Optical Quantum Sensing in Molecular Assemblies

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This project aims to create a novel class of highly sensitive, deployable quantum sensors using spin-polarized electrons and nuclear spins within molecular assemblies. Molecular quantum sensors offer unique advantages over traditional sensing technologies. The inherent synthetic versatility of molecular systems allows precise spin placement, orientation, and connectivity, and also enables them to sustain nuclear spins with remarkably long intrinsic lifetimes, sometimes extending to several hours. These characteristics together provide a compelling opportunity to directly correlate spin properties with molecular design, promising substantial improvements in sensitivity and enabling new sensor deployment modes for novel application areas.

Several critical scientific and technical hurdles must be overcome to realize the full potential of molecular quantum sensors. This project addresses these challenges through three complementary research thrusts. First, this research will develop a thorough understanding of decoherence mechanisms in molecular spin systems. By employing long-lived nuclear spin states as sensitive probes, studies will identify dominant relaxation pathways and investigate their influence by temperature, magnetic fields, and doping concentrations. Second, investigations will focus on maximizing sensor packing, exploiting unique features of molecular systems to facilitate control over sensor spacing and orientation. Third, molecular quantum sensors will be deployed across various length scales—from nanoscale molecular architectures to mesoscale assembled structures and microscopic droplet emulsions. These platforms will significantly extend capabilities for physical and chemical sensing, including high-resolution magnetometry and precise detection of chemical analytes.

To accomplish these objectives, the project will employ state-of-the-art in-house instrumentation, including electron paramagnetic resonance (EPR), nuclear magnetic resonance (NMR), and optical spectroscopy, enabling precise probing and control of electronic and nuclear spins under diverse temperature, magnetic fields, and spatial length scales.

Ultimately, this research will yield a deeper fundamental understanding of decoherence in molecular quantum systems, provide novel strategies for optimizing sensor density and deployment, and enable novel dynamically stabilized non-equilibrium quantum states for enhanced sensing. The insights and technologies developed will broadly impact quantum science, supporting superior qubit designs, advanced quantum control methods, and "hyperpolarization-enhanced" NMR and EPR spectroscopies, directly advancing DOE missions across multiple scientific domains.

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

Breaking Rules of Actinide Chemistry with Extreme Conditions

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Actinide elements (elements with atomic numbers 89–103) are central components of nuclear technologies, either as fuel sources or as products of nuclear reactions. Significant unknowns persist in the chemistry of actinide elements with higher atomic numbers in part because their f-electrons defy models which apply to lighter elements, defining the “f-electron challenge”. Among these late actinides, americium (Am) holds a special position. Its properties classify it as a late actinide with reactivity that is distinct from the earlier members of the actinide series. It is also one of the heaviest elements for which bulk chemical manipulation is feasible, enabling further discovery of novel systems that break the established “rules” of actinide chemistry.

While Am chemistry is often described in comparison to lanthanide elements (atomic numbers 57–71), this research will use high-pressure techniques to reexamine the “lanthanide-like” analogy and uncover the subtle differences which are nevertheless crucial for selective chemistry. Pressure acts as an incrementally tunable handle for electronic energy, driving fundamental changes in chemistry and electronic structure that depend on the specific character of the valence electrons. This project will harness this distinct response to reveal differences between actinide and lanthanide complexes. Crucially, study of how a single chemical system changes upon compression provides a direct and self-referential comparison of properties across distinct electronic structures. The insight this engenders will help bridge the gap between predictions and the unique behavior of actinide elements with far-reaching implications for the safe handling of these elements in applications ranging from nuclear waste remediation to critical material separations and quantum information science.

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

Development of Efficient First Principles and Machine Learning Methods to Study and Predict Magnetic Topological Materials Exhibiting Dual Berry Phase Effects

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Next-generation quantum technologies—ranging from low-power microelectronics and robust spintronics to quantum computing—require a new class of materials with emergent functionalities. This project addresses that need by developing an integrated suite of advanced theoretical and computational methods to discover and design materials that exhibit both real-space and momentum-space Berry phase effects. Building on cutting-edge electronic-structure calculations, advanced machine learning methods, and large-scale numerical techniques, we will investigate the interplay between localized spin order and itinerant electronic degrees of freedom in a unified framework. Our goal is to identify the conditions and material platforms under which topological spin textures (e.g., skyrmions) strongly couple to Dirac/Weyl band structures, thereby revealing emergent phenomena that could enable dissipationless transport, novel magnetic textures, and enhanced quantum coherence.

We will systematically explore 4*f*-electron intermetallic systems—particularly Eu-based compounds such as EuAuSb and EuAuP—that hold promise for coexisting topological band structures and chiral spin orders. In this effort, we will use spin-fermion modeling informed by *ab-initio* calculations, incorporating neural-network potentials, Bayesian optimization methods, and GPU-accelerated solvers to efficiently navigate the phase space of multi-parameter electron-spin Hamiltonians in large unit cells. Key predictions regarding anomalous and topological Hall signals, spin-wave dispersions, and skyrmion lattices will be validated through collaborative experimental measurements. Our project aligns with the U.S. Department of Energy's strategic priorities in quantum materials, exascale computing, and machine-learning–assisted materials discovery.

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

Chemical Vapor Deposited superconductors on Cu-based cavities for compact superconducting radio frequency accelerators

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Superconducting radio frequency (SRF) technology enables the efficient conversion of radio frequency energy into beam energy, allowing for the production of high-power electron beams (e-beams). Currently, SRF technology, which uses pure niobium (Nb) with a superconducting transition temperature (T_c) of about 9.2 K, has been successfully developed for particle accelerators in nuclear and high-energy physics research. However, Nb-based accelerators operate at very low temperatures and require complex, large liquid helium (He) cooling systems, posing a significant barrier to the broader adoption of this superconducting technology. Using higher T_c superconductors in SRF accelerators, along with more accessible highly conducting copper-based materials, can eliminate the need for continuous liquid He cooling, resulting in more compact accelerator systems. A smaller SRF-based accelerator will revolutionize existing e-beam irradiation technologies, including applications in the food industry, medical device sterilization, wastewater treatment, and others.

This project will develop techniques to deposit high-quality, high-T_c compound Nb_3X (X = Sn, Ge, Al) superconducting films on copper-based cavities while addressing fundamental material defect limitations. Chemical vapor deposition (CVD), a scalable technique, will be used to deposit a high-temperature superconducting film ($T_c > 18$ K) less than 2 microns thick on high-conductivity copper substrates. This work will build on current advances and improve our understanding of the trade-offs and fundamental limits of thin film depositions for SRF applications. The project will actively involve industry stakeholders in translating basic research results and techniques into complex accelerator shapes for larger-scale commercial deployment.

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

Probing Dark Energy with Strong Gravitational Lensing in the era of the Vera C. Rubin Observatory

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The phenomenon of strong gravitational lensing is a powerful probe of the expansion history and scale of the Universe. The Vera C. Rubin Observatory, and its Legacy Survey of Space and Time (LSST) is going to discover tens of thousands of strong gravitational lenses, more than 200 lensed quasars, and about one hundred multiply imaged lensed supernovae per year. These numbers correspond to several e-foldings of lenses being used compared to current state-of-the-art studies. One key limitation of using strong gravitational lensing is the mass-sheet degeneracy (MSD). The research will use galaxy-galaxy weak gravitational lensing measurements of the deflector galaxies to contain the MSD. This research will test and deploy an end-to-end workflow from the LSST DR1 & DR2 data products combining strong and weak lensing measurements to provide a precise and accurate measurement of dark energy and the Hubble constant.

A measurement of time delays from a strongly-lensed multiply-imaged time-variable sources is an absolute distance indicator. The change in Einstein radius as a function of source redshift is a relative distance indicator. This proposal addresses two key limiting factors of such an analysis: (i) The radial density profile of the strong lensing deflector needs to be known precisely to accurately predict the time delays, while the strong lensing observables do not have access to this information due to the MSD. Stacked galaxy-galaxy weak lensing measurements from small to large angular scales with LSST data is able to break the MSD and contain the uncertainty on the time delays to $\sim$ 1% (Khadka et al. 2024). (ii) Strong lenses are rare and inherently a result of a selection effect in the tail of the large-scale structure mass distribution. It is crucial to understand the selection effects in the lens discovery channel to apply the needed corrections in the inference. The overarching methodology of this research is to integrate the lens search, analysis, weak lensing deflector selection, and cosmological inference components in one integrated pipeline. The research program will perform a lens search and modeling analysis based on LSST DR1 &DR2 data. All our analysis choices and population-level parameters are propagated through an end-to-end population-level simulation and compared with the discovered lenses in the LSST data set, effectively correcting for population biases. In parallel, this research will select a larger sample of self-similar deflector galaxies to perform a galaxy-galaxy weak lensing mass density profile measurement from LSST data. The relative selection function between strong and weak lensing measurements will be accounted for with the same full population-level simulation tools. Finally, the bias-corrected sampling over lensing deflector population hyper-parameters and cosmological parameters will be conducted. The time-domain data allows measurements of time delays to constrain an absolute distance, the Einstein radii distribution allows for a relative distance tomographic analysis, and finally the weak lensing data enables the MSD to be constrained to the percent level.

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

Designing Site Ensembles for Efficient Plastic Upcycling to Fuels

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Developing new methods to take complex polymeric mixed materials and convert them into chemical and fuel is challenging due to a myriad of technological and scientific issues, including the presence of mixed waste streams, contaminants, and difficulties processing polymer chains. Nanoporous solid acids, such as zeolites, are catalysts that can cleave strong carbon-carbon bonds in polyolefins, but their nano-confined structures hinder access of polymer chains to acid sites. The interplay between polymer diffusion and acid site reactivity ultimately determines the selectivity towards desired hydrocarbon products. Designing catalysts that selectively produce fuel-grade hydrocarbons requires new kinetic models that incorporate both polymer diffusion and acid site reactivity.

This project leverages advanced computational modeling and machine learning to predict the selectivity and reactivity of zeolite catalysts towards fuel-range hydrocarbons from polyolefins feedstocks. Kinetic models for depolymerization derived from theory and simulation would be transformative for catalyst discovery and optimization, yet conventional computational catalysis models face limitations for coupled reaction and diffusion. This limitation constrains the discovery of new depolymerization catalysts, as reaction and diffusion events are intrinsically convoluted in experimental observations. The modeling and kinetic theories developed in this project will advance catalyst discovery by disentangling the catalytic significance of reaction and diffusion in nanoporous catalysts. The fundamental kinetic insights obtained in this project can be applied beyond nanoporous catalysts to liquid-phase thermal and electrocatalysis on surfaces of impact to many chemical industrial applications.

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

Surface-Inspired Catalysts for Carbon Oxygenate Reduction to C_{2+} Products

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Electrochemical CO_x reduction using earth-abundant complexes presents an attractive platform for efficient formation of precursors to chemicals and fuels, simultaneously addressing energy security and industrial competitiveness. To date, the most promising catalysts for CO_x conversion to C_{2+} products—which boast higher energy density and therefore greater value—have been copper-based heterogeneous materials. However, how copper achieves these complex multi-proton/multi-electron transformations remains unknown. The objective of this work is to utilize atomically precise molecular copper clusters to map out fundamental reaction mechanisms pertinent to CO_x upgrading. Acting as excised active sites of the heterogeneous materials, these cluster architectures provide detailed insight into key bond-making and bond-breaking transformations that require multi-point cooperative binding interactions absent in mononuclear homogeneous systems. Moreover, the ability to control catalyst uniformity, combined with atomistic-level understanding, will facilitate rational development of selective catalysts for multicarbon product generation. This work will inform the convergence of molecular and solid-state catalysis as a means of discovering novel technologies for selective, scalable, and efficient energy-relevant transformations.

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

Examining Field-Altered Solvation for Contaminant Capture and Critical Element Recovery

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Solvation of dilute, high value targets such as rare earth elements (REEs) and fluorinated contaminants from aqueous samples is a critical challenge in separation science. Important solvent parameters, including pH and ionic strength, influence the chemical speciation and solubility of these molecular targets. These hinder the effectiveness and reproducibility of current separation processes including capture, especially when recovery from waste streams is sought. Recently, magnetic (B) field treatment of complex liquid mixtures and soft materials was shown to exhibit extraordinary impacts on resulting properties such as material durability, filter lifetime, and plant metabolism, over wide-ranging pH and ionic strength conditions. While the mechanisms underlying these behavior changes are unknown, the observed B-field effects clearly depend on solute-solvent interactions and solute identity. This project aims to elucidate how magnetic fields alter the solvation and aggregation behavior of high value separation targets such as REEs and fluorinated contaminants in complex aqueous systems and to subsequently exploit this B-field control to modulate separation efficiency and reproducibility. Spectroscopic tools and neutron and X-ray scattering measurements are expected to reveal how B-fields alter solvent orientation and hydrogen bonding, change the solvent and solute electric and magnetic dipolar character, and distort the solute molecular conformation and hydration shell, both in bulk solution and at solid-liquid interfaces. Beyond developing an understanding of how the chemical, structural, and dynamical properties of the system change, the alteration of solubility and solute aggregation at or near ambient conditions using B-fields could yield a novel, non-thermal separation mechanism that overcomes current challenges offered by traditional, energy-intensive separation processes.

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

Studying Moiré Quantum Phases with in-situ Sliding Tip Galvanometry

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Two-dimensional quantum materials are ultimately thin materials with outstanding performance in terms of their electronic, optical and mechanical properties. It was recently discovered that the twisting between two-dimensional materials offers further control over their band structures and many-body correlations via moiré effects, which allows the creation of a plethora of exotic quantum states, including unconventional superconductivity, strongly correlated phases, and fractional quantum states. This research project will use novel scanning microscopy techniques to study emerging quantum phenomena that exist in moiré matter beyond twisting. This research will use recently developed microelectron-mechanical system (MEMS)-based manipulators to develop a novel scanning microscopy approach called sliding tip galvanometry (STG) that enables *in situ* study of electromechanical behaviors in moiré materials with high spatial resolution and unprecedented degree of control, both electrically and mechanically. STG will be used to investigate quantum phenomena in graphene and transitional metal dichalcogenide heterostructures. The research will first explore novel electromechanical transduction mechanisms based on topological charge pumping effect, which is a process where electronic charges are transported across insulators in a quantized manner. Using this quantization, the goal of this research is to further study the spin and charge orders in the correlated energy gaps of twisted moiré materials to gain insight into their underlying mechanism. STG will also be used to study ferroelectric two-dimensional materials to understand nano-actuation and to further tailor moiré quantum materials. The results from these studies will answer fundamental questions about moiré physics and give new insight into the electromechanical coupling at two-dimensional interfaces, which is highly relevant to quantum technologies and energy science.

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

Fundamental Physics at the Quantum Limits of Measurement

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Quantum sensing technologies, which leverage non-classical states of light and matter, are a crucial ingredient in the search for new fundamental physics. While quantum sensing protocols have been constructed on paper, applying them in realistic experiments has proven to be extremely challenging, particularly due to the presence of noise and spurious background signals in real devices, and due to difficulties integrating the quantum devices with more traditional sensors. We will overcome these challenges and apply quantum sensing to a classic challenge of particle physics: detection of small recoils from single-particle interactions.

Specifically, we will construct an optically levitated nanomechanical sensor whose motion can be monitored with an accuracy limited by its quantum zero-point motion. The nanoscale mechanical element will be doped with radioactive elements, which will regularly decay and emit particles. At this quantum-limited measurement sensitivity, each nuclear decay event can be detected and recorded with very high precision. This device, integrated with a pixel calorimeter to detect any ejected nuclear decay products, can serve as a probe of numerous high energy physics (HEP) targets, in particular heavy sterile neutrinos, in currently unexplorable parameter space. Working towards an implementation of mechanical state squeezing to perform such a search at impulse thresholds below the standard quantum limit set by zero-point fluctuations, we will implement a plan that combines theory, simulation, co-design, and prototyping. The central technological goal will be a demonstration of mechanical squeezing at a few dB below the quantum zero-point in this system, bringing true quantum advantage into the domain of particle detection.

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

Radiation-Induced Heterostructure Formation

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Structural metallic materials for nuclear fission and fusion systems must withstand sustained irradiation at high temperature over long periods of time. In current alloys, the nanometer-scale defects induced by particle irradiation eventually lead to embrittlement and loss of mechanical integrity over time. So far, material design strategies to mitigate this effect have focused on introducing microstructural features through alloying or processing pathways, to either slow down irradiation-induced defects, or eliminate them into sinks before they can agglomerate and become deleterious. However, these features often suffer from their own instability in service and can only delay damage formation.

This project provides the fundamental science underpinning a new design approach to engineer radiation-tolerant alloys by leveraging radiation-induced phase decomposition (RIPS). The central hypothesis is that initiating RIPS in an originally single-phase and chemically homogeneous alloy will promote the spontaneous formation of a dense network of stable sinks during service. This strategy represents a new paradigm as it utilizes radiation as an intrinsic vector for sink formation, rather than conceptualizing it as a deleterious phenomenon and combatting its effects.

This research seeks to establish a fundamental understanding of the mechanisms that govern RIPS in a set of iron-copper-nickel-chromium (FeCuNiCr) alloys, taken as model materials. The work will focus on elucidating how the interplay between irradiation species, flux, dose, and temperature, drives phase separation under irradiation. Advanced electron microscopy techniques will be employed to characterize the irradiated microstructures from the macroscopic down to the atomic scale, and determine the governing physics of RIPS. These will be paired with nano-mechanical testing to quantify the strength and ductility of these novel materials. This work is anticipated to pave the way for the design of a new class of radiation-tolerant materials, that spontaneously form stable micro- and nanostructures in extreme environments, healing damage as it occurs.

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

Conductive Chiroptical Polysaccharides for Dynamic Infrared Electro-Reflectivity

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This project explores a new class of bio-inspired materials that combine the self-assembly and optical behavior of naturally occurring polysaccharides with the electronic functionality of synthetic conducting polythiophenes. The scientific objective is to create hybrid copolymers that conduct both ions and electrons while interacting with light in tunable and dynamic ways. A central focus is understanding how the helical order of the biopolymer backbone is maintained and propagated across larger length scales, even after the introduction of conducting sidechains, and how self-assembly affects charge transport. Chitosan, a polysaccharide derived from chitin, naturally forms helical structures that organize into chiral nematic liquid crystals, a state of matter with both fluidity and long-range helical ordering. These structures reflect specific wavelengths and polarization states of light and respond to environmental changes. However, chitosan is a poor conductor of both ions and electrons. To address this, this research relies on the chemical grafting of polythiophene sidechains onto the chitosan backbone. This design leverages chitosan's self-assembly to guide the organization of the sidechains, promoting close packing and efficient charge transport. This will be explored through three interconnected objectives: (1) developing scalable methods to graft polythiophenes onto chitosan and evaluating how composition affects self-assembly; (2) investigating how helical and liquid crystalline structures influence light absorption, emission, and reflection; and (3) exploring how multiscale order and mixed conduction affect performance and tunability under electric fields. This work aims to establish design principles for creating responsive, chiral materials that expand the capabilities of organic electronics and biopolymer-based energy devices.

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

A High-Dimensional Rydberg Quantum Simulator for Probing Gauge Theories and Their Dynamics

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Understanding nuclear physics from first principles remains one of the most significant challenges in modern science. The strong nuclear force, which binds protons and neutrons into atomic nuclei, is governed by quantum chromodynamics and gauge theories. While classical computers have made progress in calculating thermal-equilibrium properties of nuclear systems, simulating real-time, non-equilibrium dynamics--such as particle collisions, vacuum decay, and matter formation in the early universe--requires computational resources that scale exponentially with system size and evolution time, rendering these processes inaccessible to classical methods. To address these challenges, this research will employ a scalable, high-fidelity quantum simulator to study advanced nuclear physics models based on lattice gauge theories in regimes where classical computation struggles. On the hardware side, the research will leverage the unique capabilities of a Rydberg-atom quantum simulator that can rapidly assemble and control two- or three-dimensional qubit arrays using a fast, AI-optimized spatial light modulator. On the control side, the project will implement a time-varying optimal quantum control strategy based on periodic driving (known as Floquet engineering), combined with real-time qubit transport to establish long-range entanglement. This hardware-control co-optimization approach will enable effective all-to-all connectivity and support the generation of complex multi-body interactions that go beyond conventional two-body interaction models. To quantitatively certify experimental results, the research will utilize efficient system-level benchmarking and entanglement characterization protocols. The integration of large-scale qubit arrays, novel multi-body interactions, and robust validation tools will significantly advance the feasibility of simulating complex gauge theories both in and out of equilibrium, bridging the gap between quantum simulation and real-world nuclear physics, and moving toward practical quantum advantage.

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

Programmable Floquet Algorithms for Materials Research: Enhanced Qubit Coherence and Entangled State Preparation on Quantum Hardware

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Programmable noisy intermediate-scale quantum (NISQ) devices offer exciting possibilities for studying questions of both fundamental and practical importance in quantum materials research. Traditional theories based on weakly interacting particles struggle to explain experiments on strongly correlated quantum materials, such as Mott insulators with localized magnetic moments. Despite advances in theoretical methods and quantum simulation experiments, a breakthrough in materials research has remained elusive. While practical quantum applications typically require stable quantum bits with long coherence times, this research proposes innovative programmable algorithms that can harness the power of imperfect quantum simulators to tackle complex materials problems. The focus will be on studying models of quantum materials where the combined effects of competing interactions, strong correlations, and disorder create novel forms of quantum entanglement that go beyond conventional theoretical frameworks. This project will develop three complementary theoretical approaches to: (i) simulate time-periodic (Floquet) algorithms in the presence of dissipation to find ground states of interacting magnetic systems and use hybrid classical-quantum methods to investigate their equilibrium dynamics, (ii) create Floquet protocols that enhance coherence times and improve the quality of entangled many-body states while reducing unwanted quantum chaotic effects across different hardware platforms, and (iii) enable quantum sensing of correlated quantum magnets using coupled microwave superconducting devices, and detect their magnetic fluctuations.

This research combines analytical and computational methods with collaborative experimental partnerships. The theoretical insights will help create a roadmap for near-term simulation of long-range entangled ground states of frustrated magnetic systems that model correlated insulators, enabling study of their universal responses and detection of their low-energy excitations through quantum sensing. By integrating concepts across disciplines, this work aims to expand boundaries in the interconnected fields of quantum matter and information, establishing novel research directions that cross traditional disciplinary limits and create transformative advances in quantum materials research.

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

Bridging the Gap Between Scientific Datasets with Artificial Intelligence

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In high-energy physics (HEP), simulations are often used for training artificial intelligence (AI) models. Unfortunately, computational constraints, approximations, and unknown physics create unavoidable differences between simulations and real data. These differences cause simulation-trained AI models to experience a catastrophic drop in performance when applied to real experimental data. This effect is called the domain shift problem, and it is a persistent issue present in all spheres of HEP research. To unlock the full potential of AI for HEP, the development of AI methods that can generalize across datasets is paramount. This project will provide a universal AI analysis framework, designed to bridge the gap between simulated and real data and deliver timely results and depth of scientific understanding for cosmology, collider, and neutrino physics. The framework will have a modular structure and include a plethora of data, models, and task options to enable broad scientific use and solutions to any HEP domain shift problem. Notably, it will also include Graph Neural Networks (GNNs), which are uniquely well suited for work with complex and sparse scientific data, such as galaxies in astronomical surveys, or particles detected in neutrino or collider experiments. The project will capitalize on Fermilab science and computing capabilities, which are necessary to create a universal AI analysis framework compatible with the research needs and coding standards of all HEP groups. To accomplish this goal, the projects will implement and advance domain adaptation (DA) methods, which are aimed at solving the domain shift problem by enabling AI models to learn more robust features present in both simulated and real data (i.e., domain-invariant features). DA will allow AI to deliver trustworthy physics results even when trained on imperfect simulations-- it is therefore essential for real-world analysis, where simulation is always imperfect. Furthermore, while experiment- or simulation-specific features might be different between datasets, the underlying physics must be the same. Hence, using DA to learn domain-invariant features will also lead to the extraction of more physically meaningful information from the data.

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

Probing the Role of the 5f Electrons in Transuranic Reactions by Mass Spectrometry

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The chemistry of the heavy elements, most notably uranium and plutonium, is critical to many of the Department of Energy (DOE) nuclear missions. On a fundamental level, the actinide (An) row of the periodic table is the ultimate test of current chemical theory. Many difficult questions remain to unravel the unique chemistry of the 5f elements. The role of the f electron in chemical behavior has been identified as one of the grand challenges in heavy element chemistry, which refers to the difficulty of describing f-element systems in theoretical calculations. However, experimental transuranic data are limited, impacting the ability to develop theoretical methodologies. Gas phase results are the most direct experimental link to computational results and can provide the necessary experimental input to leverage theory to meet DOE missions. To accurately model actinide systems, the extent to which the 5f orbitals participate in 1) actinide bonding, 2) actinide reactivity (bond activation), and 3) from excited states must be considered.

An experiment capable of observing endothermic reactions that can handle the highly radioactive transuranic actinides is necessary to probe the role of the 5f orbitals and provide comparative data to validate theoretical models, while avoiding the limitations of other mass spectrometry methods and facilities. An inductively coupled plasma tandem mass spectrometer (ICP-MS/MS) housed within radiological facilities at Pacific Northwest National Laboratory (PNNL) can overcome both experimental obstacles. These specialized facilities are well suited to handling transuranics and expanding the capability to experimentally study actinide chemistry, while also mitigating potential risks. This instrument possesses the ability to alter the ion kinetic energy to examine the energy dependence of a reaction, so that both exothermic and endothermic reactions can be observed with a distinct high-throughput advantage that enables rapid identification of reactivity trends. ICP-MS/MS can study the actinide 1) reaction endpoints through determining thermodynamics, 2) reactivity by establishing reaction kinetics, and 3) excited state contributions to observed chemistry.

This work will use ICP-MS/MS to 1) determine the role of the 5f-orbital in actinide bonding, 2) determine the role of the 5f-orbital in actinide reactivity (bond activation), and 3) characterize actinide reactivity in “extreme” conditions. The results will improve the understanding of when 5f orbital participation is significant-both in bonding and reactivity. The observation of excited state chemistry will be used to assess the validity of traditional computational methods used to predict actinide behavior. This work will significantly increase the availability of transuranic experimental data, advancing efforts to solve the f-electron challenge and meet DOE’s nuclear missions.

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

Biosystems Design of a Genomically Recoded Chloroplast

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Engineering microbes for biomanufacturing enables the domestic production of needed fuels, chemicals, polymers, and critical minerals. A broad variety of microbes can be cultivated on biomass or waste streams for various biotechnological applications. An emerging powerful bioengineering approach called genomic recoding takes advantage of the redundancy of the genetic code to create novel proteins with new functions and catalytic capacity. To genomically recode an organism, its entire genetic code and protein synthesis machinery are modified to reassign a redundant codon to a specific non-standard amino acid, expanding the organism's biocatalytic potential beyond that conferred by the 20 natural amino acids, enabling the creation of proteins with novel properties. Genome recoding can help overcome a myriad of hurdles in biomanufacturing while also providing new tools to answer fundamental scientific questions on genotype-to-phenotype relationships and the evolution of the genetic code. To date, this technology has only been applied to a few species of bacteria that are relatively easy to genetically modify. Bacterial genomes contain millions of base pairs and significant additional work is needed to address a poorly predictable decrease in microbial fitness after genome recoding. The lack of predictive understanding of the phenotypic impacts of genomic recoding represents a key knowledge gap that must be addressed to take full advantage of its biotechnological potential. This project will address this challenge by recoding the chloroplast genome of the emerging model microalga *Picochlorum renovo*, testing the technology in a eukaryotic organism for the first time. The chloroplast is an ideal chassis for this purpose because it has a genome 50-times smaller than bacteria, and protein synthesis machinery independent of the algal nucleus. This research will apply synthetic biology approaches to synthesize a recoded genome followed by multidisciplinary phenotypic measurements, multi-omics analyses, and metabolic modeling to shed light on how altering the genetic code results in defective phenotypes and what strategies can be used to mitigate that stress. Further, the project will demonstrate the incorporation of non-standard amino acids into chloroplast proteins, enabling the engineering of new-to-nature enzymatic properties. The project will advance the US bioeconomy by developing new microbial bioproduction systems and potentially enabling the translation of the genomic recoding technology to bioenergy crops.

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

Physics of the Higgs Boson at the Highest Energies

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The Large Hadron Collider (LHC), located at the European Organization for Nuclear Research (CERN), accelerates and collides protons at the highest possible energies and intensities to probe new particles, reveal their interactions, and investigate the fundamental forces using sensitive state-of-the-art particle detectors. Thus far, LHC measurements indicate that the Higgs boson, the most recently discovered elementary particle in the Standard Model (SM) of particle physics, is responsible for electroweak symmetry breaking. The SM predicts that the Higgs boson is unique in this role and that electroweak symmetry is restored at high energies. Using the large dataset collected by the Compact Muon Solenoid (CMS) experiment during the current Run 3 program of the LHC, the research will study this high energy regime by measuring Higgs boson production and subsequent decays of the Higgs to a pair of bottom quarks that yield hadronic resonances at high transverse momentum. Consequently, three dominant Higgs boson production mechanisms will be measured simultaneously, and the first experimental test of electroweak symmetry restoration will be conducted, laying the foundation for more precise studies and measurements at the upcoming high-luminosity era of the LHC (HL-LHC) and at the proposed future particle colliders. As such, the physics output at the HL-LHC or at the future machines will depend on the associated detectors' ability to acquire and process large volumes of scientific data at high rates. This project will therefore develop custom intelligent readout electronics that contain compact and novel artificial intelligence (AI) and machine learning (ML) algorithms to analyze data on-detector, through pixelated Application-Specific Integrated Circuit (ASIC) chips or "smart pixels," which will provide an enabling technology for the fast processing and selection of the data. Critical steps towards achieving the technical readiness of on-chip artificial intelligence are planned, including AI/ML algorithmic development and tests of the ASIC's radiation tolerance to demonstrate that such smart pixel technology has the potential to operate in revolutionary detector designs and online particle selection strategies for collider experiments at the HL-LHC and beyond.

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

Speciation, Nucleation, and Aggregation in High-Ionic-Strength Electrolyte Solutions

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Speciation, nucleation, and aggregation in aqueous electrolyte solutions are essential processes that govern complex phenomena in condensed-phase environments. Molecular-level understanding of these processes is critical for controlling molecular synthesis, design, and separation, especially in high-ionic-strength solutions containing transition metals, post-transition metals, and lanthanides. These solutions exhibit intricate behaviors, such as hydrolysis, halogenation, nitration, and the formation of polynuclear ionic species, which affect nucleation and aggregation both in bulk and at interfaces.

The goal of this research is to create models of the collective properties of electrolyte solutions and to develop advanced many-body methods rooted in statistical mechanics, considering the progress in artificial intelligence. The machine learning interatomic potentials will be developed to enable the quantitative understanding of the important molecular-level information in liquids. This data will be imported into physics-informed reduced descriptions of the condensed phase to predict the collective outcomes dictated by the resulting free-energy landscape of electrolyte solutions. In addition, these reduced models will be further extended to capture the role of chemical-reaction networks and their dissipative behaviors on the phenomena, forming the basis of a systems-level modeling framework.

The outcomes of this research will be theoretical methods capable of spanning length and time scales. These frameworks will advance the understanding of how pH, ionic strength, surfaces, and external stimuli influence and optimize fundamental processes, thereby contributing to innovation in basic energy sciences in the Department of Energy.

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

Unravelling Cooperative Gas-Surface Coupling via Dynamic Temperature and Electric Field for Transformative Non-equilibrium Synthesis

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The synergy between gas-phase and surface chemistries plays an essential role in chemical and material syntheses, such as catalytic transformations of gaseous species (e.g., methane conversion, propane dehydrogenation, ammonia synthesis) and vapor deposition processes (e.g., chemical vapor deposition, atomic layer deposition, sputtering). While recent advances in in-operando characterization, advanced spectroscopic/microscopic analysis, ultrafast laser diagnostics, and multiscale modeling have significantly improved the understanding of reaction mechanisms in the gas phase, on surfaces, or both, the cooperative coupling effects between gas-phase and surface chemistries, especially at the space- and time-resolved molecular level, remain elusive. This challenge partly arises from the lack of methodologies to independently modulate the energetics and kinetics of gas-phase and surface species. Moreover, many conventional thermochemical reactions and material syntheses occur under near-equilibrium or near-steady-state conditions, offering limited control over timescales, energy levels, and their temporal patterns. This research aims to achieve a deeper understanding of the gas-surface coupling under non-equilibrium conditions through synergistic and spatiotemporal modulation of surface and gas-phase energies and their delivery patterns, thereby unlocking new opportunities for chemical synthesis and material fabrication. In parallel, this project aims to develop an active-learning-guided, high-throughput experimental platform to tailor the large parameter space of dynamic reactions, thus accelerating mechanistic explorations under complex reaction conditions. Overall, this project will provide a novel platform to investigate molecular-scale gas-surface chemical and material transformations within an underexplored non-equilibrium and dynamic regime. In addition, the decoupled control on the surficial and gas-phase energetics and kinetics will help elucidate the critical cooperative gas-surface coupling. The insights will be highly relevant to energy conversion and storage technologies, as well as transformative manufacturing of chemicals and semiconductors.

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

Modulating Post-translational Lysine Acetylation to Control Bacterial Bioproduction Phenotypes

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To develop the biotechnological advances that will propel the U.S. bioeconomy and deliver energy security, it is necessary to gain fundamental knowledge of microbial complexity. A predictive understanding of the foundational processes that allow microbes to acquire and use energy –and how these processes are regulated– is key to engineering controllable biological systems for production of valuable chemicals and critical materials. Post-translational modifications of bacterial proteins, particularly lysine acetylation, are critical yet poorly understood regulators of core foundational processes, such as central metabolism. This research will investigate how lysine acetylation influences the metabolism of the bacterium *Pseudomonas putida* and leverage this understanding to formulate strategies that prevent acetylation from hindering biochemical synthesis, thereby increasing its capacity to produce valuable chemicals. The project will apply state-of-the art synthetic biology, quantitative multi-omics, and computational modeling approaches to explore the effects of lysine acetylation during different bacterial growth stages under multiple conditions. These analyses will be enabled by a novel post-translational modification editing method that combines genetic code expansion and CRISPR interference to control protein acetylation states inside the cell. The novel approach developed through this project for studying lysine acetylation in a living bacterial cell will enable a deeper understanding of how this post-translational modification controls foundational processes in bacteria, and support the design of new biological engineering strategies. Additionally, the strategies developed to control acetylation-based regulation in *P. putida* will be broadly applicable across diverse bacteria because key enzymes involved in both lysine acetylation and the metabolic pathways required for chemical synthesis are often evolutionary conserved. Ultimately, this project will not only advance next-generation biochemical production efficiency, but also provide both foundational knowledge of how cellular processes are regulated in bacteria and a new approach to rationally control these critical processes.

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

Molecular Models to Probe the Stability and Redox Chemistry of Plutonium Oxides

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Plutonium (Pu) chemistry is complex and poorly understood, particularly in aqueous systems where pH-dependent interactions between Pu ions and water molecules lead to the formation of ill-defined solution species and solid products, including plutonium oxides. These oxides play an important role in the behavior of Pu in natural and engineered environments. Questions regarding the relative stability of these oxides and the role of redox chemistry in the formation or dissolution of plutonium oxides remain unanswered, partly due to the difficulty in characterizing the structure of dissolved solution species and bulk oxide phases. To address these questions, this project will take a molecular-level approach to understanding the formation, growth, and stability of plutonium oxides in aqueous systems by synthesizing, isolating, and structurally characterizing discrete polynuclear plutonium-oxo clusters. These polynuclear Pu clusters have atomic arrangements that directly mimic those observed in crystalline plutonium dioxide (PuO_2), allowing these clusters to serve as molecular models of plutonium oxides. Further characterization using voltammetry, spectroelectrochemistry, and solution calorimetry will provide insight into the relationships between Pu oxidation state, structure, and thermodynamic stability across a range of polynuclear Pu cluster compounds. Leveraging these molecular models of Pu oxides will allow this project to define the mechanisms and thermodynamics driving plutonium oxide formation and reactivity in aqueous systems. When combined with reported thermodynamic and structural properties of bulk plutonium oxides and an examination of changes in cluster structure over long time periods, a deeper understanding of electron transfer and chemical bonding in plutonium oxides will be gained, thus advancing the Heavy Element Chemistry program closer to unraveling the role of f-electron behavior in the actinide elements and controlling Pu chemistry in aqueous systems.

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

Discovery of new physics using electron scattering at JLab and EIC

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Nuclear physics addresses fundamental questions about the universe, including how atomic nuclei can reveal physics beyond the Standard Model. This project advances research at two premier facilities: the Thomas Jefferson National Accelerator Facility (JLab) and the Electron-Ion Collider (EIC). At JLab, the MOLLER experiment will test electron interaction theory with unmatched precision. Secondly, the PREX puzzle, involving lead nuclei, will be investigated through measurements of transverse asymmetries in medium-Z nuclei. At the EIC, objectives involve enhancing capabilities and exploring new physics observables in collaboration with theoretical and experimental communities. Critical to achieving research goals at both facilities is the advancement of Compton polarimetry. This award supports the development of a new photon detector to enable a full three-dimensional understanding of high-energy electron beam polarization. The device will be the first in the world to offer this capability and will enhance the physics reach of JLab.

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

Taming the Low-Energy Frontier for the Deep Underground Neutrino Experiment

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As the 2020s draw to a close, the US will host a multi-billion-dollar international physics project called the Deep Underground Neutrino Experiment (DUNE). Using the world's most powerful neutrino beam and two sets of detectors installed in Illinois and South Dakota, DUNE will pursue precision measurements to answer fundamental questions related to the nature of neutrinos and the origin of the universe.

Construction of DUNE will follow a staged approach, with the South-Dakota-based detectors beginning to record data a few years before the other components. While some of DUNE's physics goals can only be achieved with the full apparatus, many scientific topics may already be explored with the initial detector system alone. Some of these involve using DUNE as a telescope to measure cosmic neutrinos generated by the Sun, supernovae, and black holes. There are also a wide variety of related opportunities to search for manifestations of hypothesized new particles and forces.

The primary challenge for studying these natural phenomena is their lower energies compared to the neutrinos from the high-energy beam. However, recent demonstrations of DUNE-like detector technology have achieved remarkable performance in measuring relatively faint low-energy signals. Prospects for related scientific discovery with DUNE are therefore more limited by analysis tools than by detector sensitivity: a reliable simulation of the low-energy particle interactions of interest does not yet exist. Without such a simulation, rigorous interpretation of a future DUNE low-energy data set will remain impossible.

This research launches a broad program of scientific investigation with DUNE at low energies. Rapid development of the missing simulation capabilities will be pursued in the early years of the project. Modeling and software work will be combined with interaction measurements needed to address key gaps in the available input data. The resulting transformative upgrades to an existing simulation code called MARLEY (Model of Argon Reaction Low Energy Yields) will then be put to work immediately to search for new physics processes. Analyses studying low-energy signatures of proton decay and dark matter, made newly accessible to DUNE by the earlier stages of the project, will be designed and eventually brought to completion. Tools and techniques created during these activities will empower a wide range of additional measurements in DUNE and beyond.

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

Correlated Electron Materials with Novel Quantum Building Blocks

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Correlated quantum materials with novel functionalities must integrate competing properties, such as magnetism, ferroelectricity, superconductivity, and metal-insulator transitions, within a single compound. This poses a central challenge in quantum materials design. In some materials, correlated electronic states do not emerge from individual atomic d-orbitals but from molecular orbitals (MOs) formed across clusters of transition metal atoms. These correlated electron-molecular orbital (CEMO) materials are enabled by their diverse geometries and exhibit unique properties not accessible in conventional systems. They have already demonstrated potential in applications, for example in field-free Josephson diodes. While a few correlated electron-molecular orbital materials have been studied in isolation, this project will create a unified theoretical framework to define, identify, and systematically model this emerging class of materials. This project has three objectives:

1. Development of numerical tools to discover correlated electron-molecular orbital materials based on symmetry and bonding and to predict their properties. The methods include statistical and machine learning methods.
2. Construction of symmetry-adapted theoretical models to simulate their correlated behavior.
3. Creation of predictive frameworks for emergent magnetic and multiferroic phenomena in correlated electron-molecular orbital materials.

The integrated approach will establish the theoretical and computational foundation for the discovery and design of a new family of functional quantum materials with future applications in spintronics, microelectronics, and quantum technologies.

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

Designing Dynamic Function for Nonequilibrium Dissipative Chemistry

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The ability to build synthetic molecular machines that perform work—mimicking the active processes found in living systems—is one of the grand challenges in systems chemistry. While biological motors operate far from equilibrium, using fuel to drive motion and accomplish tasks, most of our chemical design tools are rooted in equilibrium ideas like free energy minimization. This project aims to bridge that gap by developing theoretical and computational tools for designing and optimizing synthetic systems that function away from equilibrium. Using coarse-grained molecular simulations and new optimization algorithms, the research will explore how simple chemical building blocks can be combined to create more effective molecular motors and materials. For example, the work will test how coupling multiple motors into units can enhance their performance and yield better conversion from chemical energy into mechanical work. By advancing the theory and modeling of nonequilibrium chemical systems, this research will lay the groundwork for a new generation of active, responsive materials.

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

Exploring Diverse Far-red Light Adaptations in Cyanobacteria

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While many are familiar with the idea that plants use visible sunlight for photosynthesis, it is less well known that some photosynthetic organisms can use “far-red light” which is a type of light that lies just beyond the range of what our eyes can see. Far-red light spans wavelengths between 700 and 800 nanometers and is abundant in shaded environments like dense forests and soils. Cyanobacteria have evolved several remarkable strategies to adapt to these conditions and make use of far-red light that is otherwise wasted.

This project will explore how cyanobacteria perform photosynthesis using far-red light, with the goal of understanding the molecular protein systems that make this possible. Specifically, the project focuses on three unique adaptations:

1. Low-Light Photoacclimation (LoLiP): a response in which cyanobacteria build helical antenna structures to capture extra photons in the far-red.
2. Far-Red Light Photoacclimation (FaRLiP): a process that modifies the protein complexes used for photosynthesis, allowing the light-absorbing chlorophyll composition to include far-red light-absorbing chlorophyll *f*.
3. Chlorophyll *d*-based Photosynthesis: a form of photosynthesis used by some cyanobacteria that rely on a different type of chlorophyll pigment, known as chlorophyll *d*, to capture far-red light.

To conduct this work, we will use a combination of cutting-edge tools in structural biology, including cryo-EM, spectroscopic analyses, and biochemical experiments. The research will take place at the University of Wisconsin-Madison in the Gisriel Lab, which specializes in understanding how photosynthetic proteins are built and how they work. We will also collaborate with experts in spectroscopy and computational modeling to ensure a comprehensive understanding of how these unique systems operate.

The long-term impact of this research extends beyond understanding the natural world. By uncovering how organisms thrive using far-red light, we can potentially apply these strategies to improve crop productivity in shaded or low-light conditions, such as in dense agricultural fields, vertical farms, or even future space habitats. Moreover, this work could inform the design of bioengineered systems for renewable energy production, such as photosynthetic systems that produce fuels or other valuable chemicals more efficiently.

Ultimately, this project aims to answer fundamental questions about how life adapts to its environment while opening new doors for innovation in energy, agriculture, and sustainability.

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

Deep Learning and Instrumentation for the HH Measurement at the High-Luminosity Large Hadron Collider

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The Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland provides a unique research facility to explore the fundamental laws of nature. The discovery of the Higgs boson marked a pivotal achievement, yet key questions in particle physics still remain unanswered. These include, for instance, understanding the origin of the matter-antimatter asymmetry in the universe, which potentially is connected to baryogenesis during electroweak phase transitions; the exact nature of electroweak symmetry breaking; and the Higgs potential and stability of the electroweak vacuum often linked to the ultimate fate of the universe. Studying interactions between pairs of Higgs bosons (HH) is central to answering these questions, particularly by probing the Higgs boson's self-interaction and studying the shape of its potential. This research program will leverage existing and forthcoming data from the LHC to advance the HH search using the Compact Muon Solenoid (CMS) experiment, while paving the way for extending the studies during the upcoming High-Luminosity LHC (HL-LHC) running era. A central component of the research is the development and deployment of cutting-edge artificial intelligence and deep learning (AI/DL) methods to significantly improve the signal-to-background discriminating power and associated background estimation, and to enhance the performance of real-time bottom quark identification. The integration of such AI/DL techniques is critical for the HH measurement, in studying other rare physics decay processes at CMS, and in further bolstering the broader LHC scientific program. In particular, the application of AI-driven tools can allow reaching sensitivity levels for HH production that were previously thought to be achievable only during the culmination of the HL-LHC program, enabling its exploration on a much faster timescale. Complementing these efforts, the project will also significantly advance the CMS detector upgrade for the HL-LHC, focusing on the commissioning and physics exploitation of the new High-Granularity Calorimeter (HGC). To that end, the HGC's unprecedented spatial and timing resolution will be harnessed using innovative AI/DL-based reconstruction algorithms to enable more precise measurements of particle interactions and thereby expand the HL-LHC's full scientific discovery potential. These dual studies promise to not only deepen our understanding of the Higgs boson but also unlock new avenues in searching for new physics beyond the Standard Model of particle physics.

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

Visualizing the Atomic-Scale Dynamics of Charge-Ordered Phases in Quantum Materials

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Understanding how electric charge moves through quantum materials is of critical importance to the fundamental science of solids and to unlocking their full potential for next-generation energy and quantum information technologies. Many quantum materials host a charge density wave (CDW), a collective quantum state where electrons and the crystal lattice spontaneously couple to form a new global spatial pattern. Similar to spectators acting as a collective to perform “the wave” at a sports game, applying an electric field can cause the entire CDW to slide through the material, resulting in technologically desirable properties such as non-linear current-voltage behavior and memory effects. However, crystal defects can hinder sliding by locally pinning the CDW. Although bulk probes have shed much light on the micrometer-scale dynamic properties of CDWs, a comprehensive atomic-scale investigation of sliding and pinning is still lacking. This research project focuses on forging new microscopic insights into the nature of charge transport in several charge-ordered systems through the development of current tuned scanning tunneling microscopy/spectroscopy (CT-STM/STS). By combining atomically-resolved surface imaging with simultaneous bulk electronic transport, CT-STM/STS will be used to reveal how the onset of collective charge sliding occurs and how the CDW interacts with crystal disorder in several low dimensional crystals. Applied mechanical strain and surface patterning will be explored as methods to demonstrate fine control of CDW sliding in these systems. Finally, CT-STM/STS will be used to search for novel surface CDW dynamics in crystals where bulk sliding is conspicuously absent. The results of this research will advance our understanding of current flow in charge-ordered correlated materials while also establishing CT-STM/STS as a powerful microscopy technique for visualizing atomic-scale dynamics in a host of other quantum materials.

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

Unlocking New ZZ* Decays of the Higgs Boson with Analog AI/ML Algorithms

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The Standard Model of particle physics has successfully explained many scientific phenomena in our universe, with the Higgs boson playing a central role. While many theoretical predictions involving the Higgs boson have been confirmed through high-precision measurements, several difficult-to-study decay modes remain unexplored, and key questions remain unanswered. This research will investigate unmeasured Higgs boson decays – specifically those in which the Higgs decays into Z bosons, which subsequently decay into tau leptons and electrons or muons – using the ATLAS (A Toroidal LHC ApparatuS) experiment at the Large Hadron Collider (LHC), located at the European Organization for Nuclear Research (CERN) in Switzerland. As such decays of the Higgs occur in only 1 in 10 trillion LHC collisions, distinguishing their signatures from other events poses a significant challenge. To address this, the research will develop advanced artificial intelligence (AI) and machine learning (ML) techniques to enhance the identification of the Higgs signal at ATLAS. Results from the study will enable more accurate measurements of the interaction between the Higgs and Z bosons and explore new regions of phase space to search for physics beyond the Standard Model that can not only reveal the exact identity of dark matter but further explore the matter-antimatter asymmetry in the universe. One key challenge in this measurement lies in the proper identification of tau leptons, where conventional computing methods have limitations. The project will integrate new analog AI/ML algorithms and technologies into high energy physics detector systems to perform computationally intensive mathematical operations using low-power resistive analog circuits within silicon chips. Using the ATLAS detector as a testbed, the research will establish the use of AI/ML-based particle recognition algorithms on analog systems at particle colliders and lay the groundwork for developing the next generation of advanced detectors. The technology promises to enhance the capability for measuring complex particle interactions in real-time at the upcoming high-luminosity era of the LHC and at future world-leading colliders, such as the Electron-Ion Collider or the proposed Future Circular Collider and Muon Collider.

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

Uncovering Physical Drivers Behind Graphic Structure within Nano-Seismic Catalogs

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Fractures in rock—ranging from tiny cracks to large faults that produce earthquakes—often organize themselves in strikingly similar ways across vastly different scales. These scale-invariant patterns resemble the branching seen in river deltas, leaf veins, snowflakes, or neural networks, and are governed by the physical forces shaping each system. By studying these patterns, researchers can better understand how stress accumulates and is released within the Earth.

This project will examine how small fracture events, known as nano-seismic events, form interconnected networks under varying stress and fluid conditions. Through advanced laboratory experiments, the research will generate detailed catalogs of these events that mirror the behavior of much larger seismic systems. By applying graph theory and machine learning, the work will reveal how these events connect and evolve in space and time—forming topological structures that change shape, much like how a palm tree's outline might shift toward that of a conifer.

By uncovering the organizational signatures of these fracture networks and linking them to underlying physical drivers, the project will improve the ability to predict subsurface fracture growth and help enhance seismic forecasting activities. These insights are critical for subsurface engineering efforts, such as enhanced geothermal systems and supporting the Department of Energy's mission to advance fundamental knowledge of Earth's dynamic processes.

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

Probing and Controlling Attosecond Chirality in Molecules by Multi-dimensional Coincidence Spectroscopy

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Molecular chirality plays a fundamental role in most chemical reactions and biochemical processes underlying life on earth. Over the last two decades, time-resolved spectroscopies on femtosecond and attosecond time scales have made unprecedented progress, based on advances in both laboratory- and accelerator-based light sources. However, most of these fundamental advances in attosecond science have been realized with linearly polarized light and are therefore inherently insensitive to molecular chirality. This proposal aims at applying attosecond spectroscopy tools to probing and controlling molecular chirality on the electronic time scale. More specifically, the proposed work will address three main objectives: (1) Probing electron emission asymmetry from chiral molecules with circularly polarized attosecond pulses and enhancing chiral recognition on the sub-femtosecond time scale; (2) Resolving electron scattering dynamics from dynamically evolving chiral potentials in real time; and (3) Manipulating chiral electron motion in molecules to influence chirality-sensitive photodissociation pathways. These goals will be achieved by generating and characterizing circularly polarized isolated attosecond light pulses and combining them with kinematically complete electron-ion-coincidence measurements.

If successful, the proposed studies will provide access to purely chiral electronic dynamics on the attosecond timescale, as well as the coupling between electronic and nuclear motion in chiral systems. Using the proposed multi-dimensional coincidence spectroscopy, this study aims to address some of the most fundamental questions in molecular chirality—such as the evolution of chiral electron flows within molecules, the role of electrons in inducing molecular chirality, and strategies to enhance chiral sensitivity and recognition.

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

Tailoring Phase Space Correlations for Future Accelerators

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Over the past several decades, phase space manipulation has been a key factor in advancing the performance of particle accelerators by enabling control over the spatial and momentum distributions of charged particle beams. Among various strategies, the control of correlations within phase space—such as between position and momentum or energy and time—has emerged as a critical tool for shaping beam properties to meet application-specific requirements. Most modern accelerator techniques rely on these correlations, yet existing methods are limited to linear or low-order polynomial forms. This constraint prevents access to more complex beam distributions that could significantly improve accelerators' performance such as the luminosity of particle colliders or the efficiency of acceleration. The proposed project aims to establish a new framework for tailoring phase space correlations using cosine-basis approximations. This approach removes the limitations of traditional polynomial-based methods and enables precise control of nonlinear structures in phase space. The project will implement new modulation hardware and beamline configurations to realize these correlations experimentally, with demonstration goals that include improved wakefield acceleration efficiency, generation of high-brightness electron beams, and control of multidimensional phase space. These developments will address several priorities identified for particle colliders and in general accelerator R&D roadmaps and support future advances across a range of accelerator platforms.

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

Microelectronics and Detector Simulation Co-Design to Demonstrate 4D Tracking for Future Collider Experiments

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Particle physics and the exploration of the fundamental constituents of matter described by the Standard Model of particle physics rely on high energy collider experiments like the Large Hadron Collider (LHC) at CERN (Geneva, Switzerland) to probe the universe at its smallest scale. Sophisticated detector systems are used to measure the momentum and energy of the decay remnants emerging from the collision point to reconstruct the particle interaction that has taken place and to probe for the existence of potentially new fundamental particles and forces. In order to enable future particle colliders and their experiments and to improve on measurement precision or expand their physics reach, detector systems have to be developed that can tolerate more extreme environments created by the colliders while improving their performance to explore particles at even smaller scales.

At the heart of modern collider experiments are tracking detectors that record the trajectories of all charged particles emerging from the interaction point and, in combination with a strong magnetic field, enable momentum measurement of each particle. In the past, these detectors have recorded only spatial information (3D) of traversing particles, but as the particle flux in future colliders will increase drastically to provide high statistics data, the temporal dimension also has to be used to discriminate particle tracks from each other. This gives rise to the concept of 4D tracking detectors that simultaneously measure particles with high spatial resolution (of order 50 micro-meters) as well as high temporal resolution (of order 50 pico-seconds), which up to now has only been done in independent detector systems. To pave the way for 4D pixelated tracking detectors to become feasible at the scale of a full-size detector system, this research will develop a first of its kind pixel detector readout chip in 28 nano-meter Complementary Metal-Oxide-Semiconductor (CMOS) technology to demonstrate 4D particle tracking in a test environment. The pixel detector readout chip will be designed in parallel to a performance simulation of a detector system envisioned for the potential 10 TeV Muon Collider, which sets challenging requirements specifically for the parts of the pixel detector tracking system that are closest to the beam. This co-design of readout chip and system simulation enables evaluation of the physics performance impact of readout chip design choices, such as spatial and temporal resolution, and signal processing and data compression schemes. This highly integrated design flow has never been implemented before and could drastically improve the design cycle of chip design for detector instrumentation. Once manufactured, the readout chip will serve as the basis to explore the new high precision timing paradigm in-situ, and it will aid the development of novel sensor technology and high-performance tracking detectors.

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

Maximizing Helium-3 Polarization at the Electron Ion Collider

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The Electron Ion Collider (EIC) at Brookhaven National Laboratory (BNL) will quantify the contribution of spin from quarks and gluons to the total angular momentum of nucleons. Polarized neutron beams and polarized proton beams are essential for this quantization. The most promising path to polarized neutron beams is the acceleration and storage of a polarized helium-3 beam. While polarized protons have been established at the Relativistic Heavy Ion Collider (RHIC) and its injectors for several decades, polarized helium-3 is undeveloped at RHIC or its injectors. The EIC will use the existing RHIC injectors, the Booster and Alternating Gradient Synchrotron (AGS), and repurpose the RHIC into the EIC's Hadron Storage Ring (HSR). Due to properties of the helium-3 nucleus relative to protons, helium-3 is more susceptible to polarization loss as it is accelerated. This project will investigate the polarization transmission of polarized helium-3 beams at the EIC hadron accelerator complex. Extensive simulations to optimize transmission in the Booster, the AGS, and the HSR will be performed, in addition to studies in the Booster and AGS. In the Booster and the AGS, the studies of polarized helium-3 will bring them to an energy that is three orders of magnitude higher than what has previously been achieved.

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

Bringing Light into the Equation: Engineering Strong Light-Matter Interactions for Chemistry and Materials

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Chemistry began as a descriptive science, guided by intuition and heuristics. It became predictive with the rise of quantum chemistry and first principles calculations, now accelerated by machine learning. Today, molecules, materials, and reactions can be designed by solving the equations of quantum mechanics. Yet one key player remains largely absent from theoretical frameworks: light. Often treated as a probe or tuning knob, light is rarely included as part of the system, despite its central role in processes from photosynthesis to quantum information. This is beginning to change. Recent advances reveal that strong light–matter interactions can reshape chemical reactivity and materials and device design by creating hybrid states of light and matter. These developments make light an active component of matter and call for a new framework that treats photons (i.e., light) on equal footing with electrons and nuclei (i.e., matter).

This project aims to establish a predictive framework for strong light–matter engineering. We focus on strong light–matter interactions in plasmonic systems, particularly under voltage control. Using scanning tunneling microscope break junctions (STM-BJ) as a complex yet highly controlled platform, we aim to investigate how voltage driven excitation enables new regimes of polariton formation, exciton dynamics, and long-lived coherence at the single molecule level. More precisely, we aim to explore this through a combination of fundamental understanding (i.e., mechanisms behind exciton lifetimes, mode structures, classical versus quantum effects, and laser versus voltage excitation mechanisms), bottom-up code development (i.e., implementation of nonadiabatic dynamics into the open-source software package Libra), and close collaboration with our experimental partner. The latter allows us not only to push theoretical development forward but also to ground it in experimental realities, helping to bridge the substantial gap between theory and experiment in chemistry and materials design driven by strong light–matter interactions. Building on this foundation, we extend our framework to chiral plasmonic nanocavities, an unexplored regime, to explore how structured light and symmetry breaking enable enantioselective control and quantum coherence under ambient conditions.

This work bridges quantum chemistry and quantum optics, opening new avenues for understanding and engineering strong light–matter coupling in chemistry, optoelectronics, and quantum technologies, with the ultimate goal of making light–matter engineering as systematic, predictive, and transformative as traditional quantum chemistry.

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

Unravelling the Chemistry of Non-Equilibrium Radiation-Induced Actinide Species

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Actinides are inherently unstable elements that are often encountered in the presence of other radioisotopes. Consequently, inherent ionizing radiation fields promote the formation of non-equilibrium actinide oxidation states. These states play a critical mechanistic role in the radiation response of actinide-containing systems due to their unique redox chemistry. Additionally, actinide ions have been found to directly stabilize radiation-induced radicals, leading to the formation of non-equilibrium actinide-radical complexes, adding another layer of mechanistic intricacy to unravelling the fundamental radiation-induced chemistry of the actinides. However, our basic knowledge of these non-equilibrium actinide species is limited, yet this missing information is essential for understanding fundamental actinide science and complex phenomena induced by ionizing radiation.

This program will utilize novel experimentally validated multiscale modeling techniques to elucidate the molecular-level role of non-equilibrium, radiation-induced actinide species in the overall chemistry of actinide-containing aqueous solutions to identifying the mechanisms underpinning their formation, lifetime, and chemical reactivity. This knowledge fundamentally advances our ability to efficiently utilize nuclear energy resources, ensuring that the United States remains at the forefront of nuclear energy technologies, isotope production, nonproliferation, and national security. Additionally, the insights gained will support fundamental actinide research, such as developing tailored actinide materials for catalysis, quantum information science, and nuclear medicine, where ionizing radiation impacts synthetic success and material efficiency, longevity, and recyclability.

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

Nonequilibrium Spin States Studied by Neutrons

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Understanding the behavior of quantum many-body spin systems far from equilibrium is a frontier challenge with broad implications for condensed matter physics, statistical mechanics, and quantum information science. Despite having far-reaching scientific and technological significance, nonequilibrium phenomena in driven-dissipative quantum systems remain largely unexplored. Unlike equilibrium macroscopic behavior, which can be described using a few state variables such as temperature and pressure, out-of-equilibrium quantum systems generally require a full quantum mechanical description—one that is often difficult to obtain due to the lack of tools capable of probing the microscopic dynamics. This project seizes a unique opportunity offered by recent development in laser pump–neutron probe techniques and accessible new advanced computational capabilities such as large-scale computation through supercomputers and quantum simulation via quantum computers to tackle out-of-equilibrium phenomena in quantum spin systems.

The goal of this research is to uncover how quantum interactions among spins govern nonequilibrium dynamics in low dimensional quantum magnets. This will be accomplished through an integrated approach that combines advanced neutron pump-probe spectroscopy, theoretical modeling, and state-of-the-art computational methods. The outcome of this research will offer insights into the roles of dimensionality, integrability, and quasiparticle interactions in governing decoherence and dynamical phase transitions in spin-based systems—providing a foundation for future quantum technologies.

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

Leveraging Noncovalent Interactions to Modulate Multimetallic Actinide Structures

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This research focuses on the significant role that weak forces, known as non-covalent interactions (NCIs), play in determining the behavior of heavy elements called actinides. Non-covalent interactions encompass a variety of forces, such as London dispersion forces and π-cation interactions. These forces are already well-known for their influence in fields like biology, where they help proteins fold, and materials science, where they affect the stability of various compounds. However, their potential in actinide chemistry remains largely untapped.

The primary goal of this study is to investigate how these weak forces can be harnessed to control the distance between two actinide centers and influence the way these centers electronically communicate with each other. Such control could pave the way for new methods of managing electronic communication, charge transfer, and bonding between actinide elements.

To accomplish these objectives, this work explores a variety of molecular frameworks and ligand structures to systematically study how actinides engage in electronic interactions through NCIs. This approach will allow the identification of which specific conditions and frameworks most effectively promote enhanced interactions between the actinide centers. This research aims to show how weak interactions can serve as powerful tools for manipulating and controlling the electronic behavior of actinide elements.

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

Open heavy-flavor photoproduction at the LHC and EIC for a scale-dependent characterization of nuclear matter

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Characterizing the properties of quarks and gluons, the building blocks of atomic nuclei, represents one of the foremost open questions in nuclear and particle physics. This project exploits the production of particles containing a heavy quark to achieve a scale-dependent characterization of nuclear matter at extreme densities of low-energy gluons. The program follows a two-pronged strategy. In the first stage, it exploits ultra-peripheral lead-lead collisions at the Large Hadron Collider (LHC) as a high-statistics source of photon-nucleus interactions at the highest center-of-mass energies currently achievable. These collisions, which occur when the two nuclei do not touch each other and interact only via their electromagnetic fields, will enable high-precision measurements of open-charm hadron photoproduction using the Compact Muon Solenoid (CMS) detector. In a second stage, the same observables will be measured at the US-based future Electron-Ion Collider using the ePIC detector, benefiting from the unique experimental conditions available in electron-nucleus collisions. To maximize the accuracy and physics impact of future open heavy-flavor measurements at the EIC, this project will develop advanced low-level simulations of the future Silicon Vertex Tracker (SVT). This state-of-the-art silicon detector will employ next-generation monolithic active pixel sensors and enable micrometer-level precision in reconstructing charmed and beauty hadron decays. In addition to providing new experimental constraints on the nature of nuclear matter at high partonic densities, the project will therefore strengthen U.S. leadership in high-precision silicon-pixel technology for future particle-physics experiments.

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

Understanding and Enhancing Photophysics of Singlet Fission Films Interfaced with Silicon

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Singlet fission enables the transformation of a single particle of light, known as a photon, into two electron-hole pairs, known as excitons. This novel process promises to significantly increase the efficiency with which sunlight is converted into useable energy. However, realizing the immense potential of singlet fission has been limited by major challenges in solar photochemistry. This project aims to overcome these roadblocks by developing an innovative approach to interface singlet fission films, composed of a select subset of organic semiconductors, with silicon, an inorganic semiconductor that forms the basis of most electronics. These materials systems will be utilized to elucidate and control the fundamental photophysical and molecular principles required to generate, transport, and transfer excitons with unprecedented efficiency. This project exploits cutting-edge materials discovery and state-of-the-art spectroscopy to (1) develop approaches to produce singlet fission films on silicon with ideal molecular orientation and packing for solar energy harvesting; (2) discover how exciton transfer from singlet fission films to silicon can be enhanced by engineering interfacial properties, including electronic coupling, defect passivation, and energy level alignment; (3) demonstrate new exciton transfer mechanisms by transforming excitons from dark to emissive; and (4) establish molecular design rules for improving exciton generation and dynamics. This work will enable key insight into exciton transport in organic semiconductors and exciton transfer across hybrid organic-inorganic heterojunctions. Overall, this research will provide a scientific basis for harnessing singlet fission to efficiently produce electricity, chemical fuels, and quantum coherent states for a variety of next-generation technologies ranging from solar energy generation to photocatalysis to quantum information science.

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

Electric Field Responsive Surfaces for Dynamic Catalyst Design

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Dynamic control of catalytic reactions is an emerging opportunity for responsive catalyst design, with the potential to overcome classical kinetic and thermodynamic limitations in critical chemical transformations central to the nation's energy infrastructure. Active control over the electronic characteristics of the catalyst will accelerate the catalyst design process by accessing multiple electronic environments for a single catalyst material, and facilitate real-time adjustment to process variables and outputs. Further, current catalyst design strategies are inherently limited because they rely on static changes to a catalyst's structure, lowering the energy barrier to one sluggish step of the reaction at the cost of sacrifices elsewhere in the catalytic cycle. In contrast, dynamic catalysts can adapt over the catalytic cycle, affording complementary electronic environments for energetically disparate elementary steps, offering the potential to dramatically exceed static theoretical rate limits. This work will establish an understanding of the electronic coupling of catalytic active sites with field responsive oxides including ferroelectrics for which polarization can be manipulated by external electric fields for reactions including selective methane oxidation to methanol and ammonia synthesis. To understand how electric field responsive catalysts can be leveraged for dynamic catalysis, field effects with varying dynamic timescales will be explored with *in situ* and *operando* infrared and X-ray absorption spectroscopy, including the use of Modulation Excitation Spectroscopy (MES), providing insight into the dynamic interplay between field induced changes in surface electron density with the electronic state and reactivity of supported active sites. Exploration of the broad space of reaction and field stimulus parameters will be accelerated by AI/machine learning guided autonomous experimentation. This work will establish a fundamental understanding of how catalysts on field responsive surfaces can be used to modulate catalytic outcomes and to drive reactions beyond the classical limits of static systems.

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

Maximizing Electron Beam Intensity for High-Brightness Synchrotron Light Sources

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Next-generation synchrotron light sources promise unprecedented X-ray brightness, enabling transformative advances in materials, chemical, and biological sciences. However, achieving these brightness levels requires electron beams with particle densities significantly higher than in existing synchrotrons, leading to enhanced particle interactions within the beam and with accelerator surroundings, which can degrade beam quality and limit achievable X-ray brightness. To overcome these fundamental limits, this project advances the understanding of critical beam interactions—particularly intrabeam scattering and Touschek scattering—by using innovative theoretical approaches inspired by plasma physics. It further explores new techniques using multi-harmonic radiofrequency cavity systems designed to stretch electron bunches, thus reducing their particle density and enhancing stability. By integrating theory, advanced simulations, and experimental validation at Brookhaven National Laboratory's National Synchrotron Light Source II (NSLS-II), in collaboration with other leading facilities, this research tackles critical limitations in beam intensity. The outcomes will support the Department of Energy's goals, pushing forward the capabilities of future diffraction-limited synchrotron facilities and enabling groundbreaking scientific discoveries.

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

Accelerating Large-Scale Atomistic and Continuum Simulations with Physically Consistent and Scalable Machine Learning Methods

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Modern scientific research increasingly relies on massive datasets generated by high-fidelity simulations and experiments. Machine learning (ML) approaches offer a powerful way to extract insights from these datasets. However, current ML methods often encounter practical limitations when handling large-scale scientific data, including computational inefficiencies and challenges in ensuring accurate, physically consistent predictions. To overcome these limitations, this research will: (1) create new machine learning architectures explicitly designed to efficiently scale with increasing dataset size and model complexity, and (2) develop specialized techniques to ensure rapid and physically meaningful predictions during practical use. We will validate our approach across multiple scientific domains, each characterized by complex spatiotemporal dynamics, computational demands, and the need for physically accurate outcomes. By integrating scalable ML architectures with targeted inference-time methods, our research aims to establish a broadly applicable framework that effectively balances accuracy, computational efficiency, and scalability for diverse scientific problems.

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

Decoding Fragility: How the Kinetics and Structure of Metallic Liquids Govern Solidification

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Most metallic materials are synthesized by solidification from the liquid state. Practical examples range from casting and quenching techniques, to additive manufacturing, to atomization for powder synthesis. Here, metallic liquids are the precursor, and the solidification pathway determines the product. This pathway, however, depends on the properties and atomic structure of the liquid, which are difficult to measure and poorly understood. Specifically, *liquid fragility* describes how quickly a liquid's viscosity slows down with decreasing temperature. Due to experimental challenges, there is a lack of reliable fragility data. As a result, it is currently not possible to predict liquid fragility as function of chemical composition, posing an acute knowledge gap. The recently developed Film Inflation Method (FIM) overcomes this barrier. First FIM data have revealed a complex behavior challenging conventional assumptions. This project will now harness FIM to decode fragility broadly: The fragility will be mapped across 10 new alloy systems, yielding up to 2,400 data points. Then, additional characterization (diffraction and electron microscopy), simulation (molecular dynamics), and thermodynamic modeling will be performed. This will allow to (1) build a mechanistic understanding of the fragility in metallic liquids, (2) develop new models to describe the atomic structure of liquids, and (3) uncover the impact on glass formation and crystallization. Ultimately, this will yield widely applicable predictive models to enable targeted synthesis and processing, with practical impact across various materials and alloy classes, different manufacturing methods, and a wide range of applications in electricity generation, energy storage, aerospace and propulsion, and beyond.

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

Biocontained Bacterial Spores for Controlled and Durable Plastics Upcycling

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Metabolic engineering takes advantage of the broad metabolic capacity of microbes for multiple biotechnological purposes. A growing application of microbial bioprocessing is the degradation of plastic waste and its conversion into valuable materials. However, the semi-crystallinity of certain plastics prevents enzymes from penetrating the plastic for complete degradation, leaving potentially harmful microplastics. A promising approach to address this challenge is the use of the benign bacterium *Bacillus subtilis*, which is capable of forming spores. These thick-walled structures that form inside bacterial cells allow the bacteria to withstand harsh conditions in a dormant state, and to germinate and continue vegetative growth when conditions improve. Due to their long shelf-stability and tolerance to heat and solvents, spores from plastic-degrading engineered *B. subtilis* strains can be embedded within plastics during their fabrication, and their germination induced at the desired end-of-life of the plastic for uniform degradation. This project will perform a comprehensive analysis of the solvent and heat tolerance of spores prepared from several *B. subtilis* strains and engineer new strains to improve fabrication of spore-embedded plastic biomaterials. An important component of this project is the design of an intrinsic biocontainment strategy to avoid premature spore germination, and thus early end-of-life of the biomaterial. To achieve this goal, synthetic biology approaches to expand the genetic code of selected strains will be deployed to make them strictly dependent on the presence of a non-standard amino acid (nsAA) in order to return to their vegetative state. Furthermore, novel routes to convert complex polyethylene terephthalate (PET) plastic with added co-monomers into valuable industrial diamines will also be engineered into the plastic-degrading strains. Overall, this research will not only gain fundamental understanding of spore biology for solvent tolerance and germination but also advance towards developing biological engineering approaches to produce valuable industrial chemicals from plastic waste.

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

Rigorous Quantum Simulation Tools for Correlated Attosecond Electron Dynamics in Molecules

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The recent creation of intense, ultrashort attosecond laser pulses ranging from the infrared to the x-ray regime has the potential to ultimately enable direct control of the motion of electrons and nuclei in matter to create new materials, and to develop new types of spectroscopy. To achieve these goals, it is necessary to develop a detailed theoretical understanding of the complex behavior of electrons and nuclei in molecules subject to extremely short, intense, and energetic laser fields. This requires elucidating the electron-electron and electron-nuclear correlation effects that control attosecond electron dynamics in molecules. In this proposal, we will achieve this by developing new numerical approaches to simulate attosecond dynamics based on first-principles quantum mechanics. The new tools we develop will fully include the correlated electronic motion, which will make it possible to study the rapid migration of a localized, positive charge cloud in a molecule (charge migration) and the coherent oscillation of electron holes in molecules following core ionization. Using molecules of experimental relevance such as phenylalanine and other aromatic molecules, we will explore the impact of different functional groups in molecules and ionization from different orbitals onto the electron dynamics, and we will interpret recent experiments on attosecond delays during ionization. We will gain insights from extracting orbital and quantum entanglement information from the time-dependent many-electronic wavefunction, and map them to common chemical concepts. Further, we will study how nuclear displacements influence the electronic motions, and how this affects the controllability of attosecond processes. The methods developed through this project will significantly extend capabilities to realistically simulate attosecond electron dynamics with explicit laser fields, and will clarify questions related to a fundamental understanding of coherent, correlated, and ultrafast electronic processes.

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

Chemo-Rheological Controls on Subsurface Stress Heterogeneity in Geothermal Systems

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This research explores how time-dependent rock deformation and chemical reactions affect the distribution of stress deep underground in geothermal systems. Understanding how stress evolves in these environments is essential for advancing enhanced geothermal systems, which can unlock vast energy resources by engineering hot rock formations to produce electricity. The project focuses on high-temperature rocks, where stress builds and relaxes over time due to a combination of mineral changes and mechanical strain. Laboratory experiments will simulate the extreme conditions found in geothermal reservoirs. Rock samples from active geothermal sites will be subjected to stress while chemical changes are tracked using advanced chemical tracers. These data will help scientists and reservoir engineers better understand how minerals dissolve, grow, and influence the behavior of the surrounding rock. To translate these insights to real-world applications, machine learning models will be developed to predict stress patterns using field data, such as measurements from geothermal wells. The project will also refine models that describe how granite and related rocks deform under geothermal conditions. The outcomes will improve the ability to manage and design geothermal energy systems with greater safety and efficiency. By revealing how chemical and mechanical processes interact below the surface, this work supports the Department of Energy's mission to expand abundant, reliable energy sources. It also contributes to national efforts to strengthen subsurface engineering, reduce the risk of induced seismicity, and accelerate the deployment of geothermal power as a cornerstone of the future energy landscape.

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

Multidimensional Optical Probes of Quantum Materials

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The signatures of many vital physics of quantum materials (QM) are often obscured and ambiguous in conventional material probes developed for more traditional material systems. This program aims to apply optical analogues of nuclear magnetic resonance, so-called multidimensional optical spectroscopies, for disentangling the intricate physics of QMs. We will implement these multidimensional probes across the electromagnetic spectrum to study the full range of QMs of interest to the Department of Energy toward understanding two outstanding challenges in QMs, namely that of interacting degrees of freedom and disorder.

To probe excitations at low-energy scales, we will implement multidimensional terahertz spectroscopy (MDTS) toward studying coupling and disorder of collective excitations in three-dimensional quantum materials. Initial experiments will focus on applying MDTS toward elucidating disordered quantum phases such as quantum paraelectricity and quantum spin liquidity as well as characterizing strongly coupled spin and lattice degrees of freedom. To probe electronic transitions in defect centers, we will combine multidimensional spectroscopy at optical frequencies with a scanning laser microscope to implement multidimensional optical microscopy (MDOM). Combining the capabilities of multidimensional spectroscopy with diffraction-limited spatial resolution, MDOM can both measure higher-order correlations between defect centers as well as characterize defect center disorder across all salient length scales (nm-mm). Initial experiments will focus on the physics of QMs detailed above at thermal equilibrium, and progress to studying QMs driven out-of-equilibrium with light.

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

Building a Scalable Ultrasensitive Quantum Sensor Array with High-Fidelity Remote Quantum Entanglement

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Dark matter remains a fundamental yet elusive component of the universe, defying direct detection despite extensive scientific efforts. Haloscope experiments leverage microwave cavities to probe wavelike dark matter candidates such as axions and dark photons, but their extremely weak interactions and unknown signal frequencies make detection especially challenging. Quantum information science offers promising tools to boost detection sensitivity and reduce noise, yet building a practical and scalable quantum sensor network with significant quantum advantage remains an open challenge.

This project aims to develop a novel quantum sensor array based on high-coherence superconducting radio-frequency cavities, incorporating cutting-edge quantum technologies such as high-fidelity remote entanglement, large Fock state initialization, and quantum non-demolition photon counting. These techniques will be integrated into a unified experimental platform for dark photon detection, enabling a substantial enhancement in sensitivity that scales with both the number of sensors and the stored photon number. The project will significantly improve the performance of distributed quantum sensing and demonstrate a measurable quantum advantage in dark matter detection. Additionally, outcomes from this research will guide the design of magnetically resilient, broadband-tunable devices, enabling a broader class of dark matter searches, including axion detection.

Beyond its primary focus, the developed sensor array lays the foundation for a modular quantum computing platform with high-quality interconnections, advancing distributed quantum computing and quantum communication.

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

Diodic Light-Matter Interactions Enabled by Quantum Dipoles in 2D Topological Crystals

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In the vicinity of massive objects, spacetime is curved, bending the trajectory of light and giving rise to phenomena such as black holes and gravitational waves. Analogously, the quantum world of electrons exhibits a geometrical structure encoded in their wavefunctions. This quantum geometry, characterized by quantities such as the quantum metric and Berry curvature, can fundamentally alter electronic behavior in solids. Moreover, quantum geometry is intimately connected to topological phases of matter—an area that has become central in condensed matter physics over the past two decades.

This project investigates how quantum geometric properties influence light-matter interactions and charge transport. A central focus is the generation of photocurrents, whereby light or alternating electromagnetic fields are rectified into direct currents. These effects underpin key technologies, including solar cells, terahertz and infrared photodetectors, optoelectronic sensors and energy harvesters. Conventional photocurrents rely on junction-based mechanisms—such as p-n interfaces, Schottky barriers, or tunneling junctions—to separate charges. In contrast, a new class of intrinsic photocurrents has recently been identified in homogeneous materials without junctions. These arise directly from the interaction of light with asymmetric charge, spin, and lattice configurations within a unit cell, and are fundamentally governed by the quantum geometry of electronic wavefunctions.

We aim to experimentally investigate how such intrinsic diodic light-matter interactions can emerge from quantum dipoles—specifically, Berry curvature and quantum metric dipoles. These dipoles are purely quantum mechanical constructs residing in momentum space, in contrast to classical charge dipoles that exist in real space (e.g., at p-n junctions). In this project, we will demonstrate the existence and characteristics of quantum dipole-driven photocurrents and develop their use as sensitive probes of complex charge and spin textures. Furthermore, we will establish experimental methods to actively control quantum dipoles and steer photocurrent flow. Our research combines material design and realization, advanced optical and transport measurements, theoretical modeling, and high-dimensional data approaches to advance the understanding and control of quantum geometric photocurrent phenomena.

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

Unearthing Rhizosphere Controls on Methane Emissions from Northern Peatlands

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Peatlands and other terrestrial-aquatic interfaces (TAIs) contribute significantly to the total methane (CH_4) produced from natural systems globally. However, estimates of TAI contributions to the total global CH_4 production are highly variable, ranging from 25 to 55%. This staggering uncertainty stems from a lack of process understanding of factors governing CH_4 production across these spatiotemporally heterogeneous systems. Northern peatlands are one such system that releases significant amounts of CH_4, but processes at the interface of peatland soils and plant roots, i.e., in the rhizosphere, are especially poorly understood. Roots may be an important driver of CH_4 dynamics because substrates released from roots fuel CH_4-producing microbes. Furthermore, plants act as conduits for CH_4 exchange between soils and the atmosphere. Despite their important role in CH_4 cycling, we lack measurements and models that effectively represent rhizosphere processes in northern peatlands. This research aims to close a critical knowledge gap by unearthing rhizosphere controls on CH_4 to improve our mechanistic and predictive understanding of CH_4 emissions from northern peatlands. The project will characterize global variation in CH_4-relevant root traits through field measurements and laboratory experiments. These root-CH_4 relationships will then be incorporated into peatland models, ultimately aiming to reduce model uncertainties now and into the future. Project outcomes will provide long-needed advances in our fundamental knowledge of rhizosphere processes that influence CH_4 dynamics in TAIs.

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

Structure and Function of Mitochondrial Respiratory Complexes in Brown Algae

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Brown algae—photoautotrophic organisms that evolved independently from plants and green algae—are major primary producers and key contributors to the global carbon cycle. Understanding the molecular details of their energy metabolism has strong biological, ecological and economic implications. Moreover, their distance from the green lineage allows us to expand our fundamental knowledge of bioenergetics and uncover new structure-function relationships. Despite this, our knowledge of how brown algae capture or convert energy is highly limited, particularly from the biochemical and biophysical perspective.

The goal of this proposal is to uncover the molecular basis of the bioenergetics of brown algae and provide mechanistic reasons for their differences with other photosynthetic or heterotrophic groups. My overall hypothesis is that the energy-converting complexes of brown algae have lineage-specific composition, structures and regulation that adapt them to their bioenergetic environment. We will test this with biochemical and cryo-electron-microscopy structural approaches to characterize the structure and function of mitochondrial electron transport chain complexes (complex I-IV) from *Macrocystis pyrifera* (giant kelp).

By broadening our mechanistic understanding of bioenergetics beyond the green lineage and laying the foundation for new strategies for carbon sequestration, this work will directly contribute to the DOE BES Physical Biosciences mission.

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

PECS: Protein Ensemble Compound Screening for Biothreat Response and Drug Discovery

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Proteins, dynamic molecular machines, play key roles in a wide array of important biological phenomena, from human antibiotic resistance to photosynthesis to age-related conditions like Alzheimer's disease. To control biological processes for medical or industrial applications, it is critical to understand how proteins move, change shape, and interact with other molecules. With the power of synchrotron X-rays, like those produced at Department of Energy light sources, researchers can catch glimpses of protein structures, down to individual atoms. Current methods, however, often only capture a single, static snapshot of a protein, missing crucial information that informs the structure-to-function relationship.

This research project will provide an expansive view of proteins in action, with new tools needed to capture, extract, and apply dynamics information. By leveraging advanced crystallographic techniques at the Stanford Synchrotron Radiation Lightsource (SSRL), this project will produce X-ray diffraction data revealing protein motion at the atomic level. New software, leveraging machine learning and physics-based simulations, will drive crystallography experiments to explore the protein's structural landscape and translate the data into detailed, movie-like models of how proteins work. A critical focus will be how proteins interact with potential drug molecules, explored by steering experimental conditions to induce structural changes that promote drug binding. These experimental results will be used in high-performance computing applications to rapidly predict new drug candidates for further testing. The project will focus on key proteins involved in antibiotic resistance and develop a general protocol that will extend to other applications in medicine, agriculture, and national biopreparedness, including the ability to rapidly combat emerging biothreats.

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

Randomized protocols for robust quantum optimal control and noise characterization

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Developing resource-efficient strategies to reduce noise in quantum processors is essential for their practical large-scale deployment. This project aims to design randomized quantum optimal control protocols to implement noise-resilient quantum gates and develop more efficient coherent noise characterization methods. By leveraging probabilistic protocols, our approach can significantly suppress systematic errors caused by imperfect characterization or slow-varying environmental noise, enhancing the overall accuracy of quantum gates. Additionally, these advancements enable more efficient calibration procedures without increasing resource demands, making them highly practical for scalable quantum computing. The proposed framework offers a natural integration of cost functions and optimization techniques relevant to stochastic control, including those derived from optimal transport theory. Methods for implementing noise-aware randomized control protocols will be investigated. In addition to analytical and numerical performance assessments, the protocols will also be experimentally tested on quantum hardware.

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

Embracing Performance Variability to Design Efficient, Accelerator-Rich Exascale and Beyond HPC Systems

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Modern high performance computing (HPC) systems typically use many accelerators, like GPUs, to improve efficiency. While these systems are vital for groundbreaking research in domains including HPC, scientific computing, and machine learning, they suffer from inconsistencies where even identical components deliver differing performance. This performance variability leads to significant inefficiencies: underutilized resources, longer computation times, and increased energy consumption, ultimately driving up operational costs. Thus, performance variability is a significant challenge in existing HPC systems and will become even more important in future, even larger, HPC systems. Therefore, we propose a novel approach that actively embraces and leverages this variability to transparently improve system utilization, performance, and energy efficiency of current and future HPC systems. To achieve this, we propose a solution that spans the computing stack. First, we will develop cutting-edge methodologies to accurately quantify performance and temperature fluctuations not just across different accelerators, but also across chiplets on a given accelerator. This detailed data will then inform the creation of variability-aware job schedulers for existing HPC systems. These intelligent schedulers will ensure that computational workloads are strategically matched to accelerators with similar performance and temperature characteristics, drastically reducing processing delays and significantly boosting overall system utilization and energy efficiency. Next, we will leverage our findings on current HPC system to influence the design of future HPC systems. By designing applications, hardware, and system software together, we will holistically expose and manage performance variability. This will enable dynamic adjustments to system parameters and enable intelligent workload management, further enhancing efficiency. Ultimately, by embracing performance variability we will develop more efficient, scalable, and fully utilized exascale and beyond HPC systems, and accelerate scientific discovery.

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

Improvement of optimized stellarator performance via low-Z impurity injection

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This project explores low-Z powder injection as a potential means to significantly improve the performance of an optimized stellarator, using a combination of experiments and numerical simulations. Indeed, boron (B) powder injection was recently shown to improve performances in the Large Helical Device, a non-optimized stellarator, reducing wall recycling and intrinsic impurity concentration, and more notably allowing the access to a reduced-turbulence, improved-confinement regime. A similar improvement was observed in the WEST tokamak as well, and in pulsed powder injection experiments in W7-X, although only transiently. W7-X is an “optimized” stellarator, where the magnetic field has been tailored to reduce neoclassical transport, and turbulence is the main drive of energy transport, similarly to tokamaks.

In this project, the Impurity Powder Dropper (IPD), which is being installed in W7-X and will be operative in 2026, will be used to experimentally demonstrate improvements in an optimized stellarator upon powder injection. Improvements in 3 main areas are expected: i) reduction of wall recycling and intrinsic impurities concentration, ii) reduction of turbulent transport and improvement of confinement, iii) increase of density limit through reduction of intrinsic impurities and/or edge turbulence. Leveraging the presence of an almost identical IPD system in WEST, where similar performance improvements have been observed with B powder injection, will allow us to directly compare this type of experiments in tokamaks and stellarators, highlighting common underlying physical mechanisms as well as possible differing behaviors in the two magnetic geometries.

To have a better understanding of the physical phenomena causing the expected improvement and interpret correctly the experimental results, a substantial numerical modeling effort is needed. The capabilities of the SOLEDGE3X code will be extended to include fully 3D magnetic geometry. This would allow us to model self-consistently the transport of impurities in the turbulent edge plasma of a stellarator, up to the first wall. To validate the simulation against experimental measurements, a new dedicated filtered visible camera monitoring the evolution of line radiation from B ions around the powder injection location will be installed, to be shared in between WEST and W7-X.

The interpretation of the extensive experimental database resulting from this project through the comparison with theoretical models, supported by the newly developed numerical modeling capabilities, and the unique possibility to directly compare tokamak and stellarator geometry, will provide a better physical understanding of the performance improvement via B powder injection, finally resulting in predictive capabilities that can be applied to future fusion magnetic confinement reactor scenarios, be it tokamak or stellarator.

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

Precision Studies of Neutron Spin for Flavor Decomposition

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This research explores how nucleon spin arises from its constituents, quark and gluon and their dynamics. While quark and gluon spins account for only part of the total, the distribution among quark flavors and the role of orbital angular momentum remain poorly understood. By scattering polarized electrons from a polarized ^{3}He target—an effective polarized neutron—this work will provide high-precision data to map quark spin contributions and their dependence on transverse momentum, offering new insight into the nucleon's three-dimensional structure and origin of spin. To enable these measurements, a high-field-compatible polarized ^{3}He target is being developed for use with the Large Acceptance Spectrometer at Jefferson Lab (CLAS12). This unique setup will enhance data precision and coverage, supporting broader efforts at Jefferson Lab and the future Electron-Ion Collider. Together, the experiment and target development will help resolve the longstanding nucleon spin puzzle and deepen our understanding of the fundamental structure of matter.

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

Rethinking in Silico Photoreaction Discovery Through a Seam-Driven Probabilistic Model

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In today's "Control Age," chemical innovation hinges on precisely tuning molecular properties through rational design. Photochemistry exemplifies this control, using photons to precisely trigger otherwise inaccessible rearrangements. However, despite its sustainability advantages, broader use of light-driven reactions is limited by low quantum yields and poor selectivity. Simulations have become indispensable for optimizing photochemical pathways, offering mechanistic insight and shifting the focus from post hoc explanation to predictive power. Routine *in silico* screening of new molecular systems is currently hindered by the computational cost of the tools available to explore nonadiabatic events. New strategies towards the streamlined modelling of photochemistry are urgently needed.

To address this demand, the central objective of this research is to identify predictors for conical intersection and photoproduct accessibility, and use the gained knowledge to develop an automated photoreaction discovery framework capable of quantitatively predicting photoexcitation outcomes. The crux of the work is characterizing the entire energetically accessible intersection seam (i.e., the (N-2)-dimensional manifold in nuclear coordinate space where the two electronic states are degenerate), identifying the relevant conical intersection types the seam is composed of, and mapping their connections to available photoproducts enable the comprehensive prediction of photoexcitation outcomes, including rare events. This research addresses these challenges in a three-pronged approach: (1) development of a probabilistic model for the prediction of photochemical reactivity, (2) advanced analysis of large nonadiabatic dynamics datasets to define conical intersection representativeness, and (3) implementation of efficient frameworks for comprehensive seam mapping.

By critically evaluating the delicate interplay between variables, and its calculation through cost-effective sampling, this work will pave the way for practical, predictive models that accelerate the design of light-driven molecular systems and synthetic routes. More specifically, if successful, this research will transform the way we think about photochemistry by answering the question: *what is the minimal amount of information required to predict photochemistry?*

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

Elucidating Operational and Chemical Factors Affecting the Function of Novel Polymeric Brush Active-Layer Membranes for Lithium Recovery from Aqueous Solutions

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Current methods fail to extract lithium and other critical materials from geothermal heat and petroleum industry brine streams using single-stage, energy-efficient separation methods. Separation challenges arise because of the complex chemical speciation present in the brine mixtures coupled with the presence of small, similarly charged ions. This project seeks to elucidate the mechanisms of ion separation, especially lithium from other ions, using an ultrathin polymer membrane. Two knowledge gaps regarding ion-ion selectivity in membrane-based separations are being addressed. First, membrane structure-function relationships are being determined by systematically manipulating membrane chemical compositions to probe the resulting ion selectivity. A primary focus is to determine if differences in the dehydration energy of species can be used as a basis of separation. For instance, while lithium and magnesium ions are typically difficult to separate because they are both positively charged with similar hydrated radii, they have dissimilar hydration energies. Better separation efficiency is targeted through the use of unique membrane structural gradients of charge, hydrophilicity, and pore size to sequentially unbind water molecules from ions, causing ions of lower hydration energy and higher dehydration propensity to reduce in size and permeate more easily. Second, relationships between species separation efficiency and feed stream composition are sought. Operating conditions and feed compositions, including adjustments to feed ion proportions and concentrations, temperature, and pH, are probed to mimic realistic feeds. Changes in feed composition affect membrane polymer conformation, extent of swelling, and functional group degree of dissociation and charge, impacting separation outcomes. Especially of interest is correlating membrane charge and ion adsorption capacity to flow-through ion-ion selectivity. This work addresses these knowledge gaps by leveraging the recently developed ultrathin brush active-layer membrane (BAM) platform to design a lithium-selective membrane. BAMs, which are comprised of a selective layer of densely grafted brush polymers on a mechanically robust and porous support, are produced using bottom-up surface-initiated atom-transfer radical polymerization, a technique akin to growing a membrane, monomer-by-monomer. Due to their high functional adjustability while maintaining ultra-thinness, BAMs are well-suited to elucidate fundamental structure-function relationships for ion selectivity. Crosslinker density, membrane thickness, functional group type and density, and membrane pore size are varied. Gaining a comprehensive understanding of the transport mechanisms through dense yet ultrathin polymeric membranes is expected to have implications for the development of membranes for high-value target separations involving complex solutions, especially those separating solutes with any level of charge or hydration. Such separations are important for the recovery of critical materials that face high levels of supply risk.

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

Quantum-Coherent Manipulation of Two-Level Systems via Wavefunction Engineering in a Scanning Electron Microscope

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Electron microscopes have proven to be invaluable tools for understanding the nanoworld, including the behaviors of individual atoms and molecules, as well as ensembles of these constituents. For example, cathodoluminescence and electron energy loss spectroscopy enable the measurement of band gaps and excitation energies at nanometer-scale spatial resolutions. However, fundamental information about quantum systems, like dephasing times, is generally inaccessible in electron microscopes. Typically, quantities associated with quantum coherence are measured via electromagnetic excitation, that is, with laser light. Such electromagnetic measurements have a notable limitation: the diffraction limit restricts the spatial localization of the exciting light and the resulting measurement. The central aim of this research project is to combine the nanometer-scale spatial resolution of scanning electron microscopy with the measurement capabilities of laser spectroscopy. The goal is to extend electron microscopes into the quantum realm. Specifically, a unique laser modulation system will be embedded in a customized scanning electron microscope (SEM) and will imprint density modulations onto the wavefunctions of passing electrons. If the modulation matches a harmonic, or sub-harmonic, of the resonance of a quantum system, the electrons may coherently interact with and probe the system. In this project, two common, two-level quantum systems, nitrogen-vacancy centers and quantum dots, will be probed. By carefully exploring cathodoluminescence signals, dephasing times and coupling strengths associated with these systems will be extracted at unprecedented spatial resolutions. Overall, in this project, a conventional SEM will be transformed into a unique tool potentially capable of coherently driving and measuring two-level quantum systems. This instrument, and the proof-of-concept experiments, could offer revolutionary opportunities in materials science, physics, and quantum information, as these quantum, two-level systems may, for the first time, be controllable and measurable at their natural spatial scale.

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

Structure-preserving data reduction and processing for particle representations

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Developing data reduction tools for large-scale particle datasets is essential to address the DOE Office of Science's network, storage, and computing needs in the exascale era. Unlike generic black-box compression methods, our proposed approach emphasizes preserving the intrinsic structures of particle data, thereby retaining critical kinetic physics with minimal information loss. We consider both static and dynamic particle datasets. The first thrust introduces a novel particle-based distribution representation that naturally bridges conventional particle representations and their moments, accompanied by a unique low-pass filter specifically designed for moment data. The second thrust addresses dynamic datasets through nonlinear, structure-preserving reduction techniques applicable to both dissipative and non-dissipative particle dynamics. Additionally, we will advance asymptotic-preserving model discovery by embedding multiscale structures explicitly into machine learning architectures, focusing especially on multiscale systems and closures for scale bridging. Our methodology will be validated using simulation and experimental datasets from DOE applications. Scalable deployment and open-source release of the resulting software packages are also critical objectives of this project. The outcomes of this project will broadly impact DOE mission areas, including fusion energy, accelerator physics, and nuclear physics.

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

Discovery and Synthesis of New Altermagnets for Quantum Geometric Properties

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Altermagnets represent a newly discovered class of magnetic materials that challenge the traditional dichotomy between ferromagnets and antiferromagnets. Combining zero net magnetization with spin-split electronic bands arising from unconventional magnetic symmetries, altermagnets provide a promising platform for novel spintronic functionalities. Despite their potential, the quantum geometric properties of altermagnets—particularly Berry curvature and quantum metric—remain largely unexplored. This project aims to discover and synthesize new altermagnets and to systematically investigate how their unique magnetic symmetries give rise to enhanced quantum geometric responses and associated transport phenomena.

The project is guided by the hypothesis that symmetry-protected band crossings in altermagnets, which are spin-degenerate in the absence of spin–orbit coupling, become weakly gapped when spin–orbit interaction is introduced. These avoided crossings lead to sharply concentrated Berry curvature and quantum metric features—key ingredients for anomalous and nonlinear transport. We will synthesize high-quality single crystals of altermagnetic candidates with diverse magnetic symmetries and characterize their electronic and magnetic properties. Anomalous Hall, elasto-Hall, and nonlinear transport measurements will be used to probe Berry curvature and quantum metric effects. The project will not only provide critical insights into an emerging area of condensed matter physics but also disseminate well-characterized crystals to the broader community, enabling advances in spintronics, low-dissipation electronics, and quantum information science.

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

Effects of Oxygen on Recalcitrant Carbon in Soil Aggregates: Implication for Hot Spots and Moments of Nitrous Oxide Production, Consumption, and Flux

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Anoxic microsites that develop within organic-rich soil aggregates are "hot spots" for a wide range of biogeochemical processes, including denitrification and the production and consumption of nitrous oxide (N_2O) along subsurface hydrological flowpaths. Despite the biogeochemical importance of these microsites, the development of redox gradients within aggregates and couplings between redox-sensitive reactions within aggregates and fluxes of solutes in bulk water are poorly-represented in predictive models. This project investigates the counterintuitive role that molecular oxygen (O_2) can play as an essential and often limiting factor in the development of anaerobic microenvironments within soil aggregates, due to the role of O_2 as a driver of lignocellulosic carbon degradation into more labile forms of organic carbon (OC). This introduces a feedback loop wherein O_2 exposure enhances the electron-donating capacity of aggregate carbon and thereby further enhances the consumption of O_2 and other electron acceptors, influencing denitrification and the production, consumption, and flux of N_2O. The scientific goal of this project is to build a predictive model framework that describes the role of O_2 in "unlocking" recalcitrant OC in organic-rich soil aggregates, and to use this framework to explain spatiotemporal variability in coupled nitrogen (N) and C dynamics in soils at terrestrial-aquatic interfaces. The specific objectives of this project are to: (1) Determine links between O_2 exposure, the electron-donating capacity of organic carbon in aggregates, and the source/sink dynamics of N_2O along hydrologic flowpaths; (2) Characterize micro-scale gradients in redox states and anaerobic metabolism within aggregates as a function of hydrologic regime and O_2 exposure; and (3) Connect biogeochemical gradients within aggregates to the source/sink dynamics of N_2O and other solutes along hydrologic flowpaths with process modeling. These objectives will be addressed through a series of cross-scale laboratory experiments that connect variability in hydrologic transit times and O_2 concentrations to the development of redox gradients within soil aggregates and the biogeochemical processing of N and C along subsurface flow paths. Flume experiments with synthetic organic-rich aggregates will be used to develop Damköhler number approaches to characterize the balance between reaction and transport timescales in terrestrial-aquatic interfaces as a control on the source/sink dynamics of N_2O, while detailed geochemical and microbial characterization methods will link bulk O_2 concentrations to micro-scale gradients in redox conditions and anaerobic metabolism within aggregates. Mathematical modeling will be used to connect bulk water chemistry to the development of redox gradients within aggregates through the exchange of solutes and dissolved gases.

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

How Electric Fields Influence Reactivity in Thermochemical and Electrochemical Catalysis

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Heterogeneous catalysts play an essential role in producing fuels and chemicals vital to modern society. Traditionally, strategies for optimizing the performance of heterogeneous catalysts have focused on tailoring the composition and structure of catalytic active sites. However, the environment surrounding these active sites also has a significant impact on catalytic performance. In particular, the strength of the electric field present at the catalyst surface has an important influence on measured rates. Despite their importance, the precise mechanisms by which electric fields affect catalytic reactions in both electrochemical and thermochemical systems remain poorly understood. This research aims to establish a comprehensive understanding of how interfacial electric fields alter catalytic reaction rates and selectivities. Leveraging these insights, we propose new approaches to control electric fields to enhance catalytic performance. Specifically, we hypothesize that adjusting the local electric field strength through modifications of the reaction medium will directly impact the energies of key reaction intermediates and transition states, ultimately influencing overall catalytic efficiency.

Our work leverages a combination of advanced experimental and computational techniques to gain molecular-level insights into the role of electric fields on catalytic performance. Complementary vibrational and ambient-pressure photoelectron spectroscopies will be used to directly quantify electric field strength and describe how these fields change in response to the reaction medium. Rigorous kinetic analyses and atomistic calculations will quantify the influence of these electric fields on reaction energetics. This project will yield fundamental knowledge enabling the rational design of next-generation catalysts with high efficiency through precise control of interfacial electric fields that could potentially improve catalytic technologies critical for energy conversion and chemical manufacturing.

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

Wigner-Dyson Universality Classes in Molecular Quantum Processes at Interfaces

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Modern molecular-scale fabrication techniques allow systematic control over molecular assembly synthesis on solid-state substrates, from metals and semiconductors to topological insulators and semimetals with strong spin orbit coupling. This capability opens pathways to quantum engineering of hybrid systems with enhanced charge, energy, and spin transport for transformative applications in energy conversion, quantum information technologies, and catalysis. Realizing this potential demands a detailed understanding of how quantum properties of the solid-state substrate steer molecular processes at the interface. This project will address this challenge by developing a conceptual framework for molecular interfacial science based on random matrix theory and the Wigner-Dyson universality classes, which classify quantum systems according to their time-reversal symmetry and spin-orbit coupling properties. Through large-scale computational simulations and theoretical analysis, this research program will (i) elucidate how each Wigner-Dyson class shapes molecular quantum kinetics at low-temperature interfaces, (ii) quantify the robustness of coherent quantum statistical effects under thermal fluctuations, and (iii) devise strategies for substrate-aided control of local molecular processes such as electron transfer and intersystem crossing. By connecting fundamental statistical properties of disordered quantum environments to observable molecular phenomena, this work will provide quantitative predictions describing how distinct universality classes and molecular-substrate interactions impact chemical processes. The derived theoretical framework will establish new design principles for identifying optimal substrates that control charge, energy, and spin processes in molecular systems, directly supporting the development of next-generation energy materials, quantum sensing technologies, and catalytic platforms.

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

Quantum Networking for Efficient and Robust Distributed Services

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Quantum networking is essential to unlocking the full potential of quantum information science and quantum computing technologies. Initial laboratory demonstrations have validated key quantum networking primitives, such as heralded remote entanglement generation and storage, and entanglement swapping. Current efforts—including those at DOE-supported quantum network test beds—are focused on advancing from proof-of-concept experiments to scalable, operational quantum network systems. Achieving this transition requires a functionally layered network stack with reliable, efficient, and scalable protocols that support a wide range of quantum distributed services. While several protocol stacks have been proposed, many foundational design decisions remain unresolved, particularly concerning network architecture, protocol development, and the management of hybrid quantum resources and user requests. This proposal addresses these gaps by developing new node-, link-, and network-level theories tailored to finite-resource, software-defined quantum networks. We will integrate techniques from entanglement theory, quantum information, optimization, and queuing and scheduling theory to create a comprehensive analytical framework for evaluating performance, cost, and feasibility. Project deliverables include: i) a performance evaluation toolkit to define scalability, reliability, and efficiency bounds—with and without near-term hardware constraints; ii) design principles for building robust, efficient, and adaptable network architectures and protocols, with an emphasis on enabling distributed fault-tolerant quantum computing and quantum cloud computing; and iii) an integrated software stack for implementing and testing optimized protocols on DOE quantum network test beds. By bridging rigorous theoretical foundations with deployable software, this project will accelerate the shift from lab-scale experiments to practical quantum networking infrastructure, directly supporting the DOE's mission to advance foundational quantum technologies.

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

Quantum Confined Light-Matter Interaction in Novel Magnets

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Quasiparticles, the collective excitations that emerge from the interactions of many particles, have captivated physicists for decades. Unlike the dozens of fundamental particles that are the building blocks of the known universe, quasiparticles are emergent and constantly advancing our understanding of matter and enabling technological advances. From n-/p-type doping in transistors to excitons (bound electron-hole pairs) in solar cells, quasiparticles fundamentally reshape how we manipulate semiconductor devices, which power much of modern technology. Today, a century after the birth of quantum mechanics, we are entering an exciting era where harnessing the quantum nature of matter is vital for next-generation technologies. In this endeavor, light-matter interactions play a pivotal role in both deciphering quantum behaviors of matter and promoting transformative technological advances.

This project unites state-of-the-art optical spectroscopy and near-field nano-imaging techniques to investigate layered quantum matter, with an emphasis on van der Waals (vdW) magnets. Broadband optical spectroscopies excel at uncovering novel quasiparticles and dissecting their mutual interactions across the electromagnetic spectrum (ω). The PI will utilize the newly discovered magnetically confined excitons as nanoscale probes of both the dielectric and magnetic environments, exploring correlated spin-excitations inaccessible to non-magnetic excitons.

Complementarily, near-field nano-imaging adds the crucial momentum (q) information in the dielectric response $\varepsilon(q,\omega)$, enabling real space visualization of terahertz/infrared optical responses at deep-subdiffractional length scales. By hybridizing novel confined quasiparticles with light to form polaritons, the PI will implement photonic cavity designs to further enhance and control the spatial confinement (finite q) and propagation (direction of q) of polaritons. Together, these approaches will illuminate quantum confined light-matter interactions in vdW magnets and lay the groundwork for future quantum technologies.

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

Macroscopic Quantum Mechanics and Microscopic Thermodynamics with Optically Levitated Nanoparticles

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This project is focused on foundational Quantum Information Science research involving the creation of macroscopic quantum states and the study of thermodynamics at microscopic scales. These efforts address essential scientific questions about the limits of quantum coherence and control, which are central to advancing quantum technologies and understanding how quantum principles govern physical systems at macroscopic scales.

The research will use optically levitated nanoparticles, tiny dielectric spheres held in place by laser light, as a building block to create collections of correlated quantum particles. These systems offer exceptional isolation from the environment and access to both mechanical and optical degrees of freedom, making them well suited for exploring quantum effects. The project will develop new techniques for coherent quantum control of multiple particles by combining laser trapping, structured light-matter interactions, and real-time quantum measurement and feedback. This approach, particularly coupling multiple particles to a common light field confined in an optical cavity, will enable the investigation of many-body quantum dynamics and the behavior of energy and information flow in regimes where classical thermodynamics no longer applies.

This work is expected to generate new insights into quantum correlations, coherence, and thermodynamics in engineered nanoscale systems. These results will contribute directly to the scientific foundation needed for controlling complex quantum systems and designing more robust quantum devices. In the long term, this research may lead to the development of new types of energy-efficient quantum technologies that operate by harnessing macroscopic quantum effects.

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

Magnetic Properties of Cobalt-bearing Minerals

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Cobalt is a rare and critical element for the energy transition due to its use in electrical vehicle batteries. While cobalt is known to be a permanent magnet, the magnetic properties of the more common cobalt minerals, which are mined for this element, are poorly understood. The goals of this project are to gain a better understanding of the magnetism of cobalt minerals in the context of their natural occurrence.

This project will integrate experimental and modeling data to elucidate the magnetic properties of cobalt-minerals and the wide variety of phenomena observed within natural samples. Synthetic and museum specimens of six cobalt-sulfide minerals will be magnetically analyzed to understand their properties across a range of temperatures and grain sizes. Additionally, magnetic microscopic mapping using the novel quantum diamond microscope will verify that small crystal impurities are not driving magnetic properties. Computational modeling will be performed to compare these empirical magnetic properties to those derived via calculations at the atomic and nanometer scale to understand their physical underpinning. Diving deep into the magnetism of cobalt minerals will help us understand the nature of mineral magnetism more fundamentally; most research is focused on experimental observations of iron oxides so studying cobalt sulfides through both experiments and modeling presents an exciting counterpoint.

Building upon this project's mineral magnetic analyses, rock samples from the Black Butte Deposit, Montana, United States will be analyzed to directly show applicability in understanding the formation processes of cobalt-bearing minerals and their distribution in ore deposits. In addition to using conventional and magnetic microscopes, synchrotron-based X-ray microprobes would be used to confirm mineralogical interpretations. This locality will provide a test-case to illustrate how bulk and microscopic magnetic tools could be more widely applied to understand cobalt-bearing deposits and predict resource distribution. Magnetism and magnetic properties are rarely utilized in the mining industry beyond aeromagnetics; the proposed work would highlight the utility of these tools and thus, ideally, stimulate mineral magnetism research, a field which lags far behind research on synthetic magnetic materials.

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

Hierarchical Representations of Complex Physical Systems with Euclidean Neural Networks

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Scientific data often reflects two fundamental principles: symmetry, which governs how systems behave under transformations like rotation or reflection, and hierarchy, where structure emerges across multiple spatial or organizational scales. This project develops machine learning methods that are both symmetry-preserving and hierarchy-aware to model complex physical systems, from molecules and materials to fluid flows and galaxies.

At the core of this work are Euclidean Neural Networks, a class of models that preserve the geometric symmetries of physical space. These models will be extended to capture patterns across scales by learning how to group, compress, and represent scientific data while retaining essential structural information. The project also investigates how such models can generate new data, including novel materials, molecular structures, fluid flow patterns, protein conformations, and cosmological structures, while respecting or selectively breaking symmetry. This capability supports both creative exploration and precise control of physical systems.

Key research goals include understanding how symmetry shapes learned representations, developing efficient and interpretable hierarchical models, and applying these models to tasks such as simulating physical systems, performing uncertainty quantification of simulations and measurements, and enabling search within large scientific datasets.

The resulting open-source tools will be designed for efficient deployment on DOE supercomputers, enabling large-scale analysis and simulation in support of national scientific missions. By combining geometric reasoning, scalable AI, and physical insight, this research will advance scientific discovery across scales, from atomic interactions to cosmic structure, in fields such as materials, biology, fluids, and engineered systems.

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

Engineering Photosynthetic Energy Transfer with Polariton Light-Matter Interactions

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Photosynthesis depends on a complex network of pigments embedded in proteins to absorb sunlight and efficiently direct energy through the system. While past research has revealed important details about how this energy flows, methods to systematically control and optimize these pathways have remained limited. This project seeks to overcome that challenge by developing a new photonic platform to modulate energy flow within photosynthetic systems. The approach relies on strong light–matter coupling, a phenomenon in which light confined within an optical microcavity interacts strongly with electronic transitions of the light-harvesting pigments. This interaction gives rise to hybrid light–matter states known as exciton-polaritons, which shift the pigments' energy levels and reshape the pathways of energy transfer. In contrast to traditional bioengineering methods that physically alter protein structures, this approach provides a non-invasive and tunable means of controlling photophysical dynamics. Advanced ultrafast spectroscopic techniques—such as two-dimensional electronic spectroscopy—will be employed to examine how exciton-polaritons influence energy relaxation in individual pigments, energy transfer within light-harvesting complexes, and communication between protein assemblies in both plant and bacterial systems. The outcomes of this work will provide new insights into the principles of efficient energy transfer in nature and inform the design of next-generation, bioinspired technologies for solar energy capture and conversion.

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

Designing Next-Generation Superconducting Quantum Devices via On-Device Synthesis

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Developing superconductors and superconducting devices is crucial for quantum information science, ranging from building superconducting qubits based on Josephson junctions to exploring topological qubits via the superconducting proximity effect. Two-dimensional (2D) materials and their van der Waals (vdW) heterostructures provide an emerging material platform for designing new superconducting quantum devices. In particular, highly crystalline superconductors can be synthesized directly within vdW heterostructures through a new lateral diffusion-reaction epitaxy approach, achieving atomically sharp and chemically bonded interfaces. Leveraging this on-device synthesis technique, the project will synthesize new 2D superconductors, fabricate Josephson junctions, and engineer hybrid superconducting systems. We will first employ on-device synthesis to grow highly crystalline superconductors and investigate the resulting synthesis-induced superconductivity using the vortex Nernst effect. Next, we will fabricate Josephson junctions by growing superconducting electrodes from both sides close enough to induce the Josephson effect into 2D materials, and we will study unconventional Josephson effects enabled by the highly crystalline nature of junction materials. We will then integrate the synthesis-induced superconductivity with novel quantum states in moiré superlattices to unlock new opportunities in topological quantum computation. The proposed work aims to establish a new material platform and a novel engineering pathway for designing next-generation superconducting quantum devices. More broadly, the research program will build on recent advances in two rapidly developing fields, 2D materials and quantum information science, to harness new opportunities enabled by their synergistic combination.

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

A Warm Revolution in Particle Tracking

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Silicon carbide is a promising semiconductor material for the next generation of detectors used in particle physics experiments. These experiments rely on precise tracking systems that measure the position and timing of subatomic charged particles as they pass through a detector. Future facilities will require sensors that can operate with micrometer precision, respond in billionths of a second, and remain stable over time while exposed to extremely high levels of radiation without depending on large and complex cooling systems. This research explores the potential of silicon carbide as the sensor material to meet these challenges, thanks to its wide electronics bandgap and natural resistance to radiation. These properties make it possible to build detectors that produce low background noise (known as leakage current) and function accurately at room temperature. This would simplify cooling and enable more compact, lightweight systems. However, silicon carbide has not yet been widely used in this field because it generates relatively small electrical signals in response to charged particles and is difficult to process using available techniques. It requires very high-temperature treatments and specialized equipment. This project addresses those challenges by developing a new type of silicon carbide detector known as a Low Gain Avalanche Detector, which includes an internal amplification layer to boost the signal amplitude. The fabrication process will use a technique called multi-energy, high-temperature ion implantation, performed with an accelerator at the Brookhaven National Laboratory, which is a leading center in Low Gain Avalanche Detector development. This approach allows precise tuning of the internal structure of the material without the need for complex crystal growth steps. The research is further supported by collaborations with North Carolina State University, which specializes in wide bandgap semiconductors, and Lawrence Berkeley National Laboratory, which brings expertise in detector design and modeling. In addition to advancing a promising new charged particle detection technology, this effort aims to help establish a national center for research and fabrication of wide bandgap semiconductor devices, supporting long-term priorities in the field of particle physics.

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

Conditional Kinetics: A Novel Paradigm for Multiscale and Multiphysics Modeling of Kinetic Equations

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Kinetic descriptions such as the Boltzmann and Vlasov equations are ubiquitous in the Department of Energy's (DoE) applications, including magnetic confinement fusion, nuclear fission energy, and high energy density systems. These systems are inherently complex and multiscale, where traditional macroscopic models alone—such as the Navier-Stokes equations and diffusion theory—often fail to provide the accuracy required for high consequence decision making, such as designing next-generation pulsed-power and fusion energy facilities. While the kinetic approach offers a more precise mesoscopic view of these systems, several challenges have limited its application at relevant scales. These include: 1) the need to efficiently and accurately resolve disparate spatio-temporal scales, 2) enforcing crucial physical constraints to ensure accurate long-time behavior, 3) handling tightly coupled multiphysics interactions, and 4) the exponential growth of computational cost with dimensionality, commonly referred to as the curse of dimensionality.

This project develops a novel multiscale, multiphysics framework that represents a significant advancement over existing methods for modeling kinetic equations. Our approach leverages the concept of conditional probability distributions, transforming the kinetic equation to decouple the evolution of conserved moment quantities from that of the full particle distribution function. This rigorous mathematical transformation disentangles the complex multiscale and multiphysics challenges of the kinetic equation, isolating them into more tractable companion moment equations. In this transformed system, critical mathematical symmetries—often the source of numerical difficulties—become significantly easier to address. Furthermore, the transformation reveals the underlying optimal solution structure, enabling the use of state-of-the-art low-rank tensor methods to overcome the curse of dimensionality. This capability opens the door to simulating a broader range of essential DoE applications at full system scale.

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

Chiral Effective Field Theory in the Age of Multi-Messenger Astrophysics

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In this research project, we will develop novel approaches to obtain a comprehensive and robust understanding of nuclear and electroweak forces in dense nuclear matter and atomic nuclei. With these approaches, we will address open issues that are of great importance to the theoretical description of nuclear systems: the importance of individual terms in the expansion of nuclear interactions and the range of validity of this expansion in dense nuclear matter.

Using Bayesian statistical inference, we will greatly improve models for nuclear interactions. We will develop new nuclear interaction models that account for all theoretical uncertainties and, using artificial intelligence (AI) and machine learning (ML), develop the machinery to propagate them to a wide range of nuclear systems, from atomic nuclei explored in the laboratory to dense matter explored in stellar environments. Our tools will be firmly rooted in the reliable quantum many-body computational frameworks that currently need high-performance computers to achieve high accuracy and precision. Using AI/ML, we will accelerate these codes to reduce their high computational cost. This will allow us to comprehensively study nuclear and electroweak forces in different nuclear systems and to estimate the importance of the different contributions. We will also use these studies to determine up to which densities these models remain reliable in astrophysical environments.

Our results will be critical for robust theoretical analyses of present and future multi-messenger observations of neutron stars and their mergers to constrain the dense-matter equation of state but will also have direct implications for the physics of neutron-rich atomic nuclei, probed in major experiments at the Facility for Rare Isotope Beams, and for dense nuclear matter probed at heavy-ion colliders, such as the Relativistic Heavy-Ion Collider. Furthermore, studies of electroweak processes in nuclei are important for electron scattering experiments at Jefferson Lab and other facilities in the US. Our project will also improve modeling and simulations of astrophysical processes, which will increase the fidelity of these simulations and enable us to obtain a better understanding of nucleosynthesis and the r-process in explosive astrophysical environments.

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

Probing the Chemistry of the Liquid/Vapor Interface by Infrared Action Spectroscopy of Solvent-Ion Nanoclusters

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This research investigates the unique chemical reactivity at liquid-vapor interfaces using solvent-ion nanoclusters as model systems. The project focuses on three main areas: (1) the interaction of gas-phase oxidants, such as ozone and hydroxyl radicals, with ions at the interface, exploring their role in multi-phase reactions typical of atmospheric particles; (2) the solvation structures of reaction complexes and reactive oxygen species, examining how they contribute to faster reactions and redox processes at the liquid-vapor interface; and (3) the temperature-dependent structure of water around surface-active ions, which provides new insight into the molecular interactions governing these interfaces.

This project combines electrospray ionization mass spectrometry (ESI-MS) with helium-nanodroplet isolation infrared (HENDI IR) action spectroscopy to study size-selected, charged molecular clusters. ESI-MS affords precise control over the investigated molecules, facilitating the isolation of target water-ion clusters, which can be further modified by the pickup of gas molecules within the mass spectrometer. Capture of carefully prepared ions within a helium nanodroplet cools these clusters to a near-absolute-zero temperature of -272.7 degrees Celsius. Cooling the molecules to this temperature enables the acquisition of high-resolution infrared spectra, revealing details of the molecular structure. In addition, the rapid cooling within the nanodroplet enables the preservation of high-energy or highly reactive species added to the droplet. These properties will be leveraged to study the properties of complexes inaccessible by other methods, such as those between ions and highly reactive oxygen species.

This research provides fundamental, molecular-level insights into the complex chemistry occurring at liquid/vapor interfaces, bridging the gap between theoretical models and large-scale experimental observations. Understanding interfacial reactions between ions and oxidants will enhance atmospheric models, improving predictions of atmospheric oxidizing capacity, aerosol composition, and radiative forcing, which impact air quality and climate. Furthermore, clarifying the mechanisms behind reaction acceleration and redox processes in microdroplets can inform the design of novel and efficient chemical synthesis strategies, including the conversion of typically non-reactive molecules into valuable chemical feedstocks. Finally, a more comprehensive picture of the orientation of solvent molecules around ions at the interface enables better predictions of ion reactivity in both microdroplets and aqueous aerosols.

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

Advancing the Gravitational Path Integral to Probe Quantum Spacetime

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The unification of quantum mechanics with special relativity led to the development of quantum field theory. This had a profound impact on fundamental physics since, for example, it is the framework in which the Standard Model is formulated. A satisfactory combination of quantum mechanics with general relativity has been more elusive and remains a central open problem in fundamental physics. This issue becomes particularly pressing in two circumstances: the interior of a black hole and the early universe. The goal is to develop the laws of quantum gravity through a theoretical analysis of such extreme situations and uncover their implications for our world.

Work in string theory inspired the holographic principle, a conjecture that black holes behave as unitary quantum systems with finite entropy. Growing evidence, arising from the application of quantum information techniques to black hole physics, suggests that the gravitational path integral offers a framework for quantizing gravity in a manner consistent with holography. However, the fundamental principles underlying this approach remain poorly understood. This project will compute the gravitational path integral in novel settings, aiming to clarify the structure of spacetime in regimes where classical intuition breaks down. These investigations will help lay the foundation for identifying concrete, potentially observable signatures of quantum gravity in black hole physics and cosmology.

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

VisTrust: Probabilistic Visualization of Univariate and Multivariate Scalar Data for Trusted Scientific Analysis and Discovery

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This project will research and create foundational techniques for the efficient understanding and communication of uncertainty in two- and three-dimensional (2D/3D) visualizations. This project will address the knowledge gap of how uncertainty is propagated in 2D/3D visualization by creating efficient and scalable probabilistic algorithms that can model, track, and convey uncertainty in large data.

Objective: By bridging UQ and visualization research, this project innovates theoretical and cost-efficient probabilistic techniques for 2D/3D uncertainty visualization to address challenges of state-of-the-art empirical techniques to enable scientists to perform trusted and timely data analysis.

Methods: To achieve efficient 2D/3D uncertainty visualization for trusted analysis, we propose three approaches. First, we will derive closed-form propagation of (probabilistic) uncertainty in visualization to address the lack of theory and significantly enhance algorithmic accuracy and efficiency over classical empirical techniques. Second, when closed-form visualization uncertainty is not derivable, we will research ML/AI/data-driven techniques to learn/approximate propagation of uncertainty in visualization for enhanced efficiency and scalability. Lastly, our probabilistic algorithms, combined with parallelization and cost-accuracy trade-offs, will overcome the inefficiency, limited scalability, and impracticality of state-of-the-art empirical techniques to provide reliable uncertainty-aware visualization.

Impact: At the end of the 5-year funding period, the proposed research will have created a foundation that scientists can use to efficiently visualize uncertainty in 2D/3D data for trusted analysis (VisTrust). A broad range of applications important to DOE ASCR research, including data reduction, data compression, ensemble analysis, ML/AI for science, and streaming data, will benefit from the proposed research. Specifically, our efficient and scalable uncertainty visualization algorithms will significantly reduce the time to assess uncertainty and build trust in results for these applications. Our research will be the key to overcoming the lack of a theoretical and cost-efficient framework for uncertainty visualization and to making such a framework accessible to a wider audience.

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

Thermodynamic Properties of Hot and Dense QCD Matter from Fluctuations of Conserved Charges

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Quantum chromodynamics (QCD) describes the strong nuclear force and explains how protons and neutrons bind, yet its phase structure under extreme conditions of temperature and density remains elusive. Above roughly a trillion Kelvin, nuclear matter melts into a quark–gluon plasma (QGP), the state that filled the early universe just after the Big Bang and is now recreated in the laboratory through relativistic heavy-ion collisions. Determining the phase structure of strongly interacting matter and the nature of the transition between ordinary nuclear matter and QGP is a central question in high-energy nuclear physics. This project will map the QCD phase diagram by combining first-principles lattice QCD calculations with precision studies of fluctuations and correlations of conserved charges – such as baryon number and electric charge – in relativistic heavy-ion collisions. New dynamical models will use these fluctuations to put stringent constraints on the existence and location of the long-sought QCD critical point, pinning down the boundary where the transition between ordinary matter and QGP becomes a sharp, first-order phase change. By supplementing this analysis with new constraints from lattice QCD, this research will deliver an improved equation of state of strongly interacting matter that links the hot plasma created in the laboratory to the dense matter inside neutron stars. This project benefits domestic and international facilities invested in cold and hot QCD research.

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

Monolithic Spatial Heterodyne Spectroscopy as a Robust Tool for Tritium Accountancy

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Fusion energy promises an abundant energy source, which is ideal for on-demand electricity production. Deuterium and tritium are currently the most promising fusion fuel, and the fusion fuel cycle involves a complex system dedicated to processing, extracting, and storing tritium. Since tritium is radioactive, it must be meticulously accounted for within the fuel cycle to monitor inventory throughout various system parts and its transportation to and from the plant. This meticulous accountancy is crucial for ensuring continuous operations; facilitating shutdowns, startups, and off-normal operations; adjusting inventory levels throughout offsite transfers; and meeting other operational needs. Cost-effective accountancy techniques are essential for the successful and efficient operation of fusion reactors, necessitating high-sensitivity and high-speed detection solutions that can function in rigorous environments.

A promising spectroscopic technology for tritium accountancy in such extreme environments is the spatial heterodyne spectrometer (SHS). The SHS offers high spectral resolution, a broad spectral range, and very high light throughput. SHS is suitable for miniaturization and can utilize monolithic construction techniques, which can be an advantage when spectrometer size and durability are crucial. This research aims to develop a monolithic spatial heterodyne spectrometer (mSHS) that can withstand high flux neutron environments and tritium exposure to enhance diagnostic capabilities for tritium accountancy. Developing a compact and robust spectrometer for real-time tritium accountancy will be critical to the success and operation of commercial fusion energy.

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

Quantum Optical Properties of Highly-Excited Semiconductors

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Controlling individual photons and inducing them to interact lies at the heart of future quantum technologies. From secure communication to scalable quantum computing, the ability to engineer strong photon-photon interactions is a key requirement. Yet in conventional optical materials, photons barely interact at all. This project explores an emerging solution: using Rydberg excitons—highly excited bound states of electrons and holes in semiconductors—to mediate strong optical nonlinearities and unlock new modes of quantum light control.

Rydberg excitons combine two powerful features: they exhibit the strong inter-particle forces typical of atomic Rydberg states, while being embedded in solid-state systems that are more easily integrated into scalable devices. Realizing this potential, however, remains a major challenge. These excitons exist within complex semiconductor environments that modify their behavior in ways we do not yet fully understand. To make use of Rydberg excitons as a quantum platform, we need new theoretical tools that capture how they interact with each other, and with photons, to give rise to emergent quantum optical phenomena from the few- to many-body regimes.

This project aims to build that theoretical foundation, enabling predictive models of Rydberg excitons and their role in generating and manipulating quantum states of light. The research will focus on two semiconductor systems with leading potential: cuprous oxide (Cu_2O), which hosts well-defined Rydberg excitons with long lifetimes, and transition metal dichalcogenide (TMD) monolayers, whose atomically thin geometry offers enhanced optical access. In Cu_2O, the work will explore how microwave fields, phonons, and cavity design influence many-body exciton dynamics and enable strong photon blockade effects. In TMDs, the project will investigate how geometry, interfaces, and polarization affect exciton interactions and surface wave propagation, with the goal of realizing robust, material-based sources of quantum light.

These studies will lay the groundwork for next-generation quantum optical technologies based on scalable and integrable materials. The project builds on prior advances in nonlinear optics, quantum theory, and exciton physics, and will proceed in close collaboration with experimental groups to ensure that theoretical predictions are grounded in practical feasibility and have real-world impact.

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

Controlling Metastable Phase Formation and Transformation in Multicomponent Oxide Thin Films

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Predictive control over metastable states—structural and compositional deviations from the thermodynamically most stable states—can enable access to a vast space of novel functional properties in multicomponent materials. High-entropy oxides (HEOs), composed of five or more cations in near-equimolar proportions, represent a versatile multicomponent platform for investigating metastability given their inherent chemical complexity and configurational entropy. Metastable states of HEOs featuring cation segregation, partial ordering, and compositional gradients can be created through nonequilibrium synthesis. However, the underlying mechanisms that govern the formation and stabilization of these states, as well as the link between structures and properties, remain poorly understood.

This project aims to establish fundamental design principles for metastable structural motifs in HEOs, as well as synthesis protocols to control their formation and transformation. It also seeks to develop quantitative links between metastable structures and specific functional behavior, particularly those relevant to chemical conversions and other energy-related processes. Epitaxial HEO thin films will serve as model systems to investigate how redox-active and inert cations influence oxygen vacancy formation, cation migration, and local ordering. The research will further examine how composition disorder and site-selective oxygen vacancies shape kinetic barriers and diffusion pathways during phase transformation. Finally, it will investigate how the interactions between defects and surface or interfacial composition mediate charge transfer and affect oxygen transport, driving structural reconstructions that give rise to emergent metastable interfacial phases.

This research will reveal how chemical complexity, defect landscapes, and interfacial coupling govern metastable phase formation and transformation through integrating in situ growth diagnostics with ex situ atomic-scale structural, chemical, and electronic characterization. These insights will allow for rational exploration of the vast configurational space in multicomponent systems, guiding the design and synthesis of novel metastable states to enable robust, adaptive materials for electrocatalysis, low-energy switching, tunable magnetism, and novel ferroelectricity.

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

Quantum Photonic-Phononic Transduction Empowered by Van Der Waals Layered Crystals

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Unprecedented advances in creating and controlling individual quantum entities in solid-state platforms, such as transmons in superconducting junctions, spins in silicon quantum dots, and defect-related quantum emitters in wide-bandgap semiconductors, have been witnessed over the past decade. However, it remains a long way from achieving hybrid quantum systems, due to the enormous frequency discrepancies and material incompatibilities among these diverse physical embodiments.

This Early Career Research Program (ECRP) is designed to address the challenges above by exploring quantum and non-classical states in phononic and optomechanical devices enabled by van der Waals (vdW) layered crystals, leveraging their unique quantum characteristics, extraordinary mechanical properties, and unparalleled flexibility for heterogeneous integration. A systematic investigation of device physics and dissipation pathways, in parallel with phononic engineering and topological designs, will be implemented, aiming to realize high-quality devices that are robust against fabrication-induced imperfections. Near-unity-phonon operation, phonon-quantum emitter coupling, and photonic-phononic transduction schemes will be further developed based on these device systems. The proposed research thrusts are expected to lay the scientific and technological groundwork for the realization of integrated quantum photonic–phononic circuits, opening transformative possibilities for coherent information processing, quantum signal routing, and hybrid quantum systems at the extreme scale.

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

Mechanistic Controls on the Rate and Radiative Forcing of Tree-Mediated Trace Gas Cycling

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The surface area of tree trunks and branches is nearly equal to the soil-covered surfaces across Earth's landscape. Until recently, it has not been broadly acknowledged that, like soils, these woody surfaces actively exchange trace gases (TGs) like methane (CH_4) and nitrous oxide (N_2O) with the atmosphere. Despite this recognition, mechanisms controlling TG cycling at this critical interface remain poorly understood and unrepresented in Earth system models (ESMs) or global TG budgets. This critically limits our ability to predict Earth system dynamics as even relatively slow rates of TG uptake or emission across these woody surfaces contributes to a globally significant flux given the massive surface area they represent. My goal is to establish the mechanistic and predictive understanding of tree CH_4 and N_2O cycling needed to resolve the magnitude and direction of this highly uncertain TG flux, while also better resolving whether these woody surfaces are TG sources or sinks at a global scale. This will lay the foundation for more robust predictions of ecosystem TG dynamics at global scales. My work will also span across continental-scale gradients of wood anatomy, moisture, and temperature to support predictive outcomes which are more broadly transferable as opposed to being site- or region-specific.

My overarching hypothesis is that tree TG cycling behaviors are primarily determined by the gas diffusivity and biochemistry of wood. To test this hypothesis, I will conduct field and laboratory studies guided by a model-experiment integration (ModEx) strategy using two types of models. The first are exploratory tree stem flux distribution models that will be used to generate and test hypotheses based on the physics of TG transport. I will also use data-driven, machine learning enabled models to identify the strongest predictors of stem TG fluxes, then test the transferability of these predictors across sites and biomes. The ModEx strategy will accomplish two main objectives: 1) determine how water-filled pore spaces influence gas transport mechanisms from soils, through tree stems, to the atmosphere based on wood anatomy and hydrological drivers; and 2) evaluate how TG production and consumption is affected by the redox state, moisture content, and temperature experienced by microbial communities living inside tree wood and bark. The outcome of my work will be a road map for how to feasibly represent tree-mediated TG cycling in ESMs and use mechanistic predictions to globally scale tree TG fluxes. In doing so, this fundamental research will reconcile a major gap in our capacity to predict Earth system processes, a capability that is central to a variety of critical national security and energy challenges facing our nation.

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

Machine learning for high-dimensional data exploration and model refinement in neutrino physics

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The future Deep Underground Neutrino Experiment (DUNE) has the potential to make the world's most precise measurements of neutrino oscillation and answer vital questions about the matter-dominance of the Universe and the structure of the Standard Model of Particle Physics. However, our understanding of the complex range of ways in which neutrinos interact is limited: many complex nuclear effects confuse the picture and threaten to degrade DUNE outcomes. Current models struggle to capture the full complexity of these interactions and progress is inhibited by traditional analysis methods.

This project pursues two machine learning approaches to unlock new experimental strategies for measuring and characterizing neutrino interactions. First, neutrinos at DUNE energies can eject a large number of low-energy particles or cause the nucleus to fragment. This may lead to biases in neutrino energy reconstruction, the key quantity for neutrino oscillation studies, but is unmodeled by current simulation. This project will utilize unsupervised machine learning techniques to explore the low-energy ejection space, developing hypotheses for future analysis and identifying directions for future model development. Second, the most challenging step in making neutrino interaction measurements is unfolding, the deconvolution of detector smearing and efficiency effects. Traditional approaches scale poorly to high-dimensional spaces, and introduce model-dependent bias, compromising the utility and integrity of results. This project will develop an iterative machine learning powered unfolding algorithm, for use with high-multiplicity neutrino data, to overcome these issues.

Together, these efforts will help ensure DUNE achieves its scientific goals by improving how we understand and interpret neutrino interactions, with tools and strategies that will benefit the broader high-energy physics research community.

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

Scanning Ultrafast Optical Probe and Control in Kagome Metals

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Charge density waves (CDWs) are a type of electronic ordering phenomenon where electrons create a modulation in electron density. Despite being one of the earliest discovered electronic orderings, CDW materials have not been adopted for practical applications due to the difficulty to couple it with external perturbation and its weak effect on electronic properties. The recent discoveries of CDW ordering in kagome materials AV_3Sb_5 (A = K, Rb, Cs), FeGe and ScV_6Sn_6 offer a new possibility for practical applications. The overall objective of this project is to use scanning optical microscopy to study the symmetry breaking in these Kagome metals with charge density waves and superconductivity. We also plan to use time-resolved reflectivity to study the coherent phonons to reveal the structure and symmetry of the CDW phases. Finally, we plan to use optical pulses to control the CDW phases. We aim to establish these techniques as new optical platforms to study Kagome metals with various correlated and topological properties that have been constantly emerging. This work will help to establish the comprehensive fundamental understandings of various aspects of Kagome to establish them as new platforms for quantum information science.

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

Harnessing Extreme Electric Fields to Control Anisotropic Ion Transport Near Toughened Ceramic Interfaces

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Electrified ceramic interfaces with locally intense electric fields have recently attracted significant attention for their potential to drive interface reactions, ultrafast synthesis, and ion separation under extreme conditions. Despite this growing interest, fundamental questions remain about why these intense fields drive ion motion in ways that dramatically differ from conventional transport mechanisms. This study aims to establish a fundamental understanding of the relationship between intense electric fields and ion transport dynamics. Under these high fields, moving ions and lattice structures are expected to become highly polarized, pushing the system far from low-field thermodynamic equilibrium and enabling new types of coupling between the ions and the material itself. These effects can lead to anisotropic ion motion not seen under low-field limits. To probe these phenomena, the research combines a new grain boundary doping strategy—designed to induce intrinsic extreme electric fields—with ultrafast electron microscopy and optical spectroscopy to directly observe ion–lattice interactions in real time. Key scientific outcomes expected include: 1) new methods to quantify ion-lattice coupling; 2) improved understanding of ionic transport under high-fields; 3) a new transport model that extends beyond low-field limits. This research seeks to understand ion transport and coupling dynamics under extreme electric fields. It bridges composition (heterogeneous doping), structure (ceramic interfaces and dipolar interactions), and properties (field-driven transport) to explain how material behaves in demanding energy systems such as nuclear fusion, energy storage and hydrogen production.

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

Integration of High-Throughput Experiments and Physics-Informed Machine Learning to Understand Irradiation-Induced Swelling in Metallic Glass

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Structural materials in nuclear power systems commonly experience degradation of mechanical properties due to radiation-induced swelling and damage. Metallic glasses, however, represent a unique class of structural alloys that combine the favorable properties of metals with a non-crystalline, glass-like atomic structure. Metallic glasses have demonstrated excellent resistance to radiation damage, and, remarkably, some even show improved mechanical properties under radiation exposure. Thus, metallic glasses are promising candidates for safer, more reliable structural materials in nuclear power applications. While irradiation-induced swelling in crystalline materials is well-characterized through established thermodynamic and kinetic models of crystallographic defects, the corresponding mechanisms in metallic glasses are far less understood because it is inherently challenging to define and characterize “defects” within a disordered atomic structure. The objectives of this research are to investigate how radiation influences metallic glasses at the atomic level, to elucidate the processes that lead to material swelling under irradiation, and to develop predictive models that can anticipate these effects. The research approach integrates high-throughput experimentation, state-of-the-art electron microscopy methods, computer simulations at the atomic scale, and physics-guided artificial intelligence techniques. By leveraging this comprehensive, multi-technique strategy, the project will establish an atomic-level, data-driven understanding of radiation-induced defects in metallic glasses. Insights gained from this project may accelerate the development of advanced nuclear materials that are more resistant to radiation damage, thereby enhancing the safety and performance of future nuclear energy systems.

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

Design Altermagnetic Orders in Non-Symmorphic Magnetic Crystals

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Magnetic ordering is arguably one of the most fundamental macroscopic quantum phenomena. Its intrinsic breaking of time-reversal symmetry and robust energy scales make it central to both fundamental understanding of electronic properties and the development of emerging technologies. This research program aims to design and experimentally realize new material platforms exhibiting altermagnetic orders—a novel magnetic state emerging from the interplay between antiferromagnetic spin configurations and crystallographic symmetries—by leveraging the unique properties of non-symmorphic symmetries.

We will develop hexagonal and tetragonal non-symmorphic crystals as platforms for realizing g- and d-wave altermagnetic orders. In parallel, we will establish strain-based, symmetry-sensitive thermodynamic probes for detecting signatures of altermagnetism. By tightly coupling synthesis with measurement, our goal is to expand the landscape of quantum materials capable of supporting tunable altermagnetic phases. This project directly addresses the critical shortage of experimentally viable materials for exploring altermagnetic orders and seeks to bridge the gap between experimental studies and the rapidly growing body of predicted intertwined spin and charge transport phenomena in altermagnets. The proposed material platforms span a broad range of magnetic and electronic ground states, offering the opportunity to advance the design of altermagnets with tailored magnetic/electronic symmetries and functionalities. Ultimately, these material platforms may serve as a foundation for multifunctional devices in future low-energy-consumption electronic and spintronic technologies, and open pathways toward next-generation quantum computing applications when integrated with superconducting platforms.

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

Ultrafast Structural Dynamics of Solvent-Influenced Reaction Pathways

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Understanding and controlling the flow of energy and charge within molecules is a central objective in modern chemistry. Since the vast majority of chemical and biological reactions occur in solution, solvent molecules can profoundly influence the ultrafast dynamics of solute species. These influences manifest in key ultrafast processes such as proton transfer, charge transfer, coherent vibrational motion, and intramolecular vibrational energy redistribution. By modulating energy gaps between electronic states, altering the positions of conical intersections, and enabling specific solute–solvent interactions, solvents can reshape reaction pathways and fundamentally impact molecular behavior.

This project seeks to investigate the role of solvent–solute interactions in governing photochemical dynamics on femtosecond timescales, with a particular emphasis on structural perspectives. To accomplish this, we will leverage the complementary capabilities of ultrafast X-ray solution scattering and liquid-phase ultrafast electron diffraction. These techniques provide femtosecond temporal resolution and sub-ångström spatial precision, enabling direct observation of transient structural changes in solution-phase molecular systems. Our goal is to gain insight into how solvent molecules actively participate in chemical reactions, such as mediating proton transfer through hydrogen-bonding dynamics. We also aim to understand how different solvent environments can alter or redirect reaction pathways by influencing nonradiative electronic relaxation processes. Furthermore, we will explore the structural response of solvent molecules themselves following ionization events, and how these rapid changes propagate to affect the behavior of solute molecules. By conducting experiments at Department of Energy facilities such as LCLS-II and MeV-UED at SLAC National Accelerator Laboratory, we aim to capture the coupled motion of electrons and nuclei on their natural timescales, from femtoseconds to attoseconds, and extend this understanding to increasingly complex molecular systems.

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

Development of Neutron Dark-Field Tomography to Map Nanostructures in Bulk Systems

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The performance of advanced materials and systems heavily relies on carefully architected structures spanning nano- to macroscale. Manufacturing/synthesis defects and design flaws at any of these length scales could lead to degraded material performance or even catastrophic system failure. Therefore, nondestructive techniques that can characterize a bulk system across multiple length scales, especially probing nanoscale in a centimeter-sized system are in high demand.

This research will address such needs by developing neutron dark-field tomography (nDFT), leveraging the unique time-of-flight (TOF) characteristics offered by the Spallation Neutron Source (SNS) and the advanced microfabrication capability at the Center for Nanophase Materials Sciences. This technique will employ grating interferometry to exploit the wave–particle duality of neutrons to simultaneously map structural details across multiple length scales in centimeter-sized complex systems in 3D. This unprecedented capability will bring transformative insights to advance the forefront of advanced manufacturing and energy materials, which demand an understanding of material structure and performance that spans multiple length scales. This effort will position SNS to establish international leadership in TOF-nDFT and enhance neutron imaging for a wide array of applications, advancing our understanding of materials science, structural engineering, and beyond.

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

Precision Proton Tomography on a Euclidean Lattice

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A fundamental goal of nuclear physics is to uncover the origin of the proton's mass and spin, and to understand how the strong interaction governs the confined motion and spatial distribution of quarks and gluons within the nucleon. These questions can be profoundly informed by precise multi-dimensional imaging—tomography—of the proton, which lies at the heart of the scientific missions of the Thomas Jefferson National Accelerator Facility and the forthcoming Electron-Ion Collider at Brookhaven National Laboratory. The objectives of this research are to develop a novel theoretical framework for precise first-principles calculations of the nucleon’s multi-dimensional quark and gluon structure using lattice quantum chromodynamics (QCD), and to perform these calculations on high-performance supercomputers. Compared to existing methods, the new framework offers a key simplification that not only significantly improves numerical precision but also substantially reduces systematic uncertainties. By combining this framework with other recently developed precision-enhancing techniques in lattice QCD, this project will perform systematic calculations of multi-dimensional imaging observables that depend on the transverse momentum and spin of quarks and gluons. The results will enable the construction of precise three-dimensional images of the proton and reveal the contributions of quark and gluon spin, as well as orbital angular momentum, to the proton’s spin—thus providing essential theoretical guidance and support for current and future experiments.

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

Energy and Entropy in Nonthermal Turbulent Plasmas

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Energy and entropy are two of the most fundamental quantities in physics: energy is conserved but can be redistributed amongst different components of a system, while entropy (a measure of disorder) tends to increase according to the second law of thermodynamics. Together, these two quantities impose rigorous constraints on the possible dynamics of a complex system. However, their general relationship remains elusive in nonequilibrium systems such as collisionless plasmas, which do not relax to the expected thermal equilibrium (the state of maximum entropy). The proposed work attempts to quantify the relationship between energy and entropy in collisionless plasmas that experience turbulence, where conventional approaches from equilibrium statistical mechanics do not apply. Specifically, the project will use analytical theory and kinetic numerical simulations to address the following question: when energy is injected into a turbulent plasma, what happens to the entropy as the system relaxes to a nonthermal state? The research will explore generalizations to entropy and the laws of thermodynamics for magnetized, nonthermal plasmas. The kinetic turbulence simulations will incorporate: i) varying background magnetic fields, ii) weak Coulomb collisions, and iii) expanding/ compressing domains, to evaluate the generalized relationship between energy and entropy in a controlled setting. The results from this research will be applied to model nonthermal particle distributions arising from turbulent dissipation in several contexts, including laboratory experiments at the Wisconsin Plasma Physics Laboratory and space observation from NASA and other agency spacecraft missions.

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

PREDICT (Probing and Regulating Electrochemical Dynamics at Interfaces for Correlation and Tunability)

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Electrode/electrolyte interfaces are fundamental to determining the performance, lifetime, and safety of electrochemical systems. However, understanding and controlling the chemical dynamics at electrode/electrolyte interfaces remains one of the grand challenges in this field. We aim to address this challenge through establishing a research program on PREDICT (Probing and Regulating Electrochemical Dynamics at Interfaces for Correlation and Tunability). PREDICT will integrate *operando* characterization, interface modulation, and machine learning to probe and regulate chemical dynamics at the cathode/electrolyte interphase (CEI), with a focus on high-voltage sodium-ion systems. *Operando* X-ray spectroscopy, cryogenic electron microscopy, and energy-resolved tomography will be employed to probe the CEI and bulk cathode with high spatial, temporal, and chemical resolution. PREDICT will directly correlate interfacial properties with bulk cathode transformations across electrochemical states. To regulate interfacial dynamics, PREDICT will tune the electric double layer at the cathode/electrolyte interface, focusing on designing tailored electrolytes with controlled solvation structure and introducing liquid crystal-like ordering at the interface. The designed strategy is expected to promote the formation of a uniform, inorganic-rich CEI with weak interfacial binding, thereby enhancing the cycle life of sodium- ion systems. Combining these efforts, PREDICT will employ machine learning to extract and validate interfacial and bulk descriptors, including speciation, inorganic/organic ratio, CEI thickness, interfacial energy, and fracture volume, that strongly influence the performance of sodium-ion systems. The objective of PREDICT is to build a predictive and descriptor-driven model that enables tunability of CEI in sodium-ion systems through electrolyte and interphase design. PREDICT aligns with DOE Basic Energy Sciences core interests in interfacial science, materials chemistry, and data-informed materials discovery. The knowledge generated in PREDICT will provide foundational insights that extend beyond sodium-ion systems, informing the design of advanced electrochemical interfaces in a broad range of energy technologies.

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

Leveraging Cooperative Complexation in Helical Ladder Polymers for Rare Earth Element Separation

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Separating rare earth elements (REEs) from each other is a longstanding scientific challenge due to their similar chemical properties. Improving these separation capabilities is a technological opportunity given REEs' importance in energy applications and classification as critical materials. Current REE separation strategies, which typically rely on solvent extraction and ion exchange chromatography, struggle to achieve selective separation of REEs due to their similar oxidation states and ionic radii. This project aims to address this separation science need through the design of structurally tailored helical polymers that recognize and selectively bind to REE ions. The rigid, helical, and ladder-like polymer is hypothesized to form conformationally constrained cavities that can be tailored to bind to specific REE ions. The extended, shape-persistent polymer backbone is tailored by varying its ligand composition. In so doing, the rigidity, cavity shape, and assembly kinetics that control REE affinity and selectivity are tuned. The research plan contains three research objectives including the (1) evaluation of how the complexation kinetics for REE selectivity depends on polymer molecular weight, the sequence of metal ion addition, and polymer concentration; (2) measurement of how REE binding is influenced by ligand architecture and polymer rigidity and helicity; and (3) identification of how coordinating metal centers synergistically modulate polymer conformation and REE binding. High-throughput structural characterization and machine learning methods are employed to formulate an understanding of how polymer structure leads to selective REE ion recognition and extraction. By elucidating trends in REE selectivity and binding kinetics, advancements in fundamental separation science parameters such as high REE selectivity and capacity are expected as well as a clear understanding of how the collective interactions from the polymer structure promote selective REE ion recognition. These cooperative interactions within the polymer backbone are expected to seed an innovative approach to support the Department of Energy's mission in recovering REEs and other critical materials.

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

New Physics Searches beyond 100 TeV enabled by Molecular Ion Quantum Logic

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This project aims to explore new physics beyond the Standard Model through precision measurements of trapped molecular ions. By integrating techniques from trapped-ion quantum information processing with the exceptional sensitivity of molecules, we will develop a tabletop experiment capable of probing combined Charge and Parity (*CP*) violation in the hadronic sector. The target *CP*-violating effects may originate from new particles or forces associated with energy scales above 100 TeV – well beyond the reach of current high-energy colliders.

Our approach leverages quantum entanglement to achieve high-fidelity state preparation and detection via Quantum Logic Spectroscopy (QLS). A key advantage of QLS is its molecule-independent nature, allowing broad adaptability across different molecular species. This versatility is critical for cross-validating results and disentangling the complex mechanisms of CP-violating interactions. Additionally, we will develop Centripetally-Polarized Ions in a Ring with Quantum Logic (CIRQL) trap—a chip-scale circular ion trap that continuously transports ions along the ring. This rotational motion induces polarization in the molecular ions within the rotating frame, enabling sensitivity to *CP*-violating interactions.

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

Seismic Foundation Model for Integrated Subsurface Monitoring: Pioneering Multi-Modal Learning from Seismic Networks, Borehole Arrays, and Distributed Fiber-Optic Sensing

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Understanding the Earth's subsurface structure and processes is critical for advanced energy technologies. For example, the safety and efficiency of geothermal energy production depends on accurate monitoring of how fluid migration alters subsurface conditions and rock properties. Recent advancements in seismic sensing technologies, such as dense seismic networks, borehole arrays, and distributed fiber-optic sensing, have dramatically expanded our observational capabilities, providing unprecedented data coverage for subsurface monitoring. However, these technologies also introduce significant challenges: the volume of data overwhelms traditional processing workflows, small-magnitude earthquakes often remain undetected within noise, and no unified framework exists to effectively combine the strengths of diverse sensor networks.

This research will develop a novel seismic foundation model, an artificial intelligence (AI) framework for integrated multi-modal seismic data analysis, to enable high-resolution subsurface monitoring and characterization. Large-scale foundation models have transformed fields such as computer vision and natural language processing by enabling AI systems to understand complex patterns in images and texts. Building on this paradigm, this research will develop AI models specifically designed to understand the Earth's subsurface by simultaneously learning from diverse datasets acquired from seismic networks, borehole arrays, and fiber-optic networks. This integrated approach allows the model to capture shared patterns within seismic data, moving beyond the limitations of analyzing each data type in isolation. The model's performance will be validated using real-world data from active geothermal sites and regions experiencing induced seismicity related to energy operations. The research will generate enhanced earthquake catalogs for both analyzing archived data and real-time monitoring, enabling improved tracking of fluid migration pathways and assessment of temporal changes in subsurface properties during energy operations. These new capabilities will support the Department of Energy's Geosciences research priorities in developing new approaches to understand subsurface processes that characterize the evolution of fractures associated with enhanced geothermal systems and enhanced hydrocarbon recovery.

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

Emergent Magnetism from Dynamical Spin-Lattice Coupling

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The ability to drive non-equilibrium states of matter with tailored laser pulses has emerged as a powerful strategy to access exotic phases in quantum materials. A prime example is photoinduced magnetism in systems with strong spin-lattice coupling, where selective lattice excitation can generate magnetic configurations inaccessible at equilibrium. However, the lack of direct access to lattice dynamics on ultrafast timescales and ultrasmall lengthscales severely limits mechanistic insight and hinders predictive modeling of such emergent phenomena. This missing perspective of the lattice motion also highlights a broader gap in understanding the impact of spatial heterogeneity, where lattice strains and strain gradients critically influence the transient magnetic order.

This research program aims to probe and control non-equilibrium spin configurations achieved via dynamical spin-lattice coupling across multiple lengthscales. The project involves the development and deployment of ultrafast probes capable of directly visualizing lattice dynamics—from atomic displacements to mesoscopic strain fields—and correlating them with transient magnetic responses. Three aspects of spin-lattice couplings in a nonequilibrium setting will be investigated: (i) stabilization of spin fluctuations via mode-selective phonon excitation, (ii) ultrafast strain-induced magnetic switching, and (iii) transient flexomagnetism driven by locally evolving strain gradients. Leveraging recent advances in ultrafast electron diffraction, microscopy, and time-resolved optical techniques, the research projects will address how photoinduced lattice motion can deterministically reconfigure spin textures at both the atomic scale in (i) and mesoscopic scale in (ii) and (iii). The insights gained from these studies will expand the toolbox for manipulating magnetic order in quantum materials and inform broader strategies for ultrafast control of emergent phases that are governed by the lattice degree of freedom.

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