

Dynamical Control of Chiral Superconductivity

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Superconductors are materials in which electrons pair up and move collectively without electrical resistance. In chiral superconductivity, these pairs also have a handedness, much like a preference for clockwise over counterclockwise rotation. Recent advances in tunable quantum materials raise a timely challenge: how can this handedness be deliberately controlled? Light offers a natural approach because circularly polarized light itself has handedness and carries angular momentum. Existing theories, however, largely describe light as acting on individual electrons, so its influence on superconductivity is indirect.

This project will develop a general theoretical framework for how electromagnetic fields can instead couple directly to electron pairs, including the internal pair motion that determines their handedness. A key goal is to determine how the quantum geometry of electronic states can enhance this coupling and when electromagnetic fields can act directly on the symmetry of the superconducting state. The project will also explore two complementary physical platforms in which this control can be realized and tested. In systems containing nearly flat and more mobile electronic bands, the research will determine whether handed collective charge oscillations, or chiral plasmons, can mediate chiral superconductivity and enable optical or cavity control of its handedness. In multivalley systems, the focus will be on whether interaction-driven valley polarization can reshape the available pairing states and enhance light-induced chiral pairing.

The proposed research will identify the material properties that make electromagnetic control most effective and develop experimentally testable strategies using terahertz waves and specially engineered optical cavities. If successful, these approaches could allow light to create a chiral superconducting state, select its handedness, or reverse it without physically altering the material. More broadly, the project seeks to transform chirality from an exotic property that scientists observe into a quantum property that can be deliberately controlled, advancing the Basic Energy Sciences mission to understand, predict, and control emergent properties of matter.

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

Agentic Theory: A New AI Paradigm for Formally Verified Scientific Reasoning

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In the past few years artificial intelligence (AI) has made generation dramatically faster and cheaper. Verification has not kept pace. In theoretical physics, checking a result still means experts reading it line by line, over days if not months. Moreover, as AI-generated arguments grow more linguistically plausible, their errors and hallucinations grow harder to spot. Verification is now the main bottleneck to AI-driven scientific progress.

This project targets that bottleneck with interactive theorem provers such as Lean 4: every step is written in a precise formal language and verified by a small, trusted, publicly auditable kernel. Verification stops being a social process (e.g. peer review) and becomes a computation, completed in seconds to hours. This approach has already sparked a revolution in mathematics; physics has not yet followed. Physical reasoning relies on specialized concepts and on judgment about which principles and approximations apply, and AI provers trained on mathematics perform poorly on physics. What is missing is AI that reasons at the interface between physical knowledge and formal logic.

In this work we build Agentic Theory: an open-source, multi-agent AI architecture that runs the whole generation–verification loop for physics in one system. On the generation side, a general-purpose AI model works with a smaller, open specialist that proposes physics-aware proof plans: which principles, approximations, and symmetries apply, and how to break the problem into steps. On the verification side, Lean 4 checks every step and is the sole arbiter of correctness. Failed checks flow back to the generators, which revise the plan. Lean's verdict also becomes a training signal: through reinforcement learning, the specialist learns from what survives verification. The research has three elements: (1) the two-model collaboration protocol and its feedback loop; (2) search over open libraries of formalized physics and mathematics; and (3) a multi-level reward for good plans, verified intermediate steps, and complete proofs. Two testable hypotheses guide the work: separating planning from proof writing improves performance, and training the specialist on verified outcomes improves it further.

The methods will be tested across physics, with particular attention to quantum mechanics, statistical mechanics, and thermodynamics. Expected outcomes include the open-source Agentic Theory system; three public benchmark datasets of formally stated physics problems; an open, physics-trained specialist model; and verified results contributed to Physlib – the main open-source community-maintained library of formalized physics. The project will also co-organize a conference series on formal verification in the physical sciences and train graduate students across physics, AI, and formal methods.

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Toward Resolving the f-Electron Challenge in Heavy-Element Chemistry with Spinor Krylov Algorithms on Classical and Early Fault-Tolerant Quantum Computers

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Actinides play important roles in basic energy science, yet the bonding and reactivity of their compounds remain difficult to predict computationally. In these high-atomic-number elements, relativistic effects, including spin-orbit coupling, substantially alter electronic structure and bonding; configurations involving 5f, 6d, and ligand orbitals can also lie close in energy and mix strongly. Current methods struggle to predict f-electron behavior because strong electron correlation, spin-orbit coupling, complex multiplet structure, and other relativistic effects must be treated together for predictive accuracy. The project will first determine when active spaces formed from scalar-relativistic orbitals are sufficient and when they must instead be constructed from molecular spinors obtained from a mean-field calculation that includes spin-orbit coupling. The diuranium molecule and its anion will be a leading focus, complemented by selected studies of actinide spectroscopy, uranium redox chemistry, and superheavy-element bonding. Compressed spinor Krylov methods will be applied to the selected problems and, where feasible, compared with other active-space solvers. Quantum computing methods will be pursued when a chemically meaningful prediction requires a spinor active space beyond reliable classical treatment. Spinor-based quantum Krylov algorithms will be developed and demonstrated on quantum hardware, advancing a scalable pathway toward chemically relevant calculations on early fault-tolerant quantum computers. Together, these advances will improve predictive understanding of bonding and reactivity in actinides and selected superheavy-element molecules and provide a chemically motivated use case for quantum computing.

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Quantifying Fluid Pressure Controls on Critical Mineral Formation Using Raman Spectroscopy and Experimentation

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Critical minerals such as copper, tungsten, and rare earth elements are essential for energy technologies, national security, and the modern economy. Many of these resources become concentrated when hot fluids move through rocks deep within Earth's crust. Although temperature and fluid chemistry are known to influence the process of ore formation, the role of pressure remains poorly understood. Pressure can change rapidly as fractures open and seal, potentially affecting how metals are transported and where economically valuable minerals form. However, scientists currently have few ways to directly determine the pressures influencing mineralization.

This research will develop and test a new approach for reconstructing pressures of crystallization during critical-mineral formation. The method uses mineral inclusions trapped inside garnet crystals as natural pressure sensors. Specifically, the garnet types in the proposed study form in skarn, rocks altered by hot fluids. Garnet crystals formed in these systems can form compositionally complex chemistries. Because garnet crystals can preserve these inclusions for millions of years, their physical state can provide a record of the conditions present when the garnet grew. Laboratory experiments will determine how reliably these inclusions record pressure across the range of garnet compositions common in skarn. Advanced Raman spectroscopy and scanning electron microscopy will be integrated to identify inclusions, measure their properties, and connect pressure records to mineralization processes. The resulting tools will then be applied to natural mineral deposits where garnet crystals are formed in association with important ore minerals due to the influence of hot fluids. These studies will test whether changes in fluid pressure correspond with episodes of metal transport and mineral deposition. By combining laboratory experiments with observations from natural systems, the research will establish how changes in pressure influence the economic viability of critical-mineral deposits. The project will provide new quantitative tools for understanding how mineral resources form within Earth's crust. Improved knowledge of the physical processes that concentrate critical minerals can strengthen the scientific foundation used to interpret mineral systems and guide future resource research. The work directly supports the Department of Energy's mission to advance fundamental geoscience relevant to the nation's energy and critical-mineral needs.

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

Excitonic Control of Angular Momentum and Dissipation in a Magnetic Semiconductor

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Magnetic materials can host collective spin excitations that carry and process information. Optical control of spin excitations is attractive because it provides non-contact and volumetric control over how information is carried and processed. However, current opto-spintronic approaches provide limited control over how spin motion evolves, and the control often lasts only for the duration of the optical excitation. Magnetic semiconductors provide a new opportunity to address this limitation because their electronic and magnetic properties are strongly coupled. Recent work has shown that optically generated excitons can directly exert spin torque and modify magnetic dissipation. The overarching goal of this research is to establish a fundamental understanding of this process and use it to control the flow of energy and angular momentum in magnetic materials using excitons.

The research is organized around three thrusts. Thrust 1 will determine the microscopic origin of excitonic spin torque by identifying which properties of the exciton wavefunction control the magnitude and direction of angular momentum transfer to the magnetic system. Thrust 2 will use this fundamental microscopic understanding to control non-Hermitian magnon dynamics. Thrust 3 will extend these concepts to the quantum regime by developing methods to generate, probe, and control quantum magnon states using excitons.

This research will expand opto-spintronics from controlling magnetic energy landscapes to engineering dissipation. The resulting understanding could provide a new platform for ultrafast information processing, quantum sensing, and quantum transduction.

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Interfacial Origins of Vortex Pinning and Microwave Dissipation in Superconducting Quantum Materials

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Superconducting quantum devices rely on materials that preserve quantum information with exceptionally low energy loss. Although advances in device design and fabrication have substantially improved quantum coherence, microwave dissipation associated with defects in superconducting films and buried film-substrate interfaces remains difficult to isolate. Existing approaches provide measurements of microwave loss, but directly resolving the contributions of distinct defect environments within superconducting films and buried interfaces under operating conditions remains a major challenge.

This project will investigate whether magnetic vortices can provide a new way to probe this hidden defect landscape. Vortices are quantized magnetic flux structures consisting of a region of suppressed superconductivity surrounded by circulating supercurrents. Interactions with material defects pin vortices in place, while microwave fields drive their motion and generate dissipative and reactive responses that encode information about the local pinning environment. By coupling high-precision microwave measurements in ultrahigh quality factor superconducting radio-frequency resonators with structural, chemical, and magnetic characterization, this work will test whether controlled processing variations in superconducting films generate reproducible and distinguishable vortex-response signatures associated with buried interfaces, surface structure, and distributed disorder.

This research will establish a new experimental framework for determining how microscopic defect structure governs vortex pinning and microwave dissipation in superconducting quantum materials. It will advance the fundamental understanding of driven vortex behavior at temperatures near absolute zero and reveal how buried interfaces and distributed disorder influence quantum coherence. By transforming vortex dissipation from a materials limitation into a quantitative probe, the project may ultimately inform the development of lower-loss superconducting materials for two- and three-dimensional quantum device architectures.

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

Harnessing Ternary Metal-Sulfur Clusters and Extended Materials for Scalable Fuel Synthesis

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Ternary metal–sulfur materials combining heavy Group 6 metals (molybdenum or tungsten) with mid- to late-base metals (manganese, iron, cobalt, nickel, or copper) represent a powerful platform for the synthesis of platform chemicals and fuels that address national energy and economic security needs. The immense promise of these systems lies in their compositional tunability, which theoretically permits physical properties and reactivity to be tailored on demand. However, navigating this vast compositional space presents an enormous challenge, as the design rules governing catalytic function remain poorly understood. This research leverages atomically precise ternary metal–sulfur clusters as molecular analogs to systematically map the structure–function relationships dictating catalytic performance across three energy-relevant transformations: hydrogen evolution from water, biomass conversion to aviation fuel, and ortho- to parahydrogen conversion. By harnessing well-defined cluster architectures to construct and modulate catalytic active sites, this work will establish predictive guidelines linking molecular structure to materials-level function, directly informing the development of next-generation, scalable catalyst technologies for our nation’s critical energy needs.

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

Elucidating the Mechanistic Relationships between Interfacial Interactions and Failure Properties of Multilayer Polymer Films

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Plastic films are often crucial for critical mineral extraction and longer-lasting batteries. Designing high-performance, thinner plastic films could reduce extraction costs and increase battery lifetime. To improve the performance and mechanical durability of these plastic films, multiple polymer types are stacked into a multilayer film, with layer thicknesses of less than 100 nm. However, designing a multilayer film with known mechanical durability remains challenging because the numerous nanoscale polymer-polymer interfaces that form between layers can alter failure in unknown ways. We lack this understanding because of the experimental challenges of directly measuring changes in degradation from a single interface. The overall objective of our project is to understand the mechanisms governing the durability of multilayer films by leveraging advanced mechanical characterization techniques and molecular dynamics simulations. These techniques will directly measure the influence of a single polymer-polymer interface on the durability of multilayer plastic films. This combined approach will establish fundamental relationships describing how the properties of individual layers couple with the polymer-polymer interface to affect the global durability of multilayer plastic films. Ultimately, our findings will provide new fundamental data and understanding to guide the design of high-performance plastic films.

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Multiphase Transport of Critical Minerals in Fractured Media Mediated by Gas Nanostructures

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The United States has extensive domestic critical mineral resources that are essential for advanced manufacturing, energy production, national defense, and economic competitiveness. However, many of these resources remain difficult to recover efficiently because valuable mineral-bearing fluids become trapped within complex fracture networks, rough mineral surfaces, and microscopic pore spaces where conventional transport mechanisms become ineffective. Improving recovery from these domestic resources requires a fundamental understanding of the multiphase transport processes that govern mineral accessibility in fractured geological systems and is critical to strengthening U.S. energy security, reducing reliance on foreign mineral supplies, and maximizing the value of America's natural resources.

This project seeks to establish the fundamental science governing how gas nanostructures influence the transport of critical minerals in fractured media. Unlike conventional approaches that rely on chemical additives or nanoparticles, this research investigates whether deformable gas nanostructures can fundamentally alter transport in fractured media by deforming under confinement, generating localized interfacial stresses, and promoting fluid exchange with stagnant mineral-bearing regions. The project will also investigate whether anisotropic rod-shaped gas nanostructures exhibit fundamentally different transport behavior than conventional spherical nanobubbles, providing new insight into how gas-structure morphology governs multiphase transport under confinement.

The research combines microfluidic fracture models, advanced optical imaging, and predictive transport modeling to determine how gas nanostructure morphology, fracture geometry, surface roughness, and fluid chemistry govern critical mineral transport under confinement. The resulting measurements will provide the mechanistic understanding needed to connect nanoscale interfacial processes with multiphase transport in fractured geological media.

By providing the fundamental science needed to improve recovery from domestic critical mineral resources, this work supports long-term U.S. energy security, resource independence, and economic competitiveness. The project will also educate graduate and undergraduate students at the interface of interfacial science, fluid mechanics, and subsurface energy engineering, helping develop the next generation of scientists and engineers in critical mineral and energy research.

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

Predictive Modelling of Water and Hydrogen-bond Networks in Energy Conversion

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Water is one of the most important molecules in the biosphere, sustaining life by participating in critical energy related processes such as catalysis and charge transport. In natural photosynthesis, water and hydrogen bonds (H-bonds) are indispensable and are involved in every part of the photosynthetic apparatus, such as light harvesting, charge separation and water oxidation. Despite decades of progress in understanding water properties (mostly in bulk systems), our ability to predict and control water structure and dynamics in biological channels and interfaces is very limited. This impedes our ability to build complex multi-functional biological devices modeled on photosynthesis. This project aims to (a) obtain fundamental understanding of water and H-bond networks in biological systems and (b) develop predictive models, based on machine learning and theory, to accurately determine the positions of water and protons, given the protein coordinates and environmental conditions (pH, temperature etc.). The work will utilize (1) room-temperature structural biology tools at various Department of Energy (DOE) light sources such as the Linac Coherent Light Source (LCLS) and Advanced Light Source (ALS) to map the precise positions of individual water molecules and protons and (2) machine learning (ML) technologies and DOE supercomputing resources to learn the many-body nature of water networks from structural biology datasets. Specifically, the research will determine the structure of water/H bond networks under different chemical and physical conditions (pH, charge, pore size) that influence photosynthetic function. Time-resolved methods will be used to study the changes in these networks during function of photosynthetic enzymes. Experimental studies will be carried out on several model peptide systems and photosynthetic proteins. These model peptide systems will help build a transferable set of principles applicable to more complex photosynthetic enzymes for which functional data is difficult to obtain. The ML model will be trained on both project-generated and existing data to predict water positions in channels. Theoretical models will be developed to elucidate the response of the water network to pH changes. The expected outcome is a robust set of models and design principles to predict water/H-bond structures in bioenergetic systems.

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Fluctuation-Gated Chemistry: Tracking Collective Dynamics in Aqueous Solutions

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Chemical reactions in liquids are often driven by spontaneous, collective rearrangements of dissolved ions and surrounding water that briefly create the conditions needed for transformations. These thermally driven fluctuations can control how quickly key processes occur in water and salt solutions, including ion pairing, crystallization, and proton transfer. However, the relevant motions have been extremely difficult to observe directly at atomic length scales and on the ultrafast timescales during which liquids reorganize.

This research will deliver direct, real-time measurements of collective liquid fluctuations and determine which motions control chemical change. The central experimental approach is split-pulse X-ray photon correlation spectroscopy, which uses pairs of coherent X-ray pulses to track fluctuations in microscopic liquid structure at atomic length scales with picosecond-to-nanosecond time resolution. Experiments will be conducted at the Linac Coherent Light Source (LCLS), a DOE user facility at SLAC National Accelerator Laboratory, and at complementary X-ray free-electron laser facilities, integrated with advanced molecular dynamics simulations to connect measured timescales to specific types of molecular reorganization.

Specifically, the research will: (1) measure the lifetime of intermediate-range ionic ordering in electrolyte solutions and assess whether it serves as a precursor to crystallization; (2) test solvent-gated ion-pairing mechanisms by linking ion-pair lifetimes to hydration-shell dynamics; and (3) identify hydrogen-bond network fluctuations that gate proton transfer.

By turning the foundational concept of "solvent reorganization" into measurable, length-scale-specific dynamical observables, this work will provide missing experimental constraints for modern theories of chemical reaction rates in liquids and solutions. The outcomes will deepen understanding of fluctuation-driven chemical reactivity and deliver transferable methods relevant to energy storage and conversion, catalysis, and aqueous environments important in biology and environmental science.

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Improvement of optimized stellarator performance via low-Z impurity injection

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Stellarator fusion is advancing rapidly, driven by the success of Wendelstein 7-X and growing private investments. A central challenge for a stellarator fusion pilot plant (FPP) is reliable prediction and optimization of three-dimensional magnetohydrodynamic equilibria. However, current equilibrium theory and computational practice are fundamentally misaligned. Analytic theory based on magnetohydrostatics (MHS) imposes severe constraints on stellarator configurations, while numerical solvers routinely produce high-performance equilibria that violate those constraints. This discrepancy limits the ability of theory to guide design optimization, which is essential for a viable FPP.

This project develops a new equilibrium model, MHS_α , that resolves this long-standing inconsistency. The model extends MHS by incorporating a Maxwell-Reynolds stress term associated with small-scale magnetic fluctuations. This formulation introduces a physical smoothing length α determined by the amplitude and correlation scale of non-ideal magnetic fluctuations. MHS_α may therefore be interpreted as a physically-grounded equilibrium closure distinguished by its preservation of a variational structure.

The resulting model retains the computational advantages of traditional equilibrium solvers while introducing a mechanism for smoothing singular currents at rational surfaces. Unlike implicit regularization in existing codes, MHS_α is defined explicitly at the continuum level and admits exact reductions to finite-dimensional dynamical systems. This structure enables the study of fully three-dimensional equilibria using tractable numerical and analytical tools.

The project will establish MHS_α as a viable equilibrium model through three tightly coupled efforts. First, new three-dimensional equilibrium solvers will be developed based on an exact particle reduction of the model. Second, rigorous existence theory for non-axisymmetric equilibria will be constructed, ensuring that the model avoids the mathematical limitations that motivated Grad's conjecture. Third, the model's predictive capability will be assessed by revisiting key discrepancies between theory and simulation, including quasisymmetry, omnigenity, and magnetic shear.

By providing a continuum equilibrium model that is both physically grounded and computationally tractable, this work aims to supply a missing theoretical foundation for stellarator design. MHS_α has the potential to restore consistency across theory and simulation, thereby reducing uncertainty in the design of future stellarator fusion devices. More broadly, the model provides a framework for incorporating feedback from small-scale electromagnetic fluctuations into equilibrium calculations while preserving computational tractability. This capability is particularly relevant for stellarator optimization workflows, where repeated equilibrium calculations require both robustness and physical consistency.

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

Predictive Modelling of Water and Hydrogen-bond Networks in Energy Conversion

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Life on Earth requires carbon to build the biomolecules that construct cells and store chemical energy. Accumulating carbon from inorganic sources is achieved by the Calvin-Benson-Bassham cycle, which uses the enzyme Rubisco to capture CO₂ and convert it into usable forms. Harnessing such a rare and stable species is a remarkable chemical feat, and earth's microbes have developed powerful carbon concentration mechanisms to make this process as efficient as possible. A key player is the carboxysome, a protein-based "proto-organelle" that is found in various marine and freshwater bacteria and is responsible for an estimated 10-25% of global carbon fixation. This nanoscale compartment forms on its own from a relatively small instruction set of about 10 proteins. Given this compartment's essential role, it is critical to determine how the components work together and how the compartment's strategies can be biotechnologically exploited, such as for improving carbon fixation efficiency in crops to reduce demand for water and fertilizer. Despite these goals, it is still highly challenging to get functional compartments into new organisms and create synthetic compartments that match the enzymatic loading of carboxysomes. This project aims to directly observe mechanisms of carboxysome self-assembly, interior reorganization, and damage in foreign chemical environments. The research program will harness the power of single-biomolecule trapping, microscopy, and spectroscopy to provide the ultimate sensitivity in protein detection and interaction. Successful completion of this project will provide unparalleled access into carboxysomal machinery and tools to watch their molecular dynamics in real time.

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Toward Scalable and Reliable Bayesian Inference for Intractable Inverse Problems Through Entropy and Geometry

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Across the Department of Energy's scientific missions, researchers face inverse problems: inferring what cannot be directly observed, such as subsurface material properties, seismic source mechanisms, and unresolved model parameters, from limited data and expensive simulations. Bayesian methods provide the principled framework for these problems, quantifying the uncertainty that should accompany any conclusion drawn from incomplete information. Yet in the regimes that increasingly dominate DOE science, the barrier is not only simulation cost but the coupled information-theoretic and geometric structure that determines whether a problem can be solved reliably with finite computation. This project develops a theory of Bayesian tractability that explains when and why inverse problems become hard and uses that explanation to make their solution reliable at realistic computational cost.

Four challenges arise within this joint structure: data can sharpen the solution within the range anticipated beforehand (concentration) or shift it into regions considered unlikely (displacement); the local shape of the underlying probability distribution can vary so that no single computational strategy works everywhere (geometric heterogeneity); and its length scales can differ by orders of magnitude across directions (ill-conditioning). These effects are inseparable: the data, refinements, and experimental designs intended to sharpen the solution can also displace it, distort its shape, and worsen its conditioning.

Existing methods address these challenges separately. Sequential Monte Carlo controls how the solution is refined, Hamiltonian Monte Carlo exploits local geometry, transport maps move probability mass, and optimal experimental design chooses informative data. Because each stage changes the information, geometry, and representation assumed by the next, workflows composed from these methods can be fragile. The central hypothesis is that this composition gap is a primary source of difficulty in the hardest inverse problems, and that selecting each inference and design step by its joint effect on both structures will outperform tuning those steps in isolation.

The first research thrust builds the theory: generalized information measures for robust and goal-oriented inference, diagnostics that detect when finite computational representations no longer support trustworthy conclusions, and controlled paths for moving probability from prior beliefs to data-informed conclusions. The second turns the theory into an adaptive workflow coupling sampling, transport, and design, with each step selected by its joint effect on information and geometry, kept tractable in high dimension through parallel sampling and low-rank structure. The third demonstrates the framework on DOE inverse problems in seismology, subsurface imaging, atmospheric source attribution, chaotic systems, and surrogate-mediated model calibration. The outcome will be theory, algorithms, and research software to support uncertainty-aware inversion across high-performance computing, experimental facilities, multi-fidelity modeling, autonomous laboratories, and digital twins, with diagnostics that reveal when misspecification, unresolved geometry, or approximation error is the true limit on inference.

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

Field-Directed Control of Crystallization in Polymorphic Organic Molecules

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Many energy-relevant technologies rely on the synthesis of organic molecular crystals, yet their pristine synthesis, and thereby performance, is often limited by polymorphism, the ability of a molecule to form multiple crystal structures with distinct properties. Because these polymorphs are separated by small energy differences and governed by a subtle interplay of thermodynamics and kinetics, controlling which structures form remains a fundamental processing challenge. This project addresses this challenge by investigating how external electric fields can serve as a new, tunable parameter for controlling crystallization. The central hypothesis is that weak electric fields can systematically bias molecular energetics, nucleation pathways, and growth dynamics, enabling predictive control over polymorph selection without altering chemical composition.

To test this hypothesis, this research integrates electronic structure calculations, machine learning models, and molecular simulations to examine how electric fields influence stability, nucleation, and growth. The project will produce predictive design rules and field-temperature phase diagrams, with downstream validation through in-situ experiments. By establishing electric fields as a controllable synthesis variable, this work advances fundamental understanding of phase behavior in metastable materials and informs the design of energy-relevant molecular crystals.

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

Field-Driven Molecular Mechanisms at Electrified Interfaces with Defects

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Electrified interfaces, where a solid conductor meets a liquid electrolyte, are central to electrochemistry and many energy storage and conversion technologies. Yet despite decades of study, it remains difficult to predict how molecules, ions, and electric fields organize and react in this narrow interfacial region, especially when real surfaces contain atomic-scale defects.

The objective of this research is to uncover the molecular rules that govern electrified interfaces under realistic conditions. Using platinum in salt-in-water electrolytes as a model system, the work will reveal how local electric fields, moving ions and water molecules, and atomic-scale surface defects jointly influence where atoms and molecules adsorb and how reactions proceed.

This work will develop machine-learning simulation methods that combine quantum-mechanical accuracy with the long-range electrical forces needed to describe charged interfaces. These atomic-resolution simulations will be connected to experimental measurements, helping translate observed electrochemical signals into a molecular picture.

This research will establish fundamental principles for field-controlled chemistry in complex condensed phase and interfacial molecular systems. More broadly, it will show how artificial intelligence for science, combined with physics-based atomistic simulation, can produce quantitative, experimentally testable models that strengthen the scientific foundation for electrochemistry, interfacial chemistry, and related energy technologies.

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

Developing a Scalable AI-E3SM Diagnostic Framework: Enabling Wet Urban Parameterization for Coastal-Urban Energy Resilience

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Coastal cities and suburbs across the United States face growing threats from powerful storms: flooding that can knock out electric power, and heavy rain that overwhelms the aging underground pipe networks that many older cities use to carry stormwater and sewage together. When these combined systems reach capacity, they release untreated wastewater that contains major nutrient pollution directly into nearby rivers and coastal waters, a problem known as a combined sewer overflow (CSO). The resulting pollution can further foul the water that power plants pull in to cool their equipment, forcing plants to cut back output during a storm when power demand for flood control peaks. Despite recent advances in the U.S. Department of Energy's Energy Exascale Earth System Model (E3SM), the portion of the model that represents cities does not yet track underground pipes or how CSOs reach nearby waterways. This research plans to close that gap by linking E3SM with the Storm Water Management Model, a tool widely used to simulate how stormwater moves through underground pipe networks during storms. To overcome the challenge that running detailed pipe-network simulations for each city in the country would be far too slow to include directly in a large Earth system model, the project plans to use artificial intelligence (AI) to build a fast stand-in model, trained to mimic the detailed simulations at a fraction of the computing cost. This AI model will then be dynamically coupled to E3SM's urban component, enabling it to represent how urban drainage systems respond to storms. The project will also assemble the first comprehensive national database of CSO events by using an AI tool to gather and organize thousands of local government reports, creating a benchmark for checking the model's accuracy. Two case study regions, Seattle, Washington, and Buffalo, New York, will serve as testbeds; despite their different precipitation regimes, both cities rely on aging combined systems and experience frequent overflow events. By dynamically coupling underground drainage and overflows into E3SM for the first time, this project aims to improve understanding and prediction of flooding hazards in coastal cities, laying solid foundations for protecting energy infrastructure and energy production in the roughly 700 U.S. communities.

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

Molecular Torsional Control Enhanced by Chiral Plasmonics

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Atomic and molecular systems are promising candidates for emerging quantum sensing, computation, and information technologies. Extensive studies under ultrahigh-vacuum and low-temperature conditions have driven substantial advances. The requirements of these extreme environments pose a major barrier to accessing quantum technologies. Molecules, as self-contained quantum systems, can help address this challenge. Leveraging recent advances in chiral and near-field-enhanced nanophotonic structures, this project aims to establish molecular torsional coherences outside of vacuum and at room temperature at the molecular length scale (nanometers) and ultrafast timescale (femto- to picoseconds).

Fundamentally, this project seeks to demonstrate and investigate theoretically predicted molecular torsional coherences through focused experiments and method development that combine state-of-the-art nanoscale imaging, chiral plasmonics, single-molecule magnets, and ultrafast laser spectroscopy. Specifically, torsional coherence will be demonstrated in rare-earth molecular magnets using highly amplified laser fields enabled by emerging chiral plasmonic nanostructures. Moreover, an artificial intelligence (AI) enabled denoising model will be developed to accelerate data acquisition. The overarching goal is to establish a framework for future quantum technologies based on molecular quantum coherence.

Overall, this research program aims to manipulate matter at the quantum level, thereby unlocking unprecedented possibilities and accelerating progress across numerous scientific and technological frontiers. The project addresses the DOE special-priority initiatives in Quantum Information Science. Finally, this project will contribute to STEM workforce development by providing instrumentation training and incorporating AI into experimental use for graduate students and postdocs.

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

Advanced Atomic Layer Deposition for Hard X-ray Nano-focusing Optics

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Diffractive optics are essential components at Department of Energy X-ray light sources, enabling the focusing of synchrotron beams to nanoscale dimensions for high-resolution imaging, spectroscopy, and diffraction techniques. As upgraded sources such as the Advanced Photon Source deliver dramatically higher photon flux and coherence, the fabrication limitations of existing focusing optics have become a primary bottleneck constraining spatial resolution, particularly at the higher X-ray energies required to penetrate thick or dense samples. Conventional fabrication approaches face fundamental constraints in the precision and structural quality needed to reach the next tier of performance.

This project will develop a new fabrication pathway for high-efficiency, radially symmetric diffractive X-ray optics based on atomic layer deposition (ALD), a thin-film growth technique capable of exceptional thickness control and uniformity. While ALD is well established for semiconductor applications, existing processes are far too slow to produce the thick, precisely structured coatings required for X-ray focusing optics. This research will develop new deposition and metrology processes to overcome that limitation, enabling the fabrication of optics with substantially larger apertures and higher efficiency than currently achievable with existing technologies. The resulting optics will be tested and deployed at Department of Energy user facilities, including the Advanced Photon Source and the National Synchrotron Light Source II, supporting a broad range of scientific applications.

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

Light-induced Metastability in Quantum Materials

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This project establishes a new paradigm for engineering and stabilizing light-induced metastable phases of quantum materials with technologically relevant lifetimes by combining resonant ultrafast excitations with mesoscale material engineering. To overcome the fundamental limitations of heating and thermalization, which typically restrict non-thermal states to picosecond lifetimes, PI de la Torre deploys two complementary physical strategies: exploiting large intrinsic kinetic barriers between degenerate ground states and actively suppressing thermalization pathways through the synergistic combination of resonant ultrafast excitations and mesoscale material engineering via Focused Ion Beam (FIB) nanofabrication, in-situ strain cells, and thermal bath engineering. Thrust 1 targets the reversible switching of structural chirality by harnessing the coherent dynamics of soft chiral phonons or ultrafast quenches in materials undergoing achiral-to-chiral phase transitions, with implications for next-generation optoelectronic and chiraltronic technologies. Thrust 2 targets the ultrafast stabilization of novel metastable phases in strongly spin-orbit coupled quantum materials with dynamically disordered ground states, using resonant non-linear phononic and mid-infrared electronic excitations combined with mesoscale engineering to extend phase lifetimes from picoseconds toward milliseconds. Both thrusts are supported by a methodology development component that expands the hard X-ray capabilities of the upgraded Advanced Photon Source (APS-U), including a transportable THz pump / nonlinear optical probe setup and the development of polarization-resolved Resonant Inelastic X-ray Scattering (P-RIXS) at Sector 27, providing direct experimental access to chiral, multipolar, and higher-order magnetic excitations previously inaccessible with conventional techniques.

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

Full-Fidelity Reaction Network Mapping for Chemical Kinetic Mechanisms

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Detailed chemical mechanisms for gas-phase processes provide a framework for understanding how local effects, such as pressure-dependent branching or nonthermal effects, propagate through reaction networks to produce emergent behavior. They further enable the prediction, control, and improvement of chemical processes across many domains, including synthetic, atmospheric, combustion, industrial, and plasma chemistry, chemical vapor deposition, and astrochemistry. These capabilities, however, depend on mechanisms that are comprehensive and quantitatively accurate across broad chemical conditions, which is a central challenge in mechanism development. This challenge is amplified in complex, nonequilibrium gas-phase environments.

This research program will develop a high-performance computing platform for systematic pathway exploration and concurrent high-fidelity kinetic evaluation to map the reactions that govern complex gas-phase process with quantitative accuracy. Building upon recent advances in graph-based pathway exploration, the platform will be capable of capturing important, unconventional pathways. It will do so by creating a framework for flexible, condition-dependent species definitions and thereby enable extension to broad chemical domains. By integrating state-of-the-art machine learning interatomic potentials, the platform will be able to evaluate millions of reaction pathways and identify those that are important for deeper exploration. Concurrent to network exploration, sensitive kinetic parameters will be refined using high-level energy corrections and advanced kinetic treatments that can characterize anharmonic, ring-puckering and multi-conformational, tunneling, variational, nonthermal, stereochemical, and pressure-dependent behavior. Informed by high-fidelity kinetics, the platform will be capable of accurately distinguishing the underlying processes that govern system behavior. Through these advances in mechanism development, this research program will be able to explore complex, nonequilibrium gas-phase chemistry at a large scale and with full fidelity.

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

Field-Assisted Metastable Phase Formation in Complex Oxides via Internal Oxygen Chemical-Potential Gradients

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The synthesis of complex oxides is a fundamental challenge in energy materials science. Functionality in many energy-relevant oxides is governed by metastable phases and defect populations that lie outside equilibrium phase diagrams. Conventional synthesis approaches often rely on externally controlled atmospheres and prolonged high-temperature processing, limiting access to non-equilibrium states and imposing substantial energy and processing demands. Field-assisted physical synthesis routes such as spark plasma sintering offer a promising pathway to rapid, non-equilibrium phase formation, but their application to oxygen-sensitive complex oxides remains limited by an incomplete understanding of how oxygen chemical potential evolves and influences phase formation under highly dynamic synthesis conditions.

This research aims to establish oxygen-chemical-potential-engineered, field-assisted synthesis as a predictive platform for the energy-efficient synthesis of metastable, energy-relevant complex oxides. The project will investigate internal oxygen chemical potential as a designable thermodynamic variable and determine how transient and spatially heterogeneous chemical-potential landscapes govern phase transformations, structural ordering, and microstructural evolution during field-assisted synthesis. Through complementary experimental characterization and modeling, the research will establish relationships among dynamic chemical potentials, applied external fields, and non-equilibrium phase formation. The resulting framework will advance the fundamental understanding of dynamic phase behavior and provide a synthesis-science foundation for the discovery and design of metastable complex oxides by energy-efficient physical means.

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

Theory of Thermodynamic and Transport Mechanisms Governing Ion-Selective Separations

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Transport of ions through nanoscale pores is a promising separation mechanism for the selective separation of critical metal ions. Selectivity arises from confinement effects whereby the uptake of some ions occur while connected pores provide pathways for transport through them. When pore dimensions approach the molecular scale, target and competing ions interact strongly with solvent molecules, neighboring ions, and pore walls, changing the energetic cost for different ions to enter the pore network. Because these competing interactions depend on ion size, charge, and the local pore environment; chemically similar ions can partition differently within the same material. The system is further chemically complex as the porous medium is also heterogeneous across length scales, with pores that differ in size and chemistry and networks that create distinct transport pathways. A central unresolved question is how these heterogeneities modify ion partitioning and transport and how their effects combine across pore networks to determine material-scale selectivity and permeability. As a result, this project investigates these mechanisms from individual pores to interconnected transport networks. To understand mechanisms at the pore scale, molecular interactions and local pore properties that modify ion energetics and govern ion partitioning are sought. The resulting thermodynamic description help establish how pore geometry and chemistry alter the driving forces and ion transport resistances. At the network scale, the research elucidates how pore-to-pore differences and their connectivity distribute the ion fluxes across the ion-separation medium. These results reveal when preferential ion partitioning, pore-scale transport, or network connectivity dominates separation behavior and when all three must be considered together to predict selectivity and permeability. Representative ion-separation media and electrolytes from critical-mineral recovery and aqueous waste separations are investigated. The approach combines statistical mechanics of ion thermodynamics, transport phenomena in confined pores, and pore-network modeling of heterogeneous media. Predictions are tested against molecular simulations and experimental measurements of ion partitioning and transport. By establishing how molecular interactions, pore-scale transport, and network structure combine to control selectivity and throughput, the project identifies the physical mechanisms governing separation performance in complex electrolyte mixtures. This mechanistic understanding directly addresses the mission of the Separation Science program in Basic Energy Sciences within the Department of Energy Office of Science.

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

Understanding The Role of Vibronic Dynamics at the Spinterface in the CISS Effect

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The chirality-induced spin selective (CISS) effect describes a phenomenon where chiral molecules can preferentially transmit electrons with specific spin orientations in the absence of an external magnetic field. Though the CISS effect was discovered more than two decades ago, there still exists fundamental knowledge gaps that are limiting our ability to understand and exploit electron spin polarization for controlling intermolecular interactions, chemical reactions, and molecule-surface interfacial dynamics. A central question facing the CISS research field presently is: *What are the fundamental molecular-level interactions required to create the CISS effect, and how do they arise mechanistically?* This work directly explores the idea that electronic-vibrational interactions contribute to dissipation mechanisms in molecules that are known to display the CISS effect using ultrafast coherent two-dimensional electronic-vibrational (2D EV) spectroscopy to study molecules in the bulk solution phase and at interfaces. The interface-specific chiral vibronic interactions will be targeted through the development of the sum-frequency generation detection of 2D EV signals from chiral molecules known to display the CISS effect. We propose that a direct comparison of the same chiral molecular series across bulk solution and interfacial environments using these coherent spectroscopy methods will provide crucial and unique insight into the role of vibronic interactions and the “spinterface” in the CISS effect. With relevance to Basic Energy Sciences, this project has a potentially high impact by elucidating molecular-scale chemical and physical properties and vibronic interactions governing nonequilibrium chemical reactivity, solute/solvent structure, and electron transport in chiral species where electron spin is also of interest. This basic research is central in many technological applications of interest to DOE like spintronics, quantum information and sensing, enantiospecific chemical separations and reactivity, and spin-dependent electrochemistry and catalysis.

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

Continuous-Time Physical AI as Real-Time Digital Twins for Scientific Edge Systems

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DOE science increasingly needs AI digital twins that operate within running experiments, instruments, and operational systems rather than only as offline surrogates. In many scientific-edge settings, such twins need to satisfy three requirements simultaneously: low streaming latency, low local power consumption and thermal load, and fidelity to governing physics. Conventional numerical solvers can preserve physical structure but are often too slow and energy-intensive for in-loop operation. High-capacity digital AI models can be accurate on selected tasks, but typically involve extensive data storage and movement and require substantial computing power. This project advances a different hypothesis: a scientific-edge digital twin should itself be a trainable continuous-time dynamical system, embodied in programmable mixed-signal hardware, whose learned dynamics align with the target system's dynamics so that the hardware evolves as the twin.

The objective of this project is to establish continuous-time physical AI, implemented on Dynamical System Units (DSUs), as a new scientific-edge digital-twin framework for DOE systems. A DSU is a programmable electronic dynamical system that computes through autonomous physical evolution rather than sequences of digital instructions. The project will develop the AI layer needed to turn this hardware substrate into reliable scientific twins through three integrated thrusts. First, it will create expressive and hardware-realizable continuous-time model families that faithfully capture complex spatiotemporal dynamics and provide broad support for physical boundary conditions. Second, it will develop self-adaptive learning and calibration methods to address in-service uncertainties arising from the environment, the target system, and computing hardware. Third, it will establish scalable composition methods that seamlessly coordinate sparsely interacting sub-dynamics to represent large-scale scientific systems.

The work will be evaluated on a range of canonical mathematical benchmarks and two DOE mission applications: FES nuclear fusion workflows involving simulation of fusion dynamics coupled with operational control optimization, and OE power-grid workflows involving prediction of grid behavior coupled with optimization for stable, reliable grid operation. Evaluation will proceed across PyTorch-integrated behavioral simulation, circuit-level simulation, and real-hardware validation on existing DSU prototype platforms.

The expected impact is a principled foundation for when, why, and how physical AI can be deployed for DOE scientific-edge digital twins. Rather than producing only a faster solver or a cheaper accelerator, this project will create new scientific-AI model classes, self-adaptive physical-AI methods, and scalable composition strategies for deployable digital twins. If successful, the project will enable fast, low-power, and physics-faithful in-loop inference, optimization, and control for DOE experiments, instruments, and operational systems.

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

The High Redshift Frontier in Galaxy Survey Cosmology

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With the Vera C. Rubin Observatory and the Dark Energy Spectroscopic Instrument (DESI) observations underway, the wide, nearby universe is being mapped in exquisite detail, and a frontier of genuinely new information has moved outward — to galaxies whose light has traveled for the greater part of cosmic history. DESI and Rubin offer complementary ways to access that information. On one end, the gravitational bending that reveals invisible matter accumulates along the entire path light travels, so the most distant galaxies carry the most signal. At the same time, the volume of sky available grows with distance, putting within reach the very large scales where the fingerprints of the universe's first instants would appear. This program will develop a comprehensive approach that delivers a set of distance distributions for galaxies that are both tightly concentrated and anchored to spectroscopic reality. Access to that information sheds light on key science drivers of the Department of Energy's High Energy Physics research portfolio. This research will advance our understanding of dark energy, test gravity on the largest scales, and probe the physics that seeded all structure during the universe's first instants, ultimately ensuring a stringent testing of the standard Lambda Cold Dark Matter (LCDM) cosmological model.

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

Spin and Charge Manipulation in Novel 2D Chiral Hybrid Semiconductors

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This research develops new classes of hybrid semiconductors that combine control over electron spin and optical processes at room temperature, without the need for external magnets. This breakthrough paves the way for faster, highly energy-efficient computers and optical devices, securing a critical advantage in next-generation microelectronics and advanced computing.

Modern electronics process information by moving electrical charges. However, as devices get ever smaller, they generate excess heat, pushing traditional computing to its physical limits. A promising alternative is spintronics and opto-spintronics. Instead of just moving charges, spintronics uses the magnetic “spin” of an electron to carry data with vastly lower energy requirements. Moreover, coupling optics to the spin control can enable new computing paradigms using spin and light as state variables. Historically, the major roadblock has been that controlling this spin requires extremely cold temperatures and precise conditions inhibiting commercial use.

This project explores a breakthrough solution: ultra-thin hybrid 2D semiconductors built with a specific structural “twist.” This twist is known as “chirality,” similar to how a spiral staircase or human hands have a distinct left or right orientation. Because of these chiral hybrid 2D semiconductors unique twisted geometry, these materials act as natural filters that sort electron spins and emit polarized light (i.e., with controlled state variables) at room temperatures. Crucially, they achieve this entirely without the need for external magnetic fields.

The exact rules of *how* different chiral shapes drive these behaviors remain a mystery and a basic science problem. To solve this, the research will first synthesize new chiral hybrid 2D semiconductors with varying motifs. Next, the research will integrate these custom semiconductors into light-emitting diodes (LEDs). By measuring the specific type of light these LEDs produce, the research team can effectively “read” the electron spins and map exactly how a semiconductor’s shape and chiral motifs dictate its performance.

This research is a fundamental shift in materials science that directly supports advanced computing initiatives. Mastering this structural “handedness” will provide a blueprint for designing advanced technologies as well as understanding chirality driven spin control, phenomena that may open numerous doors to new physics and applications. This ensures continued technological leadership in the highly competitive global landscape of semiconductors and advanced electronics.

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

Linking Environmental Stress to Sorghum Productivity Through Extracellular Vesicle-Driven Rhizosphere Function

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Sorghum is an important feedstock crop because it produces high biomass while tolerating challenging growing conditions. However, environmental stresses such as nitrogen limitation and high temperatures continue to reduce crop productivity. Plants depend on beneficial soil microorganisms to acquire nutrients and withstand environmental stress, but the signals plants use to communicate with these microbial communities remain poorly understood. This project investigates whether plants use extracellular vesicles (EVs) to regulate rhizosphere microbial communities during environmental stress. EVs are tiny membrane-bound particles released by cells that can safely transport biological signaling molecules between cells and organisms. While EVs have been shown to mediate communication in plant leaves and during interactions with pathogens, little is known about the roles of root-derived EVs in beneficial plant-microbe interactions. This research will determine how environmental stress changes the molecular cargo carried by sorghum root EVs and how these stress-responsive EVs influence microbial growth, activity, and community function. The project will also examine how EV-mediated changes in rhizosphere microbial communities affect sorghum growth and stress tolerance. This work will provide fundamental knowledge of how bioenergy crops communicate with soil microorganisms under challenging growth conditions. The results will advance understanding of plant-microbe interactions in the rhizosphere and provide new insights into biological processes that influence crop resilience, nutrient cycling, and biomass yield.

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

Stability of 3DOTs (Three-dimensional optimized tokamaks)

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Three-dimensional optimized tokamaks (3DOTs) represent a promising new class of hybrid stellarator-tokamak devices that aim to combine the engineering advantages of tokamaks (compact, simple coil designs) with the operational benefits of stellarators (continuous operation capability and improved stability against disruptions). However, the stability properties of these novel designs remain poorly understood, threatening the viability of next-generation compact fusion systems.

This project addresses the critical gap in stability design methods for 3DOTs through a coordinated three-thrust approach. First, we will develop comprehensive stability optimization targets by extending current hybrid optimization frameworks to include detailed computer simulations of global plasma behavior, moving beyond simplified approximations currently used. Second, we will derive analytically motivated stability criteria, focusing on sudden plasma movements (a critical instability type) that can cause machine shutdowns, which cannot be ignored in 3DOT designs despite their three-dimensional magnetic shaping. Specifically, we will develop analytical expressions describing how three-dimensional magnetic variations stabilize these plasma movements and increase achievable plasma elongation. Third, we will implement these new stability targets into the stellarator optimization framework and validate them through applications to both hybrid and conventional tokamak configurations.

The results will directly enable the transition of hybrid concepts from theoretical exploration to engineering-ready designs. By establishing systematic, physics-informed stability design methods, this work will accelerate development of commercially viable compact fusion systems. Additionally, the analytical insights and optimized design tools will have broad applicability to other stellarator and tokamak systems, advancing fundamental understanding of how three-dimensional magnetic shaping enhances plasma stability across the fusion landscape.

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

Self-adaptive multi-fidelity data-assimilation reduced-order modeling framework for complex multi-physics systems

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Advanced computer simulations allow scientists to study complex physical systems, such as high-speed flows in propulsion systems and around aerospace vehicles, that are difficult or expensive to investigate using experiments. However, even today's most powerful supercomputers cannot make these simulations fast enough for many engineering applications, and these simulations do not always accurately reproduce physical behaviors observed in the real world. This project seeks to overcome both limitations by developing a new computational framework that creates fast physics-based data-driven models and continuously improves their predictions using available experimental observations. Rather than relying on large amounts of precomputed simulation data to train these data-driven models, the new framework will automatically learn and adapt the models as the simulation progresses and as new observations become available. These capabilities will allow scientists and engineers to explore the behaviors of complex physical systems much more rapidly across a wide range of operating conditions and designs, leading to substantially shortened design cycle for next-generation energy and aerospace systems. More broadly, this research will establish new computational foundations for efficient and reliable digital representations of complex physical systems relevant to the mission of the U.S. Department of Energy.

This project will achieve this goal by integrating two complementary computational techniques: model order reduction (MOR), which produces much faster reduced-order models (ROMs) based on the limited computationally expensive simulations, and data assimilation (DA), which incorporates observations into computational models to improve their predictions. However, existing ROM methods often struggle to represent rapidly moving and strongly nonlinear sharp features, such as propagating flames, shock waves, and detonations, while existing DA methods can become prohibitively expensive for large-scale systems and unreliable when these complex sharp features are present. To address these challenges, the project will develop a unified DA-ROM framework with two major innovations. First, a self-adaptive multi-fidelity reduced-order modeling (SAMF-ROM) method will automatically construct and update ROMs during a simulation based on the evolving physics and estimated modeling errors, greatly reducing the need for expensive precomputed training data. Second, new feature-preserving DA methods will be developed to incorporate observations and more importantly perform DA operations at the reduced-state space of SAMF-ROM while accounting for complex uncertainties that cannot be adequately represented by commonly used Gaussian assumptions. Together, these advances will enable the resulting ROMs to adapt to evolving physical phenomena while using observations to continuously improve their predictive accuracy. The new methods will be developed, evaluated, and demonstrated using a hierarchy of challenging problems in turbulent combustion and high-speed aerodynamics, with the broader goal of establishing efficient and predictive computational tools for complex physical systems spanning widely different spatial and temporal scales.

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

Liquid Lithium Film Jet for High-Intensity Beams

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As beam power continues to increase, some accelerators are facing challenges intercepting high-intensity beams. Conventional solid-based devices are limited by extreme thermal loads and radiation damage. This project will address these critical issues by establishing beam-intercepting technologies with liquid lithium film jets. Liquid metal material overcomes the limitations of solids with its excellent heat transfer properties and self-healing behavior under irradiation. Particularly, lithium, one of the lightest elements, offers physical advantages such as efficient ion charge stripping and efficient production of low-energy pions, muons, and neutrons. A windowless free-surface film jet offers an ideal system for beamline applications. Although technical difficulties prevented liquid lithium from use in accelerator applications, the recent research and development at the Facility for Rare Isotope Beams (FRIB) allowed FRIB to be the first accelerator facility to use a windowless liquid lithium film jet as a charge stripper in a heavy ion linear accelerator. The proposed project will enhance this technology and drive innovation in accelerator science with broader applications.

This project will develop a new scheme for forming liquid lithium film jets, spanning a wide range of thicknesses (1-100 μm) through both experiments using simulant fluids, and computational fluid dynamics. It will also address free-surface flow instabilities, which remain largely unexplored in fluid dynamics, yet are critical for operating high-intensity beams. Based on these fluid dynamics studies, other applications using liquid lithium film jets will be developed. One promising application replaces conventional graphite targets with multiple liquid lithium film jets, serving as a production target for pions and muons with high-intensity proton beams. Another is a compact neutron source using high-intensity proton beams or laser beams. Later in this project, we will demonstrate the new film forming scheme with liquid lithium, based on our extensive experience with handling liquid lithium and systems available at FRIB.

This project's impact will extend to upgrading FRIB's charge stripper toward the future beam power ramp-up to 400 kW, where the film thickness and averaged charge state are increased, while enhancing the spatial uniformity and temporal stability. Further, it will also enable the realization of multi-MW class meson factories with pions and muons for future intensity-frontier particle physics and material science, as well as compact neutron sources for a variety of areas including nuclear physics, material science, and medical applications. Due to the uniqueness of this technology, spin-off research areas will emerge, such as free-surface fluid dynamics, extreme-heat-load thermodynamics, magneto-hydrodynamics, and liquid lithium technologies related to fusion reactor engineering.

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

Quantum Advantage in Detecting Weak Coherent Signals with Entangled Superconducting Qubits

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Entanglement is a quantum-mechanical phenomenon in which two or more qubits, the building blocks of quantum computers and sensors, share a single quantum state, such that they behave as a single interconnected system regardless of their physical distance. This interdependence makes entangled qubits a powerful tool for sensing. This project will demonstrate that an entangled 4-qubit state achieves higher detection sensitivity than the same qubits operated without entanglement when exposed to an engineered signal that mimics dark matter, and will quantify how reliably this advantage holds in practice.

A signal too weak to detect with independent sensors can be amplified by distributing it across many entangled qubits, with the enhancement growing as the number of qubits increases. For wave-like dark matter candidates such as axions and dark photons, leading explanations for the invisible matter that makes up most of the universe, this mechanism offers a detection path that complements state-of-the-art resonant-cavity searches and can operate below the standard quantum noise limit that constrains their amplifiers.

Before such sensors can be deployed in dark matter searches, the entanglement advantage must be validated and quantified under realistic experimental conditions. We propose to demonstrate this advantage through a 4-qubit experiment with two complementary sensing strategies: one amplifies the dark matter signal through a collective quantum phase that scales with the number of qubits, and the other suppresses uncorrelated background noise. An engineered signal that mimics dark matter will reproduce the expected signature, and the entangled qubits' response will be compared to that of independent qubits to quantify the quantum advantage. For both sensing strategies, subtle but significant measurement errors will also be characterized using artificial intelligence, which offers an advantage over conventional analysis when small changes in qubit behavior are hard to identify.

This demonstration is a prerequisite for deploying entanglement-based sensors in dark matter searches and fundamental research, and the characterization and quantification of correlated errors in the qubit system will inform the design of larger-scale experiments. If successful, the project would enable investigation of wave-like dark matter across a broad mass range with sensitivity beyond current technological reach. Along the way, it will also drive technological advances of broad value to quantum sensing for particle physics, including improved coherence of entangled qubits, reduction of qubit errors induced by external environmental radiation, and the application of artificial intelligence to identifying subtle errors in qubit systems. The project will also help train the next generation of the quantum workforce through education and training in quantum information science and targeted workshops.

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

Gauge Field Quantum Simulations in the Age of Controllable Quantum Noise

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Quantum simulation of lattice gauge theories has emerged as one of the main avenues of opportunity for computationally exploring non-perturbative Standard Model dynamics and many-body quantum phenomena. Challengingly, current simulation designs require vast quantum devices to maintain accurate quantum coherence over immense timescales, exceeding capabilities set by noisy error rates of present quantum technologies. However, with the vision of production-scale quantum computing on the long horizon, the advent of practical fault tolerance will fundamentally change the relationship that quantum simulations have with quantum noise—rather than simply being inundated by it, quantum devices will begin providing agency in artfully navigating its impact. Complementary to powerful universal error correction, this agency opens the door to application-aware codesign of quantum simulations within curated noise that have been infeasible in the NISQ (Noisy Intermediate-Scale Quantum) era.

With their local symmetries providing measurable error signals and their complex dynamics exhibiting hadronization and thermalization as quantum information localizes and delocalizes, the quantum simulation of lattice gauge theories is a rich context to pursue the next generation of codesign. This research program pursues opportunities at each stage of the quantum simulation design process. For early stages, this includes considering the organization of errors afforded by gauge field representations that contain finite group structure, and examining opportunities for an active role of quantum noise to focus simulations on detected field volumes in light of recent spacelike entanglement calculations. For later stages in the design process, this includes developing techniques for incorporating gauge invariance in error correction protocols to alleviate quantum memory requirements when embedding logical codespaces. Together, these directions aim to deepen our understanding of how to endure---or even collaborate with---the interconnectedness of quantum simulations and their environment, expanding the scientific reach of quantum architectures.

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

Tuning Actinide Orbital Mixing via Chemical Pressure in Solid State Frameworks

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The electronic properties of the actinides are strongly influenced by high nuclear charges and the unique behavior of valence 5f orbitals, distinguishing them from lighter elements. Studying actinide chemistry is critical because decoding these complex electron interactions enables better chemical separation processes, advances nuclear waste management technologies, enhances national security, and reveals fundamental rules governing heavy element behavior. However, understanding the behavior of the 5f electrons remains a pressing task that requires multifaceted modern experimental techniques.

This research leverages chemical pressure in solid state matrices to probe actinide orbital interactions with surrounding atoms. To illustrate the concept, chemical pressure explains the vibrant red color of chromium in a ruby's aluminum oxide matrix compared to the green color of pure chromium oxide. By embedding trace amounts of uranium, neptunium, or plutonium into rigid host crystals, such as halide double perovskites, oxides, and chalcogenides, atomic size mismatches naturally squeeze or stretch the actinide atoms, forcing 5f electrons into non-standard bonding environments. This project will combine advanced X-ray spectroscopy and optical measurements with computational modeling and machine learning tools, using AI to decode complex spectral behavior and map how these chemical adjustments alter electron energies in tunable matrices.

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

Recollision Physics of Exciton Quantum States in Low-dimensional Materials

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Ultrafast laser pulses can move electrons within a fraction of a light wave. In atoms and molecules, an intense laser field can first pull an electronic wavepacket away from its original state and then drive it back. This process, known as recollision, forms the basis of attosecond science and has enabled researchers to observe electronic motion on its natural time scale. This project will extend recollision physics from isolated atoms and molecules to excitons in low-dimensional materials. Excitons are bound electron-hole pairs that behave like atom-like quantum states inside solids. Two-dimensional materials are particularly promising because their excitons interact strongly with light and can be modified by changing the number, orientation, and composition of their atomic layers. The research will use intense mid-infrared laser pulses to drive exciton wavepackets and few-femtosecond optical pulses to observe their motion. It will determine how crystal symmetry and layer stacking control exciton recollision. The project will also investigate van der Waals ferroelectrics, whose internal polarization may steer exciton motion and retain a memory of the driving laser field. Attosecond soft-x-ray measurements at the Linac Coherent Light Source will provide element-specific views of these dynamics on sub-optical-cycle time scales. The expected outcome is a new framework for observing and controlling quantum wavepackets in solids using concepts developed in atomic, molecular, and optical physics. This work will advance fundamental understanding of ultrafast light-matter interactions and establish new approaches to coherent control and quantum measurement in low-dimensional materials.

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

Controlling Dynamic Multi-Site Redox Catalysis on Solid Surfaces

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Redox interactions between transition metal active centers underlie numerous energy chemistries including the catalytic production of industrial oxygenated chemicals. However, incumbent processes face challenges including the use of corrosive ligands, harsh oxidants, and poorly utilized precious metals, hindered by our limited understanding of multi-site redox mechanisms. The goal of this project is to elucidate and ultimately control multi-site redox function using bimetallic ion systems tethered to solid porous molecular sieves, enabling reactivity paradigms beyond traditional heterogeneous or homogeneous systems. We will test the hypothesis that the intertwined effects of reaction environment and active site structure, proximity, and mobility dictate the dynamic interactions that underlie catalytic turnover and avoid parasitic processes such as metal agglomeration. Our research approach combines precise metal-zeolite synthesis to control the properties of heterobimetallic ion systems in nanoporous voids, operando spectroscopy to directly observe redox dynamics, and mechanistic reaction studies to reveal chemical kinetic pathways. We first develop a foundational understanding of bifunctionality in canonical Wacker-type olefin functionalization reactions on solid surfaces, then use these insights to modulate redox interactions towards more demanding C-H bond activations. The fundamental principles developed here will yield a new degree of control over complex redox chemistries for energy applications including the efficient production of industrial chemicals.

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

Surrogate-Accelerated Interface Transfer Operators (SAITO) for Efficient and Robust Coupling of Heterogeneous Numerical Methods

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Many problems important to energy systems, advanced manufacturing, and the physical and engineering sciences rely on simulations that bring together interacting physical processes, such as fluid flow, structural response, heat transfer, and electromagnetics. These simulations are essential for workflows that require running many scenarios, including exploring design choices, quantifying uncertainty, and supporting the development and evolution of digital twins. At extreme scale, on leadership-class supercomputers, the cost of coordinating information exchange between components can rival or exceed the cost of solving the individual models. Even when each component model is efficient on its own, traditional coupling schemes often require many back-and-forth iterations across shared boundaries to reach a consistent solution, and they can become unstable or lose accuracy for strongly interacting processes. This project will deliver coupling methods, analysis frameworks, and tools that reduce the cost and improve the reliability of model-to-model information exchange, enabling higher-throughput studies for design, uncertainty analysis, and digital-twin workflows.

This project will develop Surrogate-Accelerated Interface Transfer Operators (SAITO), a new approach for faster and more reliable coupling of specialized simulation codes that model different physical processes or subdomains. The central idea is to build fast surrogate models for the boundary-to-boundary information exchange that closes the coupled system, replacing expensive or intrusive coupling steps with rapidly evaluated approximations that are designed to remain accurate and stable. The research has two thrusts: (1) develop hybrid-monolithic-inspired coupling methods that use reduced (surrogate) versions of component models to enable efficient testing and stability inspection; and (2) develop two complementary, nonintrusive surrogate classes for the interface transfer itself: one that learns compact representations of interface behavior from structured coupling formulations and one that treats interface exchange as a time-evolving process. Crosscutting efforts will integrate SAITOs into multirate time-advancement settings (allowing different components to march forward in time using their own optimized time steps), develop practical robustness certification tools, and evaluate SAITOs as accelerators for iterative solvers applied to tightly coupled systems. Impact will be assessed by reductions in coupling iterations, coordination points, and interface communication while maintaining accurate, stable coupled predictions.

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

AutoQEC: Algorithmic Foundations for Quantum Error Correction Design and Optimization

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Quantum computing has the potential to enable key scientific applications, such as quantum simulation, chemistry, materials, cryptography, and optimization. Because physical-qubit errors are inevitable, realizing this potential at larger scales requires systematic methods for managing them. Quantum error correction (QEC) provides a central path toward such reliability, yet practical QEC design is becoming a systems problem rather than a single code-construction problem. This project develops AutoQEC (automated QEC design and optimization), a cross-layer compiler and AI-assisted design automation framework for QEC. The scientific hypothesis is that quantum error correction can be systematically formulated as a cross-layer compilation problem, and that AI-guided algorithmic design automation can surpass manual design by efficiently exploring the QEC design space to yield implementations that are more efficient, scalable, and hardware adapted. AutoQEC will use intermediate representations, legality checks, cost models, synthesis algorithms, sample-efficient learned policies, surrogate estimators, validated simulation with decoding feedback, formal validation, and feedback-directed search to keep automated exploration grounded in QEC theory and realistic implementation constraints. The research is organized around three thrusts. First, AutoQEC will develop logical-level compilation methods for advanced QEC codes, including QEC-aware representations, constraint-aware lowering, and optimization for code-dependent logical operations. Second, it will develop hardware-aware synthesis for QEC protocols and fault-tolerant architectures, including loss/leakage-aware protocols and decoders, qubit-layout synthesis, and joint optimization of protocols and layouts. Third, it will develop closed loop synthesis for QEC codes and dynamic protocols, combining graph models, reinforcement-learning policies, surrogate-guided search, structured search, and evaluation with decoding feedback to discover code-surgery procedures, dynamic stabilizer schedules, and workload-adapted protocols. The expected outcomes are new optimization algorithms, compiler abstractions, AI-guided design automation workflows, open software artifacts, benchmarks, and quantitative evaluations showing automated QEC designs with improved resource use, latency, reliability, decoder compatibility, and hardware feasibility. Through collaborations with National Quantum Initiative centers, quantum testbeds, and industrial hardware platforms, AutoQEC will support co-design on realistic devices and broaden adoption of its software capabilities. The project's broader impact is to help turn QEC from a specialized manual craft into reusable software infrastructure, strengthen the U.S. quantum software ecosystem, support DOE-relevant scientific discovery, and train students to build reliable quantum systems.

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

Effects of High Magnetic Fields on Hydrogen Retention in Vanadium Alloys

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Vanadium alloys, such as V–4Cr–4Ti, are attractive candidate structural materials for fusion blanket applications because of their low activation, high-temperature strength, and compatibility with liquid lithium. However, their performance and lifetime can be limited by the retention of hydrogen and its isotopes, which can lead to degraded mechanical properties including embrittlement and reduced fracture resistance. In fusion reactors, structural materials must maintain reliable mechanical performance while operating under coupled extreme environments, including hydrogen ingress, elevated temperature, irradiation damage, and high magnetic fields. This project aims to establish a mechanistic understanding of how the high magnetic fields in fusion systems influence hydrogen trapping, transport, retention, and associated degradation in vanadium alloys.

In this project, V–4Cr–4Ti alloys containing controlled amounts of hydrogen or deuterium will be exposed to high-temperature and high-magnetic-field environments using world-leading magnet facilities at Florida State University and the National High Magnetic Field Laboratory. The treated samples will be characterized using advanced microstructural and chemical analysis techniques to investigate how applied magnetic fields affect microstructural evolution, particularly precipitates, grain boundaries and interfaces that can serve as strong hydrogen trapping sites, and how they modify hydrogen diffusion kinetics. These results will be integrated with mechanical testing, including tensile testing, fracture toughness measurements, and ductile-to-brittle transition temperature measurements, to assess how field-modified microstructures and hydrogen behavior affect mechanical performance. This project will provide critical scientific knowledge for predicting the lifetime and safety of vanadium alloy components in fusion blanket environments.

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

Enforcing Goal-Oriented Priors in High-Dimensional Inverse Problems

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Many critical engineering and scientific systems are distributed in nature with parameters and states varying not only in time but also in space. Examples include subsurface energy reservoirs and packed-bed reactors. Engineers and scientists must infer these distributed properties from sparse sensor observations, known as inverse problems. In practice, these inferred parameters or states are not the end goal; instead, they are typically used to make crucial downstream operation decisions such as the optimization of reactor performance. Traditionally, the inverse estimation and subsequent decision-making are treated separately, often leading to unreliable, unsafe, or suboptimal decisions, particularly when the system dimension is high while observations are limited. This project aims to develop a new mathematical and computational framework that directly incorporates downstream decision-making into the inverse problem (known as goal-oriented). It will enable more reliable, efficient, and risk-aware operations of complex distributed systems in energy, environment, and scientific discovery.

This project will advance mathematical foundations and computational algorithms to solve goal-oriented inverse problems (GOIPs) for distributed dynamical systems. Theories, methods, and algorithms will be established to address challenges including high dimensionality of the problem, scarcity of observation data, and system model uncertainty. We will establish rigorous theoretical conditions and scalable algorithms under which high-dimensional GOIPs can be efficiently solved while preserving downstream decision-making quality. Inference methods will also be developed to quantify risks to downstream performance under system uncertainties. The proposed methods will be validated on benchmark computational problems and lab-scale catalytic reactor experiments, to demonstrate the applicability to DOE-relevant systems. The resulting framework will provide broadly applicable mathematical tools for scientific computing, optimization, and uncertainty quantification communities working on decision-making under uncertainty.

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

Design Rules for Autonomous Propagation of Order in Hierarchical Biological Block Copolymers

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Many of nature's highest performing materials, like collagen, silk and nacre, achieve exceptional properties through order that propagates from the molecular scale to the macroscale. Accessing this multiscale ordering synthetically has proven challenging, even with identical building blocks: collagen dissolved and reformed from native tissue is mechanically inferior to the original material because multiscale ordering is lost upon processing. In nature, multiscale ordering often relies on elaborate cellular machinery that cannot be reconstituted outside a living cell. Synthetic multiscale order therefore requires materials whose propensity for self-organization is written into the molecules themselves. Progress has been slowed by a disciplinary divide: protein science relates sequence to structure rather than bulk behavior, while soft matter physics treats proteins as generic polymer chains, disregarding sequence altogether. Neither has yielded a material that propagates molecular symmetry into macroscopic order.

This research will pursue this goal through a new class of materials called hierarchical biological block copolymers. These materials covalently link a rigid, self-assembling protein to a flexible one. The rigid component is a shell protein that bacteria use to build protein-walled compartments that natively encase chemical reactions within cells. These proteins form six-sided tiles that assemble edge-to-edge, with recent work showing that this hexagonal symmetry can propagate outward from tiles 8 nanometers across into sheets as large as 72 micrometers, spanning four orders of magnitude. The flexible component is an elastin-like protein chain, a repeating sequence derived from the elastin protein. Because the rigid and flexible halves of the molecule repel each other but remain chemically linked, they can separate only over nanoscale distances, driving formation of regular nanoscale patterns. The central hypothesis of this work is that these two organizing forces reinforce one another, and that the flexible chains provide mobility for rearrangement into highly ordered structures. Three objectives will test this idea, determining how the intrinsic assembly of the tiles governs order in the resulting materials, evaluating how the two organizing forces compete or cooperate as the flexible chain is varied, and establishing how annealing impacts ordered regions and removes defects. Together, these studies will yield phase diagrams indicating what structures form under which conditions, and, from them, a quantitative set of design rules linking protein sequence to multiscale material organization. These design rules provide a route to controlling assembly in multiscale systems, advancing broader goals of harnessing self-assembly for the scalable manufacturing of ordered materials.

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

Hidden Fields, Broken Bonds: How Nonequilibrium Electrostatics Drives Polymer Degradation

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Polymeric ion exchange membranes and mixed ionic-electronic conductors underpin a broad range of emerging energy and electronic technologies. Their operation requires sustained ionic transport under electrical driving, which intrinsically places them out of equilibrium. Under those conditions, however, these materials tend to degrade far more rapidly than conventional stability tests predict, sometimes by orders of magnitude. Why current flow changes the chemistry of charged polymers so dramatically remains unresolved.

This research program tests the hypothesis that ionic transport in out of equilibrium conditions disrupts electrostatic screening at nanoscale structural bottlenecks inside the material, generating persistent local electric fields strong enough to reshape reaction energetics and promote degradation. Using nonequilibrium molecular dynamics, reactive atomistic models, and free energy methods, this project seeks to determine when these fields emerge and to quantify their consequences for degradation chemistry.

“Mastering Hierarchical Architectures and Beyond Equilibrium Matter” is one of the Transformative Opportunities identified by the U.S. Department of Energy’s Basic Energy Sciences program. The mechanism tested here provides a concrete route into this broader problem. Much of our intuition about materials chemistry comes from studying systems at rest, and we often assume that operation drives a material across an energy landscape whose underlying reaction energetics remain fixed. This program tests the idea that sustained driving can itself reshape that energy landscape. Establishing when and how this occurs would make operating conditions an active dimension of materials chemistry and provide principles that extend beyond charged polymers to other materials and interfaces.

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

Light-Induced Nonequilibrium in Antiferromagnetic van der Waals Semiconductors: Electronic, Excitonic, and Spin-Coupled Origins

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Magnetic van der Waals semiconductors provide a promising platform for opto-spintronics, where light can generate electronic responses involving spin. A central challenge is that different microscopic processes can produce similar optical or magneto-optical signals. Optical excitation may redistribute electronic carriers, modify excitonic correlations, alter the local electronic environment, or reconstruct spin-coupled quasiparticles. Distinguishing these possibilities is essential for understanding how light-induced nonequilibrium states form and how they may be controlled.

This project aims to determine the microscopic origin of light-induced nonequilibrium responses in antiferromagnetic van der Waals semiconductors. The project will use spin-, time-, and angle-resolved photoemission spectroscopy to directly resolve how the electronic band structure, spectral weight, transient occupation, and spin polarization change after optical excitation. These measurements will establish whether the photoresponse is dominated by one microscopic process or by a hierarchy of coupled processes.

By comparing these observables across antiferromagnetic van der Waals semiconductors with different balances of electronic, excitonic, orbital, and magnetic interactions, the project will identify which light-induced signatures are common across this material class and which are material specific. The expected outcome is a microscopic framework for opto-spintronics that clarifies how optical excitation produces electronic responses involving spin, establishes principles for controlling these nonequilibrium responses, and advances fundamental understanding of how quantum materials respond to light.

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

Leveraging Quantum Information Science for Nonequilibrium Phenomena in Nuclear Physics

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When atomic nuclei collide at nearly the speed of light, they melt into the hottest matter ever produced in a laboratory: a fluid of particles that are normally locked inside protons and neutrons. Matter in a similar state filled the universe during its first millionths of a second. In both cases, this matter begins violently out of equilibrium and then quickly settles into a liquid state. How this happens is an open question. The underlying theory, quantum chromodynamics (QCD), is well established. The obstacle is computational: describing the evolution of this matter requires tracking quantum information whose complexity grows exponentially, putting the problem beyond the reach of even the largest supercomputers. Quantum computers, however, are themselves quantum systems so they can emulate the dynamics of another quantum system without the exponential overhead. This project develops the theory, algorithms, and measurement techniques needed to turn this promise into scientific predictions. The project focuses on co-design opportunities available on near-term hardware, using simpler models as meaningful steppingstones toward the full problem. The project pursues three connected goals. The first is to design quantum simulations for hardware based on individual atoms held in place by electric fields and controlled with laser light. The project will exploit multiple atomic levels ("qudits") as information carriers, which can provide both a more efficient computational resource and a more natural representation of the underlying physics. The second goal is to establish when a quantum simulation can be trusted and when it can outperform conventional computers. The project will develop performance metrics that exploit special states embedded in the structure of the underlying theory, enabling quantitative validation in regimes where verification would otherwise be impossible. The third goal is to use these simulations to understand how hot nuclear matter approaches equilibrium and fluid-like behavior emerges. The project will investigate thermalization through the lens of quantum information: how information encoded in the initial state spreads through the system, becomes scrambled, and manifests in macroscopic thermal behavior. The results will support the interpretation of experiments at current experimental nuclear physics facilities and at the Electron-Ion Collider. They will also help determine where and when quantum computers can deliver practical scientific value for nuclear physics and identify the remaining obstacles to reaching that goal. At the same time, the project will advance quantum computing itself through new methods for simulating and validating strongly interacting quantum systems.

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

Ultrabroadband Microscopy of Multiscale Charge Dynamics in Interface-Tunable Neuromorphic Heterostructures

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Conventional computing architectures limit the scalability of data-intensive applications because data storage and processing occur in physically separate locations, requiring continuous data transfer that is both time- and energy-intensive. Material-based neuromorphic computing addresses this challenge by co-locating memory and processing within the same physical space and encoding information directly into material properties. Interfaces in 2D material/ferroelectric heterostructures provide a promising platform because synergistic polar, ionic, and electronic charge dynamics can be used to encode and process information. In these heterostructures, neuromorphic behavior emerges from the coexistence of electronic, ionic, and polar degrees of freedom that operate across distinct time and energy scales, enabling complementary mechanisms for information storage and processing.

The goal of this project is to establish a comprehensive scientific understanding of how ultrafast and slow charge dynamics evolve at 2D material/ferroelectric interfaces and how these dynamics impact capacitive states. Current instrumentation cannot capture critical nanoscale coupled charge dynamics across their full range of characteristic time scales within a single instrument. To address this gap, *ultrabroadband microscopy* will be developed by integrating specialized time-resolved near-field THz microscopy, expanded multifrequency GHz microscopy, and selected complementary low-frequency functional atomic force microscopy techniques on a single platform. Ultrabroadband microscopy will resolve nanoscale multimodal material responses across the Hz–THz frequency spectrum, a regime that is experimentally inaccessible with current approaches and of great interest to the microelectronics community to be able to access. Using this capability, the project will reveal the ultrafast and slow charge processes that govern interfacial coupling in heterostructures composed of ferroelectrics and semiconducting 2D materials, ultimately laying a scientific foundation for energy-efficient, fast, in-memory computing. Ultrabroadband microscopy, once demonstrated, will be made available to users at the Center for Nanophase Materials Sciences.

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

Elucidating the Fundamentals of (Photo-)electrocatalytic Nitrogen Transformation

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This research program will integrate electroanalytical measurement, product detection, and advanced structural characterization to develop mechanistic insights into the nature of chemical reactivity at photocatalytic interfaces, using the reduction of NO_3^- to N_2 and NH_3 as a reaction platform. Understanding of such phenomena is often limited in particulate photocatalyst systems where nanoscale dimensions can preclude the direct electrical contact used in conventional electrochemical measurements. ‘Contactless’ methods (e.g., electrochemical mass spectrometry, operando X-ray absorption spectroscopy, cryogenic electron microscopy) will be used to measure product generation rates and probe catalyst surfaces with high temporal, chemical, and structural resolution. These measurements will directly correlate potential-dependent electrocatalytic performance with the analogous photocatalyst operating conditions. Product formation rate will serve as a proxy for current, providing access to key operating characteristics without direct electrical contact under systematically varying reaction conditions. These efforts will identify the descriptors (e.g., operating potential, photovoltage, and degradation rate) that govern photocatalyst performance. These fundamental studies will enable development of a predictive photocatalyst-compatible ‘load-line’ framework, deconvoluting electrocatalytic and photovoltaic contributions to performance, and will support rational design of photocatalyst particles able to efficiently drive molecular transformations and light-to-chemical energy storage. This work aligns with DOE Basic Energy Sciences core interests in photochemistry, interfacial charge transfer, and catalysis. The knowledge generated here will provide insights that extend beyond nitrogen chemistry, informing the design of a broad range of light-driven chemical transformations.

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

Next-Generation Gaussian Processes for Scalable, Probabilistic Scientific Machine Learning

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Many of the most consequential scientific and engineering challenges within the Department of Energy (DOE) share a common structure: data is scarce and expensive to acquire, the input space is vast, and predictions must be accompanied by reliable uncertainty estimates. These conditions arise in autonomous materials discovery, fusion reactor control, subsurface flow modeling, molecular and drug design, additive manufacturing, and real-time instrument control at DOE user facilities. Contemporary machine learning methods — deep neural networks, foundation models, and their Bayesian approximations — are ill-suited to this regime: they require massive training datasets, encode physical constraints only softly through loss penalties, force structured scientific data into flat Euclidean representations, and produce uncertainty estimates that are known to be overconfident precisely where reliability matters most. No existing framework simultaneously addresses all of these limitations while preserving exact Bayesian semantics.

This project will deliver transformative probabilistic modeling capabilities across DOE's mission-critical programs. Reliable, physically consistent GP surrogates will accelerate fusion and plasma control (FES), enable principled UQ for molecular and materials discovery in sparse-data regimes (BES), and provide scalable manifold learning for large-scale molecular dynamics and DFT simulations at DOE's Leadership Computing Facilities and NERSC. By embedding physical laws directly into GP priors, the framework guarantees that statistical inference preserves the key structures governing safety-critical and high-consequence systems. The resulting posteriors enable researchers and operators to quantify uncertainty rigorously, identify where additional measurements are most valuable, and make real-time autonomous decisions with well-calibrated confidence. Through seamless integration of heterogeneous data — sensor streams, simulation outputs, and experimental diagnostics — the framework delivers robust inference even when information is sparse or fragmented. The PI's open-source platform **gpCAM**, downloaded more than 200,000 times and deployed at over 30 facilities globally, provides an immediate deployment pathway, ensuring that advances developed here reach the broader DOE community rapidly and at scale. By addressing four persistent barriers to reliable scientific ML within a single, unified framework, this project will establish Gaussian processes as a foundational, scalable, and trustworthy engine for the next generation of autonomous DOE science.

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

An Integrated Approach to Understanding the Nucleosynthesis of the p-Nuclei

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Researchers have spent decades modeling and gathering indirect evidence for the origin of the proton-rich stable isotopes—known as p-nuclei— but the specific astrophysical sites and mechanisms responsible for producing the p-nuclei remain unresolved. This multidisciplinary project will uniquely integrate cosmochemistry, experimental nuclear physics, and theoretical modeling—as well as world-class characterization and experimental facilities—to advance understandings of the origin of the p-nuclei and of stellar nucleosynthesis in the multi-messenger era. It will: (1) identify and characterize oxygen-rich pre-solar grains—with a focus on measuring isotopic ratios of important trace elements; (2) Experimentally measure previously inaccessible key nuclear reaction rates critical to p-nucleosynthesis; and (3) in collaboration with multiple astrophysical modelers, will integrate the new isotopic and reaction data into existing nucleosynthesis simulations to establish more stringent constraints on the astrophysical conditions in which the p-nuclei are made—and thereby potentially confirming or eliminating proposed sites.

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

Integrating Coupled Large Lake-Atmosphere Dynamics into E3SM: Understanding Coastal System Predictability with Human Process Interactions

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Large lakes strongly influence regional weather and water resources, yet many Earth system models fail to capture their dynamic nature, limiting our ability to predict conditions in surrounding urban and rural areas. This project addresses that gap by enhancing the Department of Energy's Energy Exascale Earth System Model (E3SM) to better understand and predict the interactions of large lakes with the atmosphere, land, cities, and human activities in the Lake Michigan coastal region. It achieves this by placing a 'zoom lens' over the area, integrating a new, dynamic model of Lake Michigan-Huron with a high-resolution model of the local atmosphere and urban-rural landscape. This approach improves simulations of lake breezes, thunderstorms, lake-effect rain and snow, and urban heat dynamics while also capturing how regional changes can influence the broader Earth system. Crucially, the coupled system also incorporates the influence of human activities, such as urban growth, land-use change, energy demand, and heat released by power plants and data centers. Using this comprehensive tool, the project runs extensive simulations spanning weeks to years to understand how these interconnected natural and human processes affect temperature, rainfall, snowfall, and heat waves. Artificial intelligence methods enable the efficient exploration of many possible conditions, identifying key sources of uncertainty and assessing how they affect predictions. The resulting scientific understanding, software, and modeling capabilities will improve predictions for large-lake coastal systems and can be applied to other large lakes across the United States and around the world.

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

Chemical Dynamics Governing Energy Dissipation in Dual Cross-link Networks

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Elastomers are permanently cross-linked polymers with glass transition temperatures below ambient conditions. In energy relevant applications these materials must preserve high elasticity at small strains while dissipating substantial energy under large deformations. Conventional elastomers dissipate energy primarily through backbone segmental motions, but this mechanism is ineffective at elevated temperatures. Dual cross-link networks (DCNs), which combine permanent and dynamic cross-links, address this limitation by introducing cross-link exchange as an additional mode for energy dissipation. By chemically modulating the cross-link lifetime τ_{XL} , a function of exchange kinetics, dissipation may be activated across targeted ranges of temperature and strain rate. A critical unresolved question in understanding DCN physical chemistry is the molecular origin of τ_{XL} . Existing theories typically assume that τ_{XL} is directly coupled to the segmental relaxation time τ_{seg} , yet recent results indicate that these two timescales may be partially or fully decoupled. This project tests the causal hypothesis that the backbone and cross-link chemistries independently define τ_{seg} and τ_{XL} , respectively, and that macroscopic energy dissipation maximizes when the applied mechanical strain rate aligns with either characteristic timescale. This hypothesis is evaluated by combining polymer synthesis, theory, simulations, and multi-scale characterization involving Department of Energy user facilities. The project involves three parallel aims. (I) Theory and simulations are developed to map the relationship between τ_{XL} and deformation. (II) τ_{XL} is measured using linear rheology and X-ray photon correlation spectroscopy. (III) Large nonlinear deformations are applied to evaluate how macroscopic stress dynamically alters cross-link exchange and energy dissipation. Overall, this work establishes DCNs as a versatile platform for understanding how cross-link reactivity and topological fluctuations govern dissipation in extreme out-of-equilibrium operating environments.

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

Unraveling Emergent Separation Mechanisms in Complex Solvent Environments

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Existing separation processes are energy-intensive and inefficient for the separation of dilute, similar sized guest species. To overcome this fundamental separation science challenge, novel materials that exhibit emergent separation properties that lead to improvements in gas selectivity or uptake by amplifying or correlating molecular processes are needed. Select compositions of porous liquids, nanoporous particles suspended in solvents that are sterically or chemically excluded from their internal porosity, have exhibited these promising emergent separation properties. However, the fundamental mechanisms that cause these properties remain poorly understood, limiting the rational design and optimization of mixed liquid-solid materials for critical separations. Therefore, it is hypothesized that emergent separation properties arise from the dynamic interplay of partial solvent infiltration and solvation networks at nanoporous particle interfaces, which collectively modulate guest molecule binding and interfacial transport across solvated and non-solvated domains. Three critical features of porous liquids are evaluated: (i) the structure of the external solvated interface, (ii) mechanisms of time-dependent solvent infiltration, and (iii) mass transport across solvated and non-solvated domains. To achieve these goals, integrated generative adversarial network machine learning techniques and molecular dynamics simulations are used to understand how defect driven solvation and solvent gradients at nanoporous interfaces mediate selective separations across interfaces. Next, high throughput computational screening are used to identify solvent-nanoporous particle combinations that exhibit partial and time-dependent pore infiltration to uncover oversolubility mechanisms within nanoconfined pores that are then validated with positron annihilation spectroscopy. Finally, artificial neural networks are used to assess spatially varied transport through heterogeneous porous liquid structures to understand the role of transport pathways through unsolvated and partially solvated internal porosity. Overall, this project advances our fundamental understanding of how solvent-particle microenvironments influence guest binding and transport, while also developing predictive capabilities needed to accelerate the discovery of tunable separation systems with emergent properties that overcome challenges in traditional separation processes.

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

Illuminating the Beauty of Quarks

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The Large Hadron Collider (LHC), located at the European Organization for Nuclear Research (CERN), provides a unique testing ground for the standard model (SM) of particle physics through high energy particle collisions. With the unprecedented volume of data that has now been collected, the LHC community's priorities are increasingly shifting towards precision measurements. An understanding of jet formation is essential to this effort, with direct impacts on the associated experimental uncertainties for Higgs boson measurements, searches for physics beyond the SM, top quark physics, and other key physics processes. The challenges of describing both perturbative and nonperturbative effects in quantum chromodynamics are particularly pronounced for the heavier bottom (b) quark, with additional theoretical challenges related to the additional mass scale and experimental complications in reconstructing heavy flavor hadrons.

This research fills critical gaps in the understanding of heavy flavor jet formation through measurements of dead cone effects in b-quark jets and gluon splitting to heavy flavor quarks using the Compact Muon Solenoid (CMS) experiment at the LHC. Precision physics requires a precision understanding of detector reconstruction, and this project will thereby develop novel particle reconstruction strategies for CMS through transformer algorithms. In turn, these will address key challenges in hadronic reconstruction, including mitigating effects from multiple particle interactions per LHC collision crossing, disentangling contributions from overlapping signals, and incorporating secondary vertex information in the analysis. Looking beyond the LHC, this research will enable the next generation of precision physics studies at future colliders by developing readout and digitization techniques for AC-coupled low gain avalanche diodes (AC-LGADs), which combine picosecond timing resolution with micron-level spatial precision. Together, this work promises to provide new insights into jet formation, reduce theoretical modeling uncertainties for key processes, advance precision particle reconstruction at collider experiments, and establish new and innovative capabilities for studying hadronic final states with next-generation silicon-based detectors.

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the DOE Established Program to Stimulate Competitive Research.*

Real-Space Quantum Geometry of Altermagnetic Textures: A Route to Spin Control at Zero Magnetization

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Altermagnets are a new class of magnetic materials in which electrons with opposite spin respond differently even though the material has no net magnetization. Current theory explains this behavior in uniform crystals. What remains lacking is a theory of how altermagnetic textures – spatial variations of the magnetic order – affect electronic spin transport. Recent experiments are beginning to image these textures, making it timely to develop a theory of real-space spin control in textured altermagnets.

Most work on spin transport in magnetic textures relies on effective electromagnetic fields to describe the motion of electron spins. This project investigates a different route in altermagnetic textures: an emergent spin-dependent geometry in real space. The central idea is that spatial variations of altermagnetic order can steer electrons with opposite spins along different paths. This behavior can be pictured as motion through a curved landscape whose shape depends on spin. The resulting geometry provides a new principle for controlling spin at zero magnetization. It also offers a way to use spin transport to reveal the symmetries of the altermagnetic order. The research will develop this framework along three directions: (1) formulating a microscopic theory of real-space quantum geometry and determining its consequences for spin transport; (2) identifying ways to control spin transport with electric fields; (3) exploring spin control in systems that combine altermagnetic and superconducting materials.

This research will combine theoretical calculations and numerical simulations to connect models of altermagnetic textures with measurable spin-transport properties. Input from materials modeling (density functional theory) and experimental collaborators will help connect the theory to candidate materials and experimentally feasible measurements. By advancing the fundamental understanding and control of quantum materials, the work supports the mission of the U.S. Department of Energy's Basic Energy Sciences program. More broadly, the project will establish a theoretical roadmap for real-space spin control in altermagnets and guide near-term spin-transport experiments in textured quantum magnets.

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

Characterization and Control of Magnetic Symmetry in Spin-polarized Materials

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The recent discovery of the magnetic materials now termed “altermagnets” has marked a seismic shift in our understanding of magnetic symmetry. Theory predicts that these materials will have spin-polarized electronic states with a characteristic momentum dependence, without the need for a net magnetic moment. This discovery has prompted intense interest due to the potential for novel electronic and spintronic devices, taking advantage of the fast switching speeds of antiferromagnets while avoiding problems due to stray fields. However, despite recent theoretical progress there are significant gaps in knowledge between the high-level symmetry arguments and actual material implementations. A central issue is the magnitude of the energy splitting between the spin-polarized electronic states. While symmetry arguments indicate whether the splitting is allowed, they give no indication of its size. If splitting is present but extremely small, it is unlikely to be useful for applications. Recent theory work has suggested that magnetic multipolar order may be the microscopic quantity which is responsible for the unconventional altermagnetic properties. However, despite its increasingly central role in theory, altermagnetic multipolar order has never been experimentally detected.

These altermagnetic multipoles can be visualized as a magnetization density distribution that is the same on each atom, with a shape reflecting the altermagnetic symmetry. We propose to search for these multipoles using polarized neutron scattering to map out the magnetization density, applying an analysis technique designed to isolate the ‘ferromagnetic’ component which will contain the multipolar density. The multipoles are also expected to be implicated in the coupling between altermagnetic domains and external fields. Manipulating domains is a crucial experimental barrier which must be overcome for the construction of useful devices, since the presence of magnetic domains causes cancellation of the altermagnetic electronic properties. Advanced in-situ x-ray and neutron scattering techniques will be used to quantify the coupling between magnetic domains, multipolar order and applied fields, for the purpose of controlling the magnetic domains. This work will be crucial for connecting theory with real world application: designing materials with optimal altermagnetic properties and manipulating altermagnetism for use in real devices.

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

Quantum Computing Primitives for Molecular Simulations with Dual-Species Atom Arrays

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This project will develop new quantum simulation tools that use measurement and controlled dissipation to more naturally capture important features of molecular systems.

Quantum simulation of molecules is one of the most promising applications of quantum computers. The basic idea is compelling: because molecules themselves obey the laws of quantum mechanics, quantum hardware should be naturally suited to describing their behavior. Yet translating this idea into useful simulations has proven difficult for reasons that go beyond simply building larger and better quantum computers. Molecular systems have strong physical constraints, complex correlations, and interactions with their environments that are often inefficient to represent using conventional quantum circuits.

Rather than forcing these features of molecular physics into a general-purpose circuit model, this project will explore quantum simulation strategies that are naturally matched to them from the outset. In particular, the research will investigate measurement as a tool for preparing, verifying, and steering quantum states within physically relevant molecular configurations, and engineered dissipation as a tool for controlling quantum systems and reproducing the effects of their environments. These ideas will be developed using a programmable quantum simulator based on arrays of two different atomic species, Yb and Rb, whose complementary roles provide flexible resources for measurement, control, and interactions with a programmable quantum environment.

The project will establish and experimentally test a new set of quantum simulation primitives built around measurement, dissipation, and environmental coupling. These capabilities will provide a framework for exploring computational approaches that more closely reflect the structure of the physical systems being simulated.

For molecular science, this work could open new routes toward quantum simulations of complex chemical and biological systems. More broadly, the measurement- and dissipation-based tools developed here could expand the capabilities of quantum processors, opening new approaches to quantum simulation, control, and computation across a wide range of scientific problems.

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

Continuum and Lattice Approaches to Generalized Symmetries

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Symmetry organizes the particles and forces of nature, and for a century physicists assumed every symmetry transformation could be reversed. Quantum physics says otherwise: a symmetry transformation can merge distinct states into a superposition, erasing the memory of where it began. Such a non-invertible symmetry cannot be undone yet remains exact and predictive. These remarkable symmetries have now been found in the theory of quarks, providing a new explanation for the decay of a subatomic particle. This research project will investigate how non-invertible and other generalized symmetries may overcome a longstanding obstacle to representing the fundamental laws of physics on a computer. One of the most surprising discoveries of twentieth-century physics was that interactions among elementary particles distinguish left from right: the laws of physics can look different through a mirror. This property, known as chirality, lies at the heart of the Standard Model. Yet chirality is exceptionally difficult to preserve when physicists translate the physics laws into discrete systems that computers can simulate. Guided by generalized symmetries, this research project aims to reveal hidden forms of chirality and open new paths toward simulations that faithfully retain nature's distinction between left and right. More broadly, it will establish generalized symmetries as powerful new tools for high-energy physics, condensed-matter physics, and quantum information science.

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

Predictive Quantum Dynamics of Programmable Iron-Sulfur Cluster Networks and Multi-Exciton Energy Transduction Enabled by First Principles Stochastic Quantum Chemistry

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Molecular computation and multi-excitonic light energy transduction have the potential to dramatically improve energy use and generation. The objective of this research program is to develop a fully *ab initio* computational platform to understand and model these dynamical processes in a predictive and chemically-specific manner, by integrating accurate stochastic quantum chemistry with exact non-Markovian quantum dynamics. The methodology will be used to demonstrate how logic operations, such as an AND gate, can be realized by a programmable chemical network that exploits field-gated electron transfer between polynuclear iron-sulfur cluster nodes. In addition, the methodology will enable first principles modeling of photocatalytic processes such as singlet fission (converting a single photon into two excitons) and the reverse process known as photon upconversion, with the capability of accurately modeling the entangled multi-excitonic intermediate states and their manipulation by magnetic field effects.

From a fundamental chemical physics perspective, these seemingly disparate quantum phenomena involve prominent many-electron correlation effects (such as spin entanglement and superexchange mechanisms) and strongly coupled electronic and vibrational degrees of freedom, necessitating theoretical advances in both correlated electronic structure and open quantum dynamics techniques. The research plan involves the development of algorithms, accelerated by machine learning strategies, to extract the physical parameters needed for field-driven open quantum dynamics simulations from an *ab initio* quantum Monte Carlo method that is both accurate and scalable to relatively large system sizes. The Hierarchical Equations of Motion formalism will then be deployed and extended as necessary to, e.g., explicitly account for prominent breathing modes and the manifold of low-energy spin states. Taken together, this state-of-the-art computational platform has the potential to reveal new design principles for next-generation optoelectronic materials with efficiencies beyond conventional limits, and to advance the prospect of energy-efficient molecular computing architectures that operate near the fundamental thermodynamic limits of information processing.

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

Terahertz Near-field Spectroscopy of Twisted 2D Materials and Few-layer Heterostructures

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This project investigates heterostructures of two-dimensional (2D) and few-layer materials with terahertz spectroscopy. Certain materials naturally form layered structures in which sheets with atomic thickness are weakly held together by van der Waals interactions. These layers can be isolated, and many combinations can be stacked and assembled at desired twist angles. The protocol of layer-by-layer assembly has been used to enable a wealth of emergent phenomena, ranging from superconductivity and other correlated electronic states to polar vortex lattices. However, producing high-quality uniform heterostructures of stacked 2D materials that cover large areas remains challenging. Studying promising heterostructures of layered materials, therefore, currently requires probes capable of interrogating local properties. Terahertz spectroscopy is a particularly sensitive probe of a broad range of effects, including polar lattice vibrations and the electrodynamics of superconducting condensates. However, the large wavelengths of terahertz radiation make conventional far-field spectroscopy challenging for materials and heterostructures that are smaller than the terahertz wavelength. This project uses and develops near-field methods for terahertz spectroscopy that can investigate the local properties of heterostructures of 2D and few-layer materials. These techniques enable terahertz spectroscopy at sub-micron length scales, which is well suited to interrogate twisted 2D and few-layer materials. The project will investigate opportunities to engineer polar textures in heterostructures of ferroelectric oxyhalide materials, which are promising candidates for memory devices, polarization and heat transport. Intense terahertz radiation, with finite momentum, will be used to control and interrogate heterostructures of 2D and few-layer materials. The project will also support the development and use of low-temperature near-field terahertz spectroscopy to investigate layered superconducting heterostructures where evidence time-reversal symmetry breaking has been reported. The results will enhance the understanding of few layer ferroelectric or superconducting heterostructures, which offer promising platforms for next-generation microelectronics, memory, and quantum devices.

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

Visualizing Ferrons at the (Sub)nanoscale

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Collective excitations governed by coupled spin, lattice, orbital, and charge degrees of freedom in quantum materials are important to many energy-efficient technologies. For example, magnons, which are collective spin excitations, can route information in spintronic devices at low power by moving magnetic excitations rather than electrons. An analogous class of collective excitations in ferroelectric materials, called ferrons, has recently emerged as an important area of study. Ferrons are collective excitations of polarization fluctuations that carry a dipole moment and can be controlled with an electric field. They have been spectroscopically detected in van der Waals ferroelectrics, but their detection in three-dimensional ferroelectrics has remained challenging because of their complex polarization configurations. This research project will reveal the (sub)nanoscale ferron landscape in three-dimensional ferroelectrics using modified scanning transmission electron microscopy–electron energy-loss spectroscopy. Specifically, the research will determine how ferron energy and dispersion are affected by different polarization configurations and applied electric fields. The objectives of this research are to identify ferron types and their characteristic energies at different polarization textures, measure ferron dispersion, and establish their tunability with electric fields. These studies will provide a mechanistic understanding of (sub)nanoscale ferron behavior and a foundational understanding of how ferrons transport energy in three-dimensional ferroic materials. More broadly, the microscopy techniques developed through this research could enable the detection of weak excitations that are otherwise obscured by much stronger signals, advancing basic research in quantum materials and future energy-efficient information technologies.

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

Medium-Mediated Physical Learning in Nonreciprocal Active Materials

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Active materials are built from components that consume energy and generate motion. These systems can spontaneously organize into collective patterns and mechanical responses, but most synthetic active materials cannot yet acquire a new function from experience. A central challenge is therefore to understand how a material can adjust its own behavior through local physical interactions, retain the resulting function, and recover it later without centralized computation.

This research will establish the physical principles of medium-mediated learning in active materials. The central idea is that individual active building blocks can adjust their activity in response to physical signals carried by the surrounding material. The medium can then play three roles: it can transmit information about the collective state, couple individual units to one another, and retain a physical memory of past activity. The research will determine whether these local feedback processes are sufficient for an active material to acquire useful collective functions.

Three objectives will address this question. First, the research will determine how fluid flows transmit the information required for learning and which collective responses can be controlled through those flows. Second, it will test whether viscoelastic materials, whose mechanical stresses relax over time, can provide an intrinsic form of memory that enables active materials to learn delayed and time-dependent responses. Third, it will determine how nonreciprocal interactions, in which the response between two components is not symmetric, expand the range of behaviors that can be learned, including directional motion and self-sustained dynamics.

The work will combine theory, computer simulations, and experiments using programmable active spinners in fluids and viscoelastic materials. Because the activity and interactions of individual spinners can be controlled directly, this platform makes it possible to connect simple local learning rules to the collective behaviors that emerge at larger scales.

The expected outcome is a general physical framework for designing active materials that can acquire, retain, and recover function through their own dynamics. By revealing how local activity, physical feedback, material memory, and nonreciprocal interactions produce coordinated behavior, this research addresses the U.S. Department of Energy Basic Energy Sciences mission of understanding and controlling how interacting building blocks organize into functional materials.

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

Cancer and Encapsulation as a New Paradigm for Chelating Emerging DOE Medical Radionuclides

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The rapid expansion of targeted radiopharmaceuticals, together with advances in isotope production, has created an unprecedented arsenal of valuable medical radionuclides that span the periodic table. Many of these radionuclides, developed through the support of the U.S. Department of Energy (DOE) Office of Isotope R&D and Production (IRP), possess attractive nuclear decay properties and half-lives well suited for treating and imaging a broader spectrum of cancers. Yet, most remain unrealized, stalled in the “valley of death” between production and clinical application, because of longstanding challenges in designing molecules that can securely bind and deliver these radioactive isotopes to disease sites. This project will develop and evaluate new chemical approaches to address these challenges and expand the range of radionuclides that can be used in nuclear medicine. The research combines molecular design, chemical synthesis, radiolabeling studies, and stability testing to improve our understanding of how molecular structure influences radionuclide stabilization. The knowledge generated through this work will strengthen the scientific foundation needed to advance emerging DOE-produced isotopes into biomedical research and future clinical applications.

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

The Role of Entropy in the Interfacial Cohesion of Metals and Alloys

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Interfacial decohesion governs the failure of metals and alloys in technologies critical to the Nation's energy security, including the ductile-to-brittle transition in body-centered cubic alloys, brittle fracture in intermetallics, cavitation at duplex boundaries, and precipitate–matrix decohesion. The classical Rice–Wang theory attributes interfacial cohesion to free energy changes from solute segregation, but entropic contributions are often neglected because of computational cost and the scarcity of experimental data needed to fit the thermodynamic properties. However, there is growing evidence of excess entropy, suggesting non-negligible entropic contributions to both segregation and cohesion.

This project aims to provide a fundamental understanding of how excess entropy in solute segregation to grain boundaries and free surfaces influences interfacial cohesion in metals and alloys, both directly, by altering segregation free energy and embrittlement potency, and indirectly, by controlling fracture path and interfacial structure. The project objective is to develop an atomistic framework that incorporates the spectrum of segregation site energies at interfaces in metals and alloys, and to quantify the role of entropy in interfacial cohesion via thermodynamic modeling and free energy quantification methods enabled by machine learning interatomic potentials. This research addresses interfaces of increasing structural complexity, from simple high-angle tilt boundaries to intermetallic and duplex grain boundaries containing multiple bulk and interfacial site types. The project will also examine the role of entropy under small structural perturbations (strain) and during structural transitions.

By establishing the fundamental enthalpy–entropy relationships that govern segregation and cohesion at surfaces and interfaces, the project will clarify the thermodynamic mechanisms behind interfacial decohesion and provide predictive frameworks for segregation and defect engineering. These frameworks will yield the interfacial free energies essential to modeling interfacial failure in extreme environments relevant to energy applications.

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

Exciton-Spin Coupling for Optical Control of Spin States in Low-Symmetry vdW Heterostructures

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Controlling magnetism with light could enable faster, more energy-efficient technologies for information processing, sensing, and communication. This project will establish atomically thin magnetic semiconductors as a platform for controlling magnetic states with light. It will focus on low-symmetry two-dimensional magnetic semiconductors, in which optical, magnetic, and structural properties are strongly interconnected. The research will first identify how light-generated excitons couple to magnetic order. We will then use twisting and interfacial coupling to create systems with multiple competing magnetic states and test whether these states can be selectively and reversibly switched by light. The work will combine strain tuning, moiré and interfacial engineering, magneto-optical spectroscopy, and nanoscale magnetic and structural characterization. The project will establish a predictive framework for designing optically controllable spin states in quantum materials. It will reveal how reduced symmetry, atomic-scale structural reconstruction, and interfacial coupling shape magnetic energy landscapes that can be controlled by light. The resulting design principles and optical control strategies could enable faster, lower-power, and non-contact approaches to manipulating magnetism in future spintronic and optoelectronic technologies.

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

Physics-Guided, Hardware-Aware AI for Adaptive and Scalable Control of Accelerators

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Particle accelerators and high-power lasers enable researchers to probe the building blocks of matter, design new materials, and search for new physics. Facilities coming online this decade will demand real-time control far more accurate and intelligent than exists today. These machines must sense and correct disturbances acting on several time scales at once. Those corrections are still tuned by hand or found by trial and error. Newer artificial intelligence (AI) methods often ignore both the machine's physics and the limits of the electronics that must run the algorithm in real time. The objective of this research is to bring the two together: AI guided by the physics of the system it controls, matched to the hardware's speed, timing, and memory limits, and retrained continuously from streaming data as conditions drift. The aim is not one controller for all machines, but a shared methodology and reusable modules — from signal processing to operator tools — retuned for each application.

Three different systems will test the approach. In high-temperature superconducting magnets at Berkeley Lab's U.S. Magnet Development Program, machine learning can spot a quench — a local loss of superconductivity — seconds before conventional protection reacts, in time to protect the magnet. In superconducting radio-frequency cavities at Fermi National Accelerator Laboratory, the electric field and mechanical resonance are linked and must be handled as one problem. At Berkeley Lab's most powerful laser, jitter recently left nearly a third of an experiment's data unusable; holding position, angle, and focus steady together is what prevents that loss. In every case the controller must scale from one magnet, cavity, or beamline to a full assembly, so the same method can steady a whole machine. The approach must also travel between machines: in a fourth demonstration, with Northern Illinois University at Argonne National Laboratory, the same framework will control the shaping of an electron beam.

The work builds on and further develops advanced control electronics — including Marble, the Berkeley Lab open-source platform now running at SLAC National Accelerator Laboratory, Argonne, and Fermilab — and adds the physics-guided AI layer. Algorithms, firmware, and a common data standard will be released as open source for others to adopt. Together these results establish intelligent real-time control as a foundational capability for next-generation accelerators and laser facilities, and more broadly for other complex scientific instruments.

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

Sea-breeze intrusion in coastal cities: from urban boundary layer structure to building energy demand

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Cities located along coastal bays, such as Baltimore, Maryland, are characterized by sharp contrasts in surface properties. Their impervious and often hotter surfaces are surrounded by cooler rural areas and coastal waters, creating strong differences in surface temperature. These temperature contrasts can generate local atmospheric circulations, such as sea and bay breezes, in which cooler air moves toward warmer land, transporting and mixing heat, moisture, and pollutants across the urban environment. As a cool breeze advances into a city, its interaction with buildings modifies how far the cooler air penetrates, how wind mixes heat within the city, and how urban temperatures and building cooling demands respond. Yet current weather and energy modeling systems do not adequately represent how these circulations interact with the built structure or how these interactions affect heat exchange between urban surfaces and the atmosphere. These limitations introduce uncertainty into predictions of the evolution of the lower atmosphere, cloud development, and building cooling demand in coastal cities. To address these questions, the planned research will leverage observations from the Department of Energy Atmospheric Radiation Measurement (ARM) Coast-Urban-Rural Atmospheric Gradient Experiment (CoURAGE) combined with high-resolution numerical simulations. The graphics processing unit (GPU)-accelerated Energy Research and Forecasting (ERF) model will serve as the primary computational framework for reproducing atmospheric conditions observed in Baltimore at very high spatial resolution, including airflow and heat transport around buildings and their interaction with regional weather. Results from these detailed simulations will be translated into a new representation of urban heat exchange using a hybrid physics-machine learning approach that combines physical understanding with information from simulations and field observations. These improved representations will be incorporated into urban modeling capabilities in ERF and the DOE EnergyPlus building energy model to evaluate how more accurate representation of urban-atmosphere interactions affects predictions of building energy use, including during extreme heat events. The planned research will provide new understanding of how processes occurring at the scale of individual buildings interact with coastal and regional weather and will improve the ability of weather and energy models to predict urban heat and energy demand in coastal cities.

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

Revealing Cross-Scale Impacts of Short-Duration Coastal Extreme Events on Long-Term Energy System Evolution Through AI-Enabled Coupling of Earth and Human System Models

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Frequent, short-duration extreme events in coastal systems generate nonlinear, path-dependent, and potentially lasting impacts on interconnected energy, water, and land systems. However, existing frameworks lack methods to translate frequent, high-impact, short-duration extreme events simulated by Earth system models into digestible information that can be used for human system models. Earth system and longer-term human system models remain poorly connected across temporal scales. This gap remains difficult to fill because of the complexity of how the impacts of extreme events can propagate across varying temporal scales and intertwined systems, particularly in coastal regions with onshore and offshore infrastructure networks. The objective of the planned work is to understand how short-duration extreme events propagate beyond the temporal scale of the originating event and influence the evolution of interconnected human systems. A new, customizable, Artificial Intelligence enabled model – Temporal Integration of Disasters and Energy Systems (TIDES) – will be developed to integrate extreme-event signals from the Energy Exascale Earth System Model (E3SM) into the Global Change Analysis Model (GCAM). This modeling framework, E3SM-TIDES-GCAM, will be used to simulate longer-term human systems evolution in response to short-term shocks. The Gulf Coast will serve as the case study region because of its dense population in large cities, the concentrated critical energy infrastructure located both onshore and offshore, and the frequent occurrence of extreme events. The planned work will enable a new class of questions to be addressed: whether repeated, tightly sequenced coastal extreme events can alter infrastructure vulnerability, resilience investment, technology adoption, regional energy transitions, and land-use trajectories in ways that are not recoverable from the existing modeling framework.

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Structural Origins of Emergent Order in Moiré Materials

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When two atomically thin crystals are stacked with a slight twist, their overlapping atomic patterns form a larger repeating pattern called a moiré pattern. These moiré materials host collective electronic behavior that neither layer shows on its own, including superconductivity and ferroelectricity. In every moiré material, the atoms and layers naturally stretch, buckle, slide, and vibrate, spontaneously settling into intricate new arrangements. This structural motion is a fundamental and universal aspect of moiré materials and may be the key to understanding the origin of their collective electronic behavior. However, a single moiré pattern can span millions of atoms, far too many for standard quantum mechanical calculations to handle. As a result, most existing theories treat the atoms as frozen in place, leaving out this potentially crucial ingredient.

This research will develop a multiscale framework that carries this structural information from individual atoms up to the full moiré pattern, treating the motion of the atoms on equal footing with the electrons by combining quantum mechanical calculations with machine learning to make simulations of millions of atoms tractable. The framework will address three open questions in moiré physics. First, why do chemically similar moiré semiconductors settle into very different electronic states? Second, do atomic vibrations contribute to moiré superconductors? Third, what mechanism underlies a recently discovered ferroelectric memory effect in stacks of graphene and boron nitride? This effect stores an electric polarization that can be tuned continuously and retained without power, a promising foundation for future low-power computer memory. All predictions made by this research will be tested in close collaboration with experimental groups.

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