron transfer stem from characterization of organisms that respire minerals as a sink for electrons in place of oxygen during respiration. However, microbes are also capable of the reverse process, oxidation of redox active substrates, or extracellular electron uptake (EEU). In this case microbes use an inorganic substrate as an electron source of electrons. The biophysics of EEU in most systems is poorly understood. The overarching goal of this work is to advance our understanding of the genetic and biochemical basis of microbial EEU in microbes across physiologically and phylogenetically diverse strains.

This work builds off our recent high throughput genetic studies. In Shewanella oneidensis MR-1—a model system capable of bi-directional extracellular electron transfer—we recently identified two distinct genes critical for EEU that will be purified to test the biochemical and electrochemical properties using thin film electrochemical techniques. The results of this work will help us understand the role of these proteins in EEU and bi-directional electron transfer—processes important for understanding Shewanella physiology, and its utility for biotechnology applications.

This work will also apply our high throughput genetic techniques (i.e., Tn-Seq) to investigate a novel mechanism of electron uptake in an environmentally isolated marine microbe, Pseudomonas stutzeri—a facultative autotroph capable of processive electron uptake when compared with other model systems. Though exploratory, we expect this work to point to a novel EEU pathway with the potential to expand our understanding of EEU metabolism and biochemistry.

This work will also investigate the EEU phenotypes of proteins implicated in M. barkeri electron uptake from electrodes. Previous electrochemical work in Methanosarcina demonstrated a low redox potential electron uptake process that couples CO_2 fixation to methane production. This work will leverage Methanosarcina gene deletion mutants to investigate the role of specific proteins in EEU. This will provide insights into the potential for non-cytochrome based mechanisms of EEU, and may identify potential targets for engineering enhanced electron uptake rates in Methanosarcina.

The expected outcomes of this work will expand our understanding the mechanisms of EEU in diverse microbial systems. We will gain insight into novel redox processes, as well as the ecology and biochemistry of extremely important, applied and environmentally relevant groups of microbes.

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

Ion Acceleration by Quasi-Parallel Magnetized Collisionless Shocks

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Collisionless shocks are ubiquitous in astrophysical environments, from the bow shock created as the solar wind impacts the Earth's magnetic field to the expanding shockwave of a supernova remnant. Unlike the shockwaves generated by aircraft as they go supersonic, collisionless shocks form through electromagnetic effects in systems where collisions between particles are rare. Additionally, these shocks often form in pre-existing magnetic fields, so that the shock dynamics are highly dependent on the direction the shock propagates relative to the background magnetic field. Of particular interest are quasi-parallel shocks, in which the shock propagates primarily along the background magnetic field, and which are considered a possible source of the some of the highest energy cosmic rays (i.e., ions) observed in the universe. However, we currently lack an understanding of key aspects of how these ions are accelerated to extreme energies, with multiple competing theories and incomplete hints from satellite observations of shocks in space. Additionally, recent advances have enabled collisionless shocks to be created experimentally using high-powered lasers, but quasi-parallel shocks have yet to be created in the laboratory. To address the challenge of quasi-parallel shock acceleration, this research will combine laboratory experiments, state- of-the-art numerical modeling tools, shock theory, and spacecraft observations. The primary objectives will be to demonstrate quasi-parallel shock formation in the laboratory, measure shock-accelerated particles, and compare the results to numerical simulations and observations of astrophysical shocks. To accomplish this, the experiments will use the largest lasers in the world, combined with intense magnetic fields, to achieve for the first time the conditions for quasi-parallel shock formation and particle acceleration. This work will open up a new class of experiments on particle acceleration and will lead to significant advances in our fundamental understanding of strongly-driven, magnetized plasmas.

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

Functionalization of 2D Materials Heterostructures for Solar Energy Conversion

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Solar-driven catalytic water-splitting processes provide clean, renewable, and sustainable forms of hydrogen for generating electricity via fuel cells. The most daunting challenge in the solar-driven catalysis process is the dearth of photocatalysts that simultaneously provide high efficiencies as well as long-term durability in the highly corrosive conditions needed for the photocatalytic reactions. A promising approach to push the limits of solar-energy-to-hydrogen conversion efficiency is to utilize record-breaking photoabsorbers to maximize the capture of sunlight then use an outstanding and robust catalyst to drive the catalytic reaction at a superior reaction rate. However, the interfaces of bulk photoabsorbers and catalysts are poorly understood. This research aims to expand our understanding of heterostructures of record-breaking photoabsorbers, like silicon, gallium arsenide, and cadmium telluride, and two-dimensional (2D) materials which excel as catalysts due to high specific surface area and a wide range of tunable properties. Through high-throughput *ab-initio* simulations and physics-based machine learning modeling, the atomic-scale structure, electronic-structure, and interface physics of 2D-bulk material heterostructures will be studied and curated in an open-source database. The physics-based machine learning models and the computed data will be used for a data-driven discovery of water-splitting photocatalytic heterostructures that push the limits of catalytic reactivity and at the same time yield corrosion-resistant durable heterostructures with massive solar energy capturing capacity. In particular, for this data-driven photocatalytic heterostructure discovery, this research will study (a) the role of an electric field at the 2D-bulk materials interface in enhancing the reactivity of the 2D catalysts, (b) the corrosion-resistance of 2D materials that can form protective barriers to the inherently corrosive photoabsorbers and (c) the fundamentals of heterostructures' interface-physics that yields massive numbers of photogenerated electrons to facilitate the water-splitting reaction.

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

Vibrational Dynamics and Relaxations in Glass-forming Liquids

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The important applications of glasses are ubiquitous in our daily lives, ranging from rewriteable optical storage media to amorphous silicates for optical fibers to encapsulation of nuclear waste. Glasses are solids, like crystals, but uniform and without long-range order, like liquids. The easiest way to make a glass is to heat a material until it is a molten liquid, then cool it to room temperature quickly enough to prevent the atoms from forming a periodic (crystalline) structure. As the liquid cools, it reaches a point when the material stops flowing and becomes a glass. This important transition occurs at the glass transition temperature. How the remarkable properties of glasses arise from the nature of the glass transition is one of the central questions in condensed mater physics. This is a challenging problem to address because the liquid, right before it becomes a glass, is not stable. Observation of the dynamics of the atoms in this unique, metastable phase requires new experimental tools. This research addresses this problem with a cutting-edge application of neutron scattering techniques uniquely available at the Spallation Neutron Source at Oak Ridge National Lab. Experiments on a range of glasses will address gaps in our knowledge of the microscopic dynamics of so-called supercooled liquids near the glass transition. A new understanding of the dynamics of glass-forming liquids will help shape our theories of phase transitions and states of mater and is central to predicting the important properties of glasses that we exploit for a wide range of applications.

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

Quantum Field Theory Tools for Gravitational Wave Science

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The emergence of gravitational wave science has opened a new direction in theoretical high energy physics: leveraging quantum field theory (QFT) to develop new tools for state-of-the-art calculations of gravitational wave signals. Future gravitational wave observatories will detect millions of binary mergers per year with sensitivity far beyond the current limits of the LIGO/Virgo/Kagra (LVK) facilities, ushering gravitational wave science into an era of precision. The possibilities for new and unexpected discoveries in astronomy, cosmology, and particle physics are staggering, but hinge crucially on complementary advances in our theoretical modeling of gravitational wave sources. This research program will apply modern tools from theoretical high energy physics, which have been honed over decades for precision studies of quantum chromodynamics (QCD), to develop a precise and systematically improvable framework for gravitational wave signals. This will complement results from numerical relativity, and enable precision measurements at future gravitational wave detectors, including searches for new physics. In turn, applying QFT in this new territory will uncover new theoretical structures and tools that can deepen our understanding of fundamental aspects of QFT.

This project brings together the mathematical and physical tools of theoretical high energy physics to tackle significant problems in gravitational wave science, with the following objectives: 1) Formulate gravitational wave phenomenology as a problem in QFT, and apply tools from theoretical high energy physics such as effective field theory, scattering amplitudes, and advanced multiloop integration. 2) Provide precise predictions for black hole and neutron star binaries, including corrections from radiative, spin, and tidal effects. These analytic results will complement results from numerical relativity to produce state-of-the-art gravitational waveforms. 3) Identify theoretical structures that emerge in the classical regime of scattering amplitudes and develop them into active tools for computation. Examples are the high-energy limit, and nonperturbative relations to classical solutions and to background spacetimes.

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

Selective Degradation of Polymer Waste to Commodity Chemicals

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While plastics have enabled our modern society, the scale of commercial polymer production, dismal recycling levels, and the absence of environmental degradation pathways have led to the vast accumulation of plastics in the environment. This proposal leverages fundamental principles of organic chemistry to convert polymer waste into valuable commodity chemicals. Using polymer waste as a commodity chemical feedstock lessens dependence on fossil fuels and remediates plastic buildup in the environment. We will develop selective strategies for valorizing polymer waste using the fundamental kinetics and thermodynamics of C–H bonds and abstraction agents. We will convert commercial polymers into divergent commodity chemical streams through selective C–H abstraction and modulation of reaction conditions. We will also demonstrate selective valorization in mixed polymer waste based on kinetic and thermodynamic selectivity principles. Successful demonstration of these fundamental science approaches will motivate new recycling approaches and research into the chemical upcycling of commercial polymer waste.

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

Bulk Synthesis of Rare-Earth-Free Tetrataenite Permanent Magnets

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This project will elucidate the underlying factors driving the recent first bulk synthesis of Fe-Ni L10 ordered tetrataenite permanent magnets, a breakthrough discovery that had been sought for nearly five decades before being announced this last year. Fe-Ni tetrataenite magnets have the potential to replace the rare-earth permanent magnets currently powering electric vehicle motors and wind turbine generators, though the only bulk samples of this material had previously been found in meteorites. Previous bulk synthesis approaches were not able to overcome the extremely long diffusion times (millions of years) required to achieve the L10 ordered phase in the binary Fe-Ni system, since overcome by incorporation of phosphorus within the casting process. Such a scalable casting-based approach defies previous scientific consensus regarding viable processing routes for producing this ordered phase transformation, and at this moment there is little scientific understanding of the underlying mechanisms governing the processing route, which is imperative to further development. This project will test key hypotheses regarding the fundamental mechanisms that have enabled, for the first time, the bulk synthesis of tetrataenite, and identify the combination of factors necessary to reliably reproduce the effect. Through a deeper fundamental scientific understanding of the processing science, the long-term goal is to devise a scalable processing route for bulk tetrataenite permanent magnets tailored to optimize their superior magnetic properties. Fe-Ni is the only known earth-abundant system with the potential to rival the energy product of rare-earth element permanent magnets, which are critical to multiple clean energy technologies and the global transition to renewable energy, yet suffer from strategic supply issues, brittleness, and susceptibility to corrosion.

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

Virtual Scientific Companion for Synchrotron Beamlines

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Synchrotrons are particle accelerators that generate extremely intense x-ray beams to enable discoveries on the atomic and molecular level across energy science, quantum materials, life science, and more. Synchrotron X-rays can, for example, reveal the internal 3D nano-structure of integrated circuits or human cells as well as capture the dynamics of battery or photovoltaic operation. The high demand and oversubscription of these specialized synchrotron beamlines call for dexterous and efficient control of experiments for maximized productivity and sustainable top-level performance. Advances in artificial intelligence and machine learning (AI/ML) can be utilized for effective user facility operations and accelerated material discovery. However, the full potential of AI/ML can only be realized when humans are kept in the loop and natural language (NL) is the most intuitive and efficient way for humans to communicate. This research will introduce a new paradigm of NL-controlled scientific exploration with joint human-AI effort. Specifically, a virtual scientific companion (VISION) based on natural language processing will be developed to transcribe NL voice to text, acquire and analyze data, visualize results, and provide advanced learning algorithms and physics modelling to suggest optimal experiment design or hypotheses. VISION will synergistically partner humans with computer controls for augmented human-AI-facility performance at synchrotron beamlines and beyond, initiating a new era where NL-based communication will be the only needed interface for scientific experimentation and design.

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

The Molecular Building Block Sampling Approach for Polymorphic Free Energy Calculations

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Polymorphism, the possibility of molecular crystals to have two or more crystalline phases with different molecular agreements (e.g., packing and orientation of molecules) but identical in the chemical formulation, has immense scientific and practical importance in chemistry, materials science, and the pharmaceutical and semiconductor industries. Therefore, it is a vital task in the academic scientific field and industry to identify different polymorphs and obtain their thermodynamic properties, such as their relative populations. However, tackling molecular crystals is among the most challenging computational chemistry tasks, especially for flexible molecules exhibiting conformational polymorphism. In this research program, we will develop a novel enhanced sampling method for molecular dynamics simulations called the Molecular Building Block Sampling Approach for tackling challenging temperature-mediated polymorphic transition in molecular crystals that state-of-the-art crystal structure prediction methods cannot describe. This free energy method will give us access to thermodynamic properties such as free energy landscapes and relative stabilities of polymorphs at finite temperatures. The novelty of the technique lies in biasing directly local order parameters that can describe both the inter-molecular and intra-molecular degrees of freedom of the molecular building blocks of the crystal. This is a paradigm shift compared to conventional enhanced sampling methods that employ global collective variables that describe the state of the whole system. The outcome of this research program will be a novel enhanced sampling method for tackling challenging polymorphic transition that can be applied to a wide range of experimentally relevant molecular crystal systems. All methodological development resulting from the proposed project will be made publicly available in open-source codes such as the PLUMED enhanced sampling code.

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

Exploring Nonlinear Electrodynamics in Layered Topological Semimetals at Radio Frequencies

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Nonlinear light–mater interactions in the RF frequency range have become an important research frontier for the advancement of quantum information and energy-sustainability technologies, such as superconducting qubit coupling, nonlinear parametric amplification, and RF energy harvesting. These functionalities require the presence of strong nonlinearities at RF frequencies, which are, unfortunately, very limited. This research program aims to investigate novel quantum-geometrical properties and the associated nonlinear RF processes in emergent layered topological semimetals. These materials arise as a new and promising platform owing to their exotic topological band structures and large quantum geometry, which can significantly influence and potentially enhance nonlinear light–mater interaction in the RF regime. The study will focus on characterizing, modeling, and understanding the fundamental relationship between RF electrodynamics, lattice symmetry, and quantum geometry. In addition, the project will unravel the fundamental mechanisms and quantify the contributions of various intrinsic factors and external stimuli on the nonlinear RF process. To achieve this, we will employ a combination of advanced spectroscopies and transport measurements. The success of this research will advance the understanding of nonlinear phenomena in quantum materials and establish a foundation for the development of broadband, powerless, and efficient energy microelectronics.

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

Probing Electronic Structure in Actinide-Transition Metal Nitride Clusters

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How metals interact with one another affects observed physical properties, such as magnetism. Systems with short metal-metal distances, including metal-metal bonding, tend to exhibit unusual physical properties. The bonding of the actinides is intermediate between the largely covalent transition metals (TMs) and the largely ionic rare earths, leading to the "f-electron problem", which is how much or how little the f-electrons participate in bonding interactions. Recent attention has focused on the bonding and electronic structure of mono-metallic actinide (An) complexes. Unprecedented physical properties have been observed in AnTM alloys, but the insolubility of the later has prevented detailed studies, which will be reflected by this research. The more covalent TMs are generally better at sharing and delocalizing electrons, while the more ionic rare earths typically exhibit highly localized electrons. Using a molecular platform of small cluster complexes with three or four metals, the electronic communication and f-electron (de)localization for homometallic U or Pu clusters will be examined. Study of analogous heterometallic Ti- U and Ti-Pu compounds will give insight to An-TM interactions. Direct TM-An and An-An interactions are poorly understood. Studying intra-metal interactions gives insight to energy generation, nuclear fuel cycle efficiency, and better catalyst design.

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

Luminosity Maximization with Flat Hadron Beams

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The US Electron-Ion Collider (EIC) has been approved by the Department of Energy as the next major scientific facility. The EIC to be built at Brookhaven National Laboratory (BNL) will serve as an ultimate electron microscope to probe the detailed physics inside the nucleus. The success of a collider is measured by its luminosity, which quantifies the number of physics events generated during collisions. The EIC plans to achieve high luminosity by utilizing a flat hadron beam, aligning it with the electron beam to enhance interactions. However, a flat hadron beam has never been demonstrated in a real machine. Maintaining a flat hadron beam presents challenges. The phenomenon of emittance growth and coupling can result in an increase in the vertical size of the beam, ultimately causing the flat hadron beam to become disrupted. This project focuses on investigating factors that can cause emittance growth and coupling in a hadron storage ring, specifically looking at intra-beam scattering, magnet non-linearity, and beam-beam interaction. By conducting experiments at the Relativistic Heavy Ion Collider (RHIC) and developing a powerful simulation code, researchers aim to better understand and control these phenomena. The insights gained from this project have the potential to improve the design and operation of future colliders and advance simulation tools for scientific research.

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

A Programming Framework for Large-Scale Graph Data Analytics on GPUs and New AI Accelerators

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Graph-theoretic algorithms and graph machine learning models are essential tools for addressing many real-life problems, including scientific ones such as bioinformatics, genomics, climate science, and combustion science. DOE's Office of Science has prior investments in large-scale graph analytics such as the EDGAR and ExaGraph projects, and the CSCAPES institute, but these efforts aimed at isolated tools for a limited number of graph analytic algorithms. In contrast, this ECRP project aims to develop a general programming framework called Graph4All that (1) makes it easy to implement various graph-theoretic algorithms and graph machine learning models, and that (2) scales well with computing resources including GPUs and AI accelerators invested in by DOE in recent years for supercomputing. This is especially important to fully unleash the supercomputing power at DOE, such as the GPU-rich supercomputers and ALCF AI testbed.

There are, however, challenges in implementing such a programming framework since graph algorithms are inherently heterogeneous. We identify three categories of graph operations frequently used in a real graph analytics pipeline: (1) vertex analytics, (2) structure analytics, and (3) graph machine learning. These operations are often related and used together in a graph analytics pipeline. Currently, the think-like-a-vertex (TLAV) computing model dominates the market of graph-parallel systems, but they are inefficient for structure analytics. Moreover, there lacks a TLAV system that effectively utilizes sparse-matrix-based operations on GPUs to speed up graph computation. The PI pioneered a new think-like-a-task (TLAT) computing model for structure analytics, but the model relies on backtracking search which is not suitable for GPU execution. Industrial systems for training big graph neural networks (GNNs) are based on cloud infrastructures rather than GPU supercomputers, and they are still diverged in the design choices.

Graph4All will be general by providing convenient programming models such as TLAV, TLAT and aggregate-update for users to write their parallel graph algorithms easily, and run at scale efficiently on GPU supercomputers and new AI accelerators. The software stack of Graph4All will follow a layered design to maximize module reuse. The technical merit and novelty of Graph4All are: (i) Graph4All aims to become a unified programming framework for heterogeneous graph operations in all types of vertex analytics, structure analytics, and graph machine learning, where each graph operation can be implemented with its most proper programming model to maximize out the efficiency on CPUs, GPUs and new AI hardware. (ii) Graph4All addresses the challenge of adapting backtracking-based TLAT systems for GPU execution, by designing a new GPU-efficient subgraph-extension execution framework that operates on subgraphs. To address the challenge that GPUs have limited global memory while subgraph extension may generate huge numbers of intermediate subgraphs, advanced techniques are designed including chunking with a dynamic chunk size adjustment strategy, and expansion-prefix sharing to reduce the redundant space and computation. A hybrid CPU-GPU computation solution will be explored to utilize both CPUs and GPUs. (iii) hardware-efficient execution methods will be designed for the TLAV computing model, such as GPU execution based on SpGEMM, and tensor-algebra formulation for execution on new AI hardware. (iv) GPU-efficient distributed GNN training methods will be designed to minimize data transmission and maximize efficiency, with techniques such as hybrid

model parallelism + data parallelism, vertex embedding caching with bounded staleness, mini-batch sampling, and subgraph partition shrinking with GNN layer number. Distributed GNN inference will also be optimized using machine learning compilation. (v) The project will explore graph compression and gradient compression techniques, graph visualization functionalities based on WebGPU, and a topology-aware communication scheduling.

Graph4All will have significant and broad impact since (i) it will be the first comprehensive and unified framework supporting all operations in vertex analytics, structure analytics, and graph machine learning, which are frequently needed to work together in a graph processing pipeline, (ii) it will be the first comprehensive framework supporting these operations on GPU supercomputers, (iii) as a software infrastructure, its programmability and extensibility will significantly speed up graph-parallel research in ASCR area, especially facilitating the use of GPU supercomputers and new AI hardware, (iv) the tools developed on top of Graph4All will allow domain scientists to conveniently customize and combine them to conduct flexible graph analysis pipeline, to speed up scientific discovery with minimal efforts.

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

Interactions of QDs' Fast Light in Rb Vapors for Hybrid Quantum Information Science and Technology

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One of the fundamental challenges towards implementing scalable Quantum Information Science and Technology (QIST) systems is to distribute entanglement in a fast and reliable way. To achieve this, key developments are required, mainly, quantum light sources emitting identical single photons at telecommunication wavelengths, and stationary-to-flying qubit interconnects. This project addresses these challenges by developing fast light-matter interconnects made of alkali atomic ensembles and quantum dots (QDs) single photons. This hybrid system combines advantages of the long coherence times and ease of operation of alkali memories with excellent light emission properties of self-assembled semiconductor QDs. To enable these and address current limitation of QDs technology, we will co-design photon sources to be suitable to work at telecommunication and atomic wavelengths. Additionally, we will engineer devices to ensure spectral and bandwidth tunability of the fast photons. We will then investigate the interaction of the co-designed fast photons with atomic vapors theoretically and experimentally, using quantum optical techniques, such as time-resolved interferometry and spectroscopy. This project will bring fundamental understanding of interactions between fast photons and atomic vapors that can be used for QIST applications in quantum-secure communication, distributed quantum computing, and quantum sensing.

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

Multiscale Ecosystem for Molecular Quantum Electrodynamics

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The control of chemistry and molecular properties with light has been a long-standing Holy Grail for decades. Only recently, new possibilities have emerged with polariton chemistry, where quasiparticles known as polaritons form due to strong coupling between molecules and the quantized radiation field inside an optical cavity. Theoretical investigations, especially on-the-fly simulations of polariton dynamics, are essential to understand the underlying mechanisms and universal features of such hybrid light-mater systems. However, the complexity of these systems, marked by multiple coherent and dissipative interactions across different time and length scales, makes modeling a significant challenge. In response to this multiscale challenge, we propose to develop a comprehensive, scalable multiscale ecosystem bridging quantum optics, computational electromagnetics, and quantum chemistry. The aim is to deliver advanced multiscale modeling capabilities for describing self-consistent interactions in light-mater hybrid systems within the rigorous framework of molecular quantum electrodynamics on DOE exascale computers. We plan to create a modular and scalable package, facilitating transferability to any new hardware without extensive recoding and allowing for easy inclusion of new advancements. Such developments will leverage our experiences developing nonadiabatic dynamics, exascale computing, multiscale modeling, molecular quantum electrodynamics theory, and high-performance computing facilities at Los Alamos National Laboratory. Envisioned applications to molecular systems such as organic donor-acceptor aggregates will demonstrate the ability to steer fundamental energy and charge transport processes and modify the outcome of photochemical reactions. The successful completion of this project will substantially enhance current theoretical and modeling capabilities for polariton chemistry. It will move beyond widely used approximations, ensuring self-consistency between light and mater, deepening our understanding of recent experiments in cavity-modified chemistry, and facilitating the design of innovative materials through strong light-mater coupling. Moreover, the developed multiscale modeling can be applied to broader light-mater interaction problems (such as plasmon chemistry, light-control of quantum transport, and photon-mediated information transfer/transduction), benefiting fields such as chemistry, physics, materials, energy, and quantum information science.

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

Using Kilometer-Scale E3SM to Investigate Air Pollution Impacts on Coastal Storms

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Coastal urban communities face a significant threat from the combined forces of air pollution and coastal storms. There is an ongoing debate among scientists regarding the potential link between human- generated air pollution and the intensification of storms. This phenomenon, known as the aerosol invigoration effect, has the potential to wreak havoc on our coastal urban areas, putting economies and properties at risk. Unfortunately, current global climate models cannot represent this effect due to the coarse grid resolution that fails to capture the intricate details of storm dynamics and microphysics. With advancements in computational power, a new generation of climate models has emerged, allowing for more detailed and accurate simulations at the kilometer scale. One such model is the DOE's Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM). Motivated by this new opportunity, this project plans to use SCREAM within a hierarchical modeling framework to assess the magnitude of the aerosol invigoration effect on coastal storms and gain a mechanistic understanding of the impacts. To that end, a series of observation-informed numerical experiments will be performed to evaluate the fidelity of the SCREAM in reproducing observed coastal storms, elucidate the physical mechanisms behind the invigoration effect, and examine how large-scale dynamics modulate this phenomenon. These modeling activities will improve the predictability of coastal-urban systems by (1) advancing fundamental understanding of air pollution impacts on coastal storms and (2) establishing a well-tested analysis framework for guiding the development of DOE high-resolution models.

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

Imaging Emergent Phenomena in Two-Dimensional Magnets Using Single-Spin Quantum Microscope

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In the last few decades, unprecedented progress has been made in controlling the quantum coherence of single electrons or atoms, and moreover in observing the quantum correlations between them. These advances present opportunities for a new era of "quantum sensors" that exploit the extreme sensitivity of electron states to their environment, achieving resolutions that are ultimately limited by the duration with which such states can remain quantum coherent or by the number of such states that can be entangled. The objective of this research project is to leverage the exceptional attributes of the nitrogen-vacancy (NV) center in diamond, possessing a coherent single electron spin in a robust solid-state form factor, for the high-resolution and high-sensitivity magnetic imaging of novel material samples. A unifying theme is to transcend now well-established measurements of static magnetizations in single two-dimensional materials by exploring emergent magnetic phenomena that arise under nonequilibrium optical excitation or through superconducting proximity effects and twist engineering. The project will identify novel, energy-efficient mechanisms to toggle magnetic devices through a unique pump-probe optical platform. In addition, it will address key questions on the reproducibility of exotic transport phenomena through the NV center's capability to resolve micro to nanoscale inhomogeneity, extricate current flow from static magnetization, and operate with continuous field and temperature tuning. More broadly, the project will advance measurement schemes to expand the scope of applicability of NV magnetometry to condensed mater systems and contribute to the preparation of a trained workforce at the forefront of technological progress.

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

Advancing Quantum Sensors and Sensor Networks with High-Efficiency Transduction

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Quantum transducers enable the conversion of quantum information and signals between different physical platforms. In the field of sensing, microwave-optical quantum transducers are particularly significant in expanding the capabilities of superconducting quantum sensors, as they combine the strengths of microwave and optical photons. This research program will significantly improve the bidirectional conversion efficiency between microwave and optical fields, advancing quantum sensors and distributed sensor networks for dark mater searches and addressing technological requirements for fundamental physics experiments, including counting single photons and amplification without adding noise. To accomplish these objectives, novel techniques utilizing hybrid platforms are envisioned. These platforms integrate quantum devices based on superconducting radiofrequency (SRF) cavities with very long photon lifetime and electro-optic converters. Extensive simulations and analyses demonstrate that this approach can achieve high conversion efficiency while operating at the quantum threshold. This work will significantly enhance the sensitivity of dark mater searches, including axion-to-photon conversion (haloscope) experiments, by converting microwave signals into optical photons and improving single-photon detection beyond the limitations of the Standard Quantum Limit (SQL). The outcome of this research will have broader applications across various scientific fields and will impact critical areas such as national security and quantum communication.

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

Ultrafast Mechanisms of Chirality Control in Electronic Materials

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Exploring and controlling the chiral properties of materials through light-mater interactions represents a critical frontier in materials research. Chiral phases, characterized by distinct left or right-handed states, hold tremendous potential for transformative applications in fields such as optoelectronics and quantum technologies. Chirality can be understood as a property that distinguishes an object from its mirror image, much like our hands. For example, a chiral molecule or material cannot be superimposed onto its mirror image. This research aims to understand and manipulate chiral order that emerges in several quantum materials with diverse structures and length scales. By employing advanced techniques such as extreme-ultraviolet ultrafast spectroscopy and ultrafast electron diffraction, we will investigate the emergence, stabilization, and dynamics of chiral order during and following light-mater interaction. This research harbors tremendous potential for scientific breakthroughs and technological advancements. By unraveling non-equilibrium chiral states, we will gain profound insights into the structure-function relationship of chiral quantum materials. The findings will pave the way for innovative applications, including optically rewritable non-volatile memories and energy-efficient computation units based on switching chiral order operating at high speeds, surpassing conventional electronics. Moreover, our investigations into chiral dynamics and the emergence of order in materials with varying length scales will drive the exploration of tailored chiral material systems to meet specific technological demands.

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