Advanced Materials to Enable Next-Generation High-Power Accelerators

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This research will develop advanced materials for beam-intercepting devices such as beam windows and particle-production targets to improve the performance, reliability, and operation lifetimes of next-generation accelerator target facilities. The microstructure and thermomechanical properties of novel high-entropy alloys and nanofiber materials will be specifically tailored to enable high-power secondary particle beam production in future facilities like the 2.4-megawatt Long-Baseline Neutrino Facility. This research project will combine in-beam experiments with complementary simulations to develop radiation damage and thermal shock tolerant materials, two of the leading cross-cutting material challenges that disrupt the performance and lifetime of beam-intercepting devices. Iterative simulations to optimize the material composition, physics performance and beam-induced thermomechanical response will guide the material design and fabrication processes based on established figures of merit. Ensuing material irradiation experiments using low-energy ions and prototypic high-energy protons, followed by extensive post-irradiation material characterization, will assess and qualify the materials for use in future high-power target facilities. These novel beam-intercepting materials, continuously bombarded by particle beams, will have to withstand an order-of-magnitude increase in beam intensities. With conventional materials already limiting the scope of experiments, the development of robust materials beyond the current state-of-the-art is crucial. The novel materials will enable the reliable operation of future world-leading accelerator facilities essential to support new high energy physics scientific discoveries.

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

Advanced methods for hybrid meson searches

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The strong nuclear force binds the fundamental quarks into composite hadrons, such as protons and neutrons, and is effectively responsible for 99% of the mass of the visible universe. Even though it is described by the theory of quantum chromodynamics (QCD) within the Standard Model of particle physics, it bears many unsolved mysteries. Confinement and the large interaction strength at low energies prevent the deduction of the hadron spectrum from first principles. Simplified models successfully describe the observed ground-state mesons and baryons as quark-antiquark or three-quark bound states, respectively, but no known mechanism in the theory forbids combinations of four or five quarks into so-called tetra- and pentaquark states. Furthermore, the carriers of the strong interaction, the gluons, can potentially contribute to the spectrum of hadrons. They can manifest themselves in the form of pure gluonic bound states, known as glueballs, or the excited gluonic field may contribute to the quantum numbers of so-called hybrid mesons. States with quantum numbers that cannot be realized by conventional quark-antiquark combinations are known as exotic mesons, which serve as unmistakable signs for hadrons beyond the simple quark models. The existence of glueballs, multi-quark states and other exotic excitations in the hadron spectrum is one of the most important predictions of the Standard Model that has not yet been confirmed experimentally. The primary objective of this research is the experimental study of these novel forms of nuclear matter within the spectrum of hadrons to further the understanding of the dynamics of the strong interaction. The Gluonic Excitation Experiment (GlueX) at the Thomas Jefferson National Accelerator Facility (Jefferson Lab) was specifically designed to study the light-quark meson spectrum and to confirm or refute the contribution of hybrid mesons. To unveil the full potential of its high-precision data and ultimately to achieve its scientific mission, novel approaches must be developed and applied, using advanced analysis methods and high-performance computing. This research project will advance Jefferson Lab as a world-wide center of expertise in the field of hadron spectroscopy. The award will invest in a state-of-the-art computing infrastructure, which will be reserved to carry out this research. Advanced methods such as machine learning and artificial intelligence will be used and studied systematically. The project also includes the development and implementation of novel real-time data processing and analysis schemes for the next generation of nuclear physics experiments.

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

Vera C. Rubin Observatory: from Commissioning to Cosmology

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Our observed universe is one statistical realization of the fundamental laws of nature enacted on the grandest scale. As observational cosmologists, we survey increasingly large volumes of the universe to help ascertain those laws with improved accuracy and precision. Experiments at the cosmic frontier have demonstrated that measurements of the cosmic expansion history and growth of structure are sensitive to physics beyond the Standard Model, including the nature of dark energy, massive neutrinos, the initial conditions of the Universe (e.g., inflation), and the particle properties of dark matter. Continuing this enterprise, the Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST) will catalog more galaxies and collect precision lightcurves for more supernovae during its first year of operation in 2024-2025 than all previous cosmic surveys combined. This research is dedicated to realizing the potential of LSST to explore the dark universe by performing value-added science validation studies during Rubin Observatory commissioning to enhance operational readiness, developing, validating, and characterizing cosmology-ready data products that will be the foundation of Dark Energy Science Collaboration (DESC) cosmology analyses using the first LSST Data Releases, and leveraging expertise in pixel-level to catalog-level analyses to advance two dark energy probes, namely, galaxy clustering and cosmography with strong gravitational lensing.

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

Mechanisms of Hydrogen Interaction with Earth Materials in Subsurface Storage Formations

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Hydrogen storage in subsurface porous formations is a promising means of large-scale, long-term energy storage. Saline aquifers are particularly appealing storage reservoirs because of their geographic prevalence, low cost, and large potential storage capacity. However, hydrogen storage has not yet been carried out in such formations. In part, this is because interactions between injected hydrogen, formation fluids, and reservoir minerals are not well understood. These reactions will control the fate of injected hydrogen and ultimately operational feasibility, efficiency, and risk. Through advanced laboratory experiments, this project aims to enhance understanding of hydrogen-brine-mineral interactions under conditions pertinent for hydrogen storage in subsurface saline formations. This work will enhance fundamental understanding of reaction rates and mechanisms as well as impacts on formation properties. The knowledge gained on hydrogen interactions with earth materials will be critical to design and implementation of hydrogen storage systems.

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

Ab Initio Vibrational Dynamics of Strongly Anharmonic Materials

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The atoms that compose molecules and crystalline materials are always vibrating. The quantum mechanical manifestations of these vibrations are called phonons. The properties of phonons, especially how they interact with one another or with electrons in the material, determine a number of technologically important properties, including those of solar cell materials that efficiently absorb light, thermoelectric materials that can turn waste heat into usable electricity, or superconducting materials that can transport electricity without resistance. Unfortunately, predicting these promising behaviors by computer simulation is very difficult when these vibrational interactions are strong. This work will develop a new computational method that will be able to simulate the vibrational properties of crystalline materials accurately and efficiently, called vibrational dynamical mean-field theory. This method is the analog of an existing state-of-the-art method for the quantum mechanical description of strongly interacting electrons, indicating a promising future in the simulation of strongly interacting phonons. This computational method will be implemented in an efficient, open-source software package and, upon completion, will be used to study halide perovskites for solar energy, thermoelectric materials for the recovery of waste heat, and hydrogen-containing materials for high-Tc superconductivity.

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

High performance adaptive multiscale simulation with data-driven scale selective subgrid parameterizations

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In many complex multiscale simulations, a fundamental mismatch exists between computational *resolution,* which is governed by the availability of computing resources, and the physical *scales* of the dynamics that must be simulated for a particular application. To maintain physical fidelity and realism, when the scales of a dynamically significant physical process cannot be resolved by a simulation, that process's effects must still be accounted for in some way. Frequently, such processes are parameterized by subgrid-scale (SGS) models derived from observational data or theoretical scaling arguments that are associated with specific assumptions about the scale of the process relative to computational resolution. As computing resources continue to grow and to permit increasing resolution, physical processes can transition from unresolved, to semi-resolved, to resolved, and the use of SGS models can become a source of error and uncertainty. Adaptive algorithms dynamically adjust the computational resolution to the evolving scales in a multiscale simulation at reduced cost relative to uniformly high resolution simulations, but face two challenges. First, some applications simply contain too large a range of scales to resolve; second, adaptive strategies are difficult to generalize across application areas. We address both challenges with new approaches to adaptive multiscale simulation and SGS models. We will develop new theoretical connections between adaptive algorithms and a recently developed ``equation free'' data-driven approach to SGS modeling. Ultimately, our goal is to provide application-independent adaptive strategies capable resolving a broad range of scales in many different applications such as coupled climate simulations and fusion reactor design, and of choosing an appropriate SGS model based on the availability of computing resources as a simulation evolves to enable the highest possible simulation fidelity.

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

Synthetic Membrane Biology in Microbial Cell Factories

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Yeasts and bacteria can be engineered to function as cell factories for the production of next-generation biofuels and biochemicals. Like all organisms, microbial cell factories are compartmentalized by cell membranes composed of lipids and proteins. These structures are only a few nanometers thick yet play critical functions during bioproduction. Membranes serve as the molecular microenvironment for the Electron Transport Chain (ETC), which is composed of a number of protein complexes and other molecules that carry out cellular respiration to provide energy to the cell. Therefore, membranes play a key role in controlling the rate of energy-producing reactions in central metabolism. They also act as the primary chemical interfaces with the extracellular environment, regulating the transport and efflux of internally produced molecules. The overall goal of this project is to engineer the structure and properties of cell membranes to improve the performance of industrially relevant microbes. The project's first objective is to enhance the rate and efficiency of the respiratory metabolism by engineering the organization of the ETC. Engineering efforts will define the limits of respiratory metabolism and seek to increase the production of energy-intensive next generation biofuels. The second objective is to apply the emerging biochemistry of intracellular lipid trafficking pathways to develop new transporters for the capture of valuable biochemicals produced by the engineered yeasts. Soluble transporters will be developed for terpene-based substrates and be applied to develop new efflux pathways for this class of bioproducts. The planned research activities will thus harness fundamental membrane biology to develop novel biotechnologies to advance towards the development of renewable energy production systems.

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

Innovative Core-Edge Solutions for Tokamaks

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Developing a core-edge solution for power handling while maintaining high core performance in tokamak-based fusion energy is a critical path toward this limitless source of energy. Because the core and the edge are governed by different physics, understanding how these regions interact and can be integrated represents an extraordinary challenge encompassing a wide range of spatial scales and a broad energy and temperature range. The limitation in reproducing reactor conditions in present experiments implies that most of current predictions of a reactor behavior have to rely on modelling. Radiative operation is considered essential for the operation of future fusion devices, and the achievement of core edge integration. As such, a deep physics understanding governing impurity transport and the development of tools to facilitate the achievement of a sustained regime with high radiation fraction has become a pressing issue in fusion research. The objective of this research is to tackle this challenge with a novel strategy which combines experimental activities, physical interpretation, and the development of a new tool for an integrated high fidelity modeling approach that will enable self-consistent impurity transport studies from the edge to the core. This will be applied to existing experiments for validation, and to inform and plan new experiments which will test the improved core-edge solutions identified through the validated modelling, thus ensuring the reliability of the integrated modelling also for predictions. Experiments designed to test modeling-driven, innovative solutions will open up important new directions for extrapolation and future predictions. This work will provide the scientific community with new modelling possibilities in the field of the integration between plasma core and edge and completely new and comprehensive possibilities in physics understanding of the complex physics processes which strongly impact the entire plasma behavior and the viability of present scenarios to reactor conditions.

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

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Unraveling transmutation effects in tungsten-based plasma-facing materials: a computational approach that integrates nuclear transmutation, first-principles calculations, and Machine Learning

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Establishing power sources that do not emit carbon dioxide into the atmosphere is one of the key challenges of the 21st century. Fusion, the reaction that powers the sun, is an energy source with one of the highest energy densities, thus holding great potential to help solve such a global puzzle. Despite the recent advances in plasma physics and materials science aimed at making fusion a feasible energy source, critical challenges still remain. One such challenges is the development of plasma-facing materials (PFMs), which provide the physical boundary between the plasma and vessel and are subject to bombardment by energetic neutrons which change the nuclide composition over time via transmutation reactions. The aim of this research is to establish an innovative computational paradigm for unraveling these transmutation effects in tungsten-based PFMs. The strategy for pursuing this goal is to integrate radiation-induced transmutation, first-principles Density-functional theory electronic structure calculations, and machine learning into a coherent materials design framework. The outcome of this project will be a suite of modeling tools able to predict transmutation effects and allow for inversely designed, high-performance PFMs. Furthermore, the modular nature of the tools will enable future extensions and integration with other modelling efforts, thus allowing for increased physics fidelity and the subsequent investigation, on a broader scale, of the evolving surface morphology and composition of tungsten-based PFMs in a realistic fusion environment.

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

Studying the properties of supranuclear matter with neutron stars

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Neutron stars are nuclear matter's last stand in the battle against total collapse under the overwhelming force of gravity. With masses comparable to that of our Sun yet smaller in size than the island of Manhattan, neutron star interiors drive matter to extreme conditions with densities exceeding those found in everyday nuclei. Under these conditions, the properties and even the composition of matter in neutron stars is uncertain. A wealth of observational and experimental data will become available in the next years. Collisions of neutron stars traveling at a fraction of the speed of light will be detected with gravitational and electromagnetic radiation; thermal emission from hot regions on the surface of isolated neutron stars will be observed with X-ray radiation; radio surveys will continue tracking neutron stars in binaries with white dwarfs and measure their masses; terrestrial experiments will constrain the properties of finite nuclei. At the same time theoretical nuclear calculations are reaching new levels of maturity. This project aims to develop the data analysis infrastructure and algorithms necessary in order to analyze and combine the incoming data. The objective is to determine the properties and composition of neutron star matter as well as the astronomical properties of neutron stars. Some of the key questions this research targets are how large is the pressure inside neutron stars; do deconfined quarks exist in their cores; and what is the heaviest neutron star that exists in our Universe. This project aims to use data to robustly address some of the open questions with the widest interdisciplinary interest in nuclear astrophysics: the internal structure of neutron stars, the properties of matter at the highest densities, and the astrophysical conditions of the production site of heavy elements.

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

Probing Quark Matter and Hadronization Using Energy Flow Substructure

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A hot and dense medium created in high energy nuclear collisions, referred to as the Quark-Gluon Plasma (QGP), exhibits novel properties of a perfect fluid. Its inner working is an open question, which holds the key to a better understanding of the strong interaction. Since the QGP only lasts about 10^{-23} second with a size of a nucleus, jets produced during hard scattering as sprays of energetic and collinear particles can be used to probe such medium. Modifications of such energy flow substructure due to jet-medium interaction therefore encode detailed information about QGP properties. This project uses modern machine learning algorithms to search for QGP signatures in jets, which will be guided by theoretical calculations of jet substructure using Quantum Chromodynamics. Nuclear structure and hadronization, which is the transition from quarks and gluons to final state particles, can also be identified through their imprints in energy flow substructure. The project will contribute to establishing timely and firm basis for understanding the data from the Relativistic Heavy Ion Collider, the Large Hadron Collider, and the future Electron Ion Collider.

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

Modulating Actinide Redox Chemistry with Functionalized Metal Oxide Electrodes

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Controlling actinide oxidation states is critical to the management of used nuclear material. The properties of actinides in unusual oxidation states, and the factors that affect oxidation state stability, are not well understood. During nuclear energy production, actinides heavier than uranium, including neptunium, plutonium, americium, and curium, are produced through neutron-capture processes. Compared to lanthanide fission products (which nearly exclusively exist in the +3-oxidation state), these transuranic elements can exist in oxidation states as low as +3, to as high as +6, with redox transformations that can occur with varying degrees of difficulty. This variety in possible oxidation states and oxidation state stability has created challenges for nuclear waste management.

The stability of specific oxidation states will be adjusted by attaching molecules to the actinide of interest. This will be exploited by creating electrode surfaces functionalized with molecules that bind and adjust the redox potentials of actinides to create a platform to study actinides in unusual oxidation states. The material scaffold we will use is a transparent conductive metal oxide like titania, while the attached ligands include discrete organic or inorganic molecules. We will adjust actinide oxidation states using electrochemical input (voltage), which may be combined with light input. The additional use of light excites the metal oxide electrode and can lower the voltage required to alter actinide oxidation states and improve efficiency. Initial work will focus on uranium and the factors that affect the reductive destruction of the uranyl structure to form a tetravalent uranium species. Ensuing studies will use actinides formed from nuclear power including neptunium, americium, and curium.

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

Molecular and Network Design of Liquid Crystal Elastomer Elastocaloric

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The elastocaloric effect occurs when stress is applied to or removed from a material inducing a phase transformation, causing the material to heat up or cool down. Thus, by coupling a change in entropy between two phases to an applied stress, elastocalorics provide a potential solid-state solution to replacing the vapor compression cycle of today's refrigeration. Notably, elastomeric elastocalorics are capable of achieving tremendous performance for orders of magnitude smaller applied stress than other leading elastocaloric candidates such as shape metal alloys. Relative to conventional elastomeric elastocalorics, liquid crystal elastomers (LCEs) exhibit a distinct mechanotropic phase transition, enabling excellent elastocaloric performance at small strains and stresses. However, LCE elastocaloric performance remains limited by the magnitude and sharpness of the mechanotropic phase transition. While liquid crystal small molecules and polymers undergo sharp first order phase transitions, these transitions are substantially broadened in liquid crystal elastomers. Non-homogenous internal stress fields are a primary driver of the observed continuous phase transition in liquid crystal elastomers and limit the magnitude and sharpness of the elastocaloric response. Improving the elastocaloric response requires driving the phase change towards classical first order behavior throughout the bulk of the material.

The objective of the proposed work is to experimentally develop a fundamental understanding of how structure and heterogeneity across scales control phase behavior in liquid crystal elastomers. Specifically, we will investigate the effects of structure on the thermotropic and mechanotropic phase transitions by probing (1) local network inhomogeneities arising from entanglements, dispersity between crosslink sites and uncontrolled junction functionality, (2) network 'memory' of stress inhomogeneities associated with liquid crystalline domain boundaries and the templated phase of the LCE, and (3) sequence-level molecular tuning to decouple the latent heat of the mechanotropic phase transition from the transition temperature. To achieve this, we will leverage a new LCE synthetic approach that will enable the synthesis of monodisperse sequence-controlled main chain liquid crystalline polymer precursors to create complementary tetrafunctional elastomer precursors. We will also use advanced morphological characterization techniques to identify changes in elastomer structure, phase, and heterogeneity, and to quantify the phase behavior and elastocaloric response. The understanding developed here is anticipated to provide design rules that will enable the rational design and synthesis of next-generation high performance elastomeric elastocalorics suitable for energy-efficient, solid-state refrigeration.

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

Measurement of Neutron-Induced Cross Sections of Nuclides Produced at the Facility for Rare Isotope Beams (FRIB) using the National Ignition Facility (NIF)

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This research leverages unique capabilities at two of the nation's premier research facilities, the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory and the Facility for Rare Isotope Beams (FRIB) at Michigan State University. FRIB is the only accelerator in the world capable of generating many of the nuclear isotopes that are created inside stars, whereas NIF is the world's only facility capable of recreating the conditions inside stars, which it achieves by aiming 192 laser beams onto a tiny capsule to induce nuclear fusion. When nuclear fusion occurs, material added into the target will undergo neutron-induced reactions, and nuclear cross sections can be determined by collecting samples for analysis. This project will harvest radioactive isotopes from FRIB, radiochemically purify those isotopes and add them to the inside of a NIF target capsule in order to study these same isotopes in a neutron-rich environment similar to that in stellar interiors. The measured cross sections will improve our understanding of stellar nucleosynthesis and benefit national security, both key goals of the Office of Nuclear Physics. These measurements will be among the first ever made in a true high energy density plasma and for radioactive species with short half-lives.

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

HPC-OMP-CAR: HPC OpenMP Compiler and Runtimes

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Developing and debugging scientific software are both hard for a variety of reasons. Some are intrinsic to the science involved, others, however, are simply regrettable side effects of the environments with which scientific-software developers are provided. It is unfortunate, but common in the high-performance-computing (HPC) community, that we require domain scientists to learn about low-level performance engineering, hardware stacks, and subtleties of compilers and runtimes—all on top of their actual field of study. Furthermore, this process is repeated for every new machine, every new parallel-programming model, every new scientist, and every major update of the software or hardware stack.

In this project, we will advance scientific-software development beyond the classical approach by providing an *adaptive*, *interactive*, and *smart* development environment tailored to non-expert users. We will evolve the novel compiler and runtime technology we put into the LLVM/OpenMP ecosystem to refocus scientific-application development on the science, not the programming, regardless of the parallel-programming models employed by an application. The overall goal is to automate costly aspects of traditional software development, while also providing the means for applications written in other parallel-programming models to utilize the modern OpenMP ecosystem, and thereby all our existing and upcoming extensions. In addition to *fully interoperable and portable* parallel-programming languages, we will create a first-of-its-kind knowledge base that helps software developers interact with the compiler in novel and productive ways. If we succeed, domain scientists will no longer have to become expert programmers and performance engineers with knowledge of every HPC hardware and software stack.

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

Nanoscale Quantum Sensing and Imaging of Topological Magnets

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Magnetic topological materials with spontaneously broken time-reversal symmetry, nontrivial band topology, and unconventional spin transport properties have received substantial research interest over the past decade due to their rich physics and enormous promise in technological applications. A central focus in this emerging field is the exploration of the relationship between microscopic magnetic structures and exotic material properties dictated by quantum mechanics. We propose to take advantage of the unprecedented field sensitivity and spatial resolution of nitrogen-vacancy (NV) centers, optically active spin defects in diamond, to perform nanoscale quantum sensing and imaging of emergent topological magnets. This will reveal the fundamental physics underlying the interplay between band topology, electron correlations, and magnetism. Specifically, we will image the peculiar noncollinear spin textures of antiferromagnetic Weyl semimetals and probe the Kibble-Zurek type magnetic phase transition in topologically protected condensed matter systems. We are also interested in using scanning NV microscopy to achieve concurrent imaging of local magnetic structures and electric current flow patterns in intrinsic magnetic topological insulators, to reveal the underlying mechanism behind the recently observed “high-temperature” quantum anomalous Hall effect. Our “stretch” goal is to integrate functional quantum magnets with NV spin qubits to establish quantum entanglement between distant NV spin qubits via energy dissipationless chiral edge states.

The proposed research will make important contributions to the burgeoning field of quantum materials and will significantly promote the role of magnetic topological materials in the development of transformative, next-generation quantum information technologies. By developing cutting-edge quantum sensing techniques and demonstrating their operation at broad experimental conditions, we also propose to provide a versatile NV-based quantum microscopy platform, which will extend naturally to a large family of untapped material systems and benefit the material science community in the long run by expediting progress towards future quantum technologies.

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

Integrated Physics Modeling and Online Machine Learning for Characterization and Tuning of Particle Accelerator Systems

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Particle accelerators are some of the most complex scientific instruments in existence. They serve a wide array of medical, industrial, and scientific applications, ranging from cancer treatment to understanding fundamental laws of physics. At highly-flexible accelerator-based scientific user facilities, such as the Linac Coherent Light Source (LCLS) and the Facility for Advanced Accelerator Experimental Tests (FACET-II) at SLAC National Accelerator Laboratory, requests for custom particle beam characteristics must be met within appropriate tolerances to ensure the success of each experiment. This can be challenging due to the large number of adjustable variables, nonlinear responses, and time-varying behavior of these systems. Increasingly, experiments also require fine dynamic control over the position-momentum phase space distribution of the particle beam, as opposed to tuning on approximate scalar metrics (e.g., bunch length, energy spread), or stable maintenance of a single optimal configuration. Proof-of-concept studies have demonstrated the efficacy of various techniques from Artificial Intelligence (AI) and Machine Learning (ML) in beam modeling and tuning, ranging from black-box optimization of accelerator setups with little previous data to the production of fast-executing approximations of computationally expensive physics-based simulations. A major next step is to integrate and build on these approaches to enable more comprehensive, model-informed tuning. Comprehensive ML-based approaches may be able to discover and leverage nuanced system-wide interactions, potentially leading to unprecedented ability to produce custom beam distributions and finely tune them dynamically during experiments. To see this to fruition, this research aims to advance the state-of-the-art in ML-based modeling and control of accelerators, with a heavy focus on customization of beam phase space distributions and the production of highly-transferrable learned model representations. This will involve developments in several areas, including techniques for making ML models more re-usable between accelerator systems and components, techniques for adaptation of ML models to new conditions (including, for example, physics-guided approaches), techniques for dynamic phase space control that leverage ML models, and the integration of these facets to tackle challenging phase space characterization and tuning problems for scientific users.

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

CommAwareNet: Towards Communication-Aware Smart Facilities: Designing an Energy-efficient High-data-rate and Reliable Hybrid THz/VLC Communication Architecture Reinforced with Intelligent Surfaces for Future Networks

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This Career Project will develop foundations for energy-efficient, high-data-rate, and reliable communication links for next-generation advanced wireless technologies. The Internet of Everything is emerging as a major technology that can establish a massively connected network among both human-type users and machine-type devices. Particularly, massive machine-type communication is becoming the dominant communication paradigm for numerous emerging areas, including data center networking and wireless backhaul, healthcare (e-health), manufacturing (industry 4.0), utilities, transportation (connected cars and public safety), and virtual or augmented reality for human-machine interaction applications. The rising demand for high data rates, especially in indoor scenarios and densely populated outdoor environments, will eventually overload conventional RF-based technologies. Consequently, terahertz (THz) and visible light communications (VLC) have been envisioned as promising key enablers to achieve high-speed information transmission for future 6G+ (6G and Beyond) and WiFi+ wireless systems. In particular, THz is a critical part of the overall solution thanks to its huge bandwidth to support optical-fiber-like speeds wirelessly. To achieve energy efficiency and high reliability in wireless systems, future communication networks will depend on seamless integration and operation of RF and optical systems. The best of both RF and optical worlds is needed simultaneously. Thus, there is a critical need to develop a new hybrid architecture for smart facilities (infrastructure) and environments to support the increasing throughput needs. Without such a network architecture, our ability to support the growing data demand of machine-type and human-type users will be limited, thus diminishing our productivity. Motivated by the PI's promising preliminary results, this project follows a hybrid approach that combines THz and VLC technologies reinforced with intelligent reflective surfaces (IRS) to overcome the challenges of new generation hybrid communication links. This project aims to conduct fundamental research to design, optimize, and validate a communication-aware, energy-efficient, and reliable network (CommAwareNet) architecture for future smart facilities and environments that require unprecedented high throughput needs for massive numbers of the machine- and human-type users. The scientific and technical merit of this work lies in the research required to bring the proposed transformative CommAwareNet solution into fully functional and practical architecture.

This project strongly aligns with DOE's advanced wireless networking objectives and the ASCR Advisory Committee's recommendations to broaden the research base and extend its national leadership in advanced computing. This research is expected to have outcomes that have far-reaching impacts ranging from a communication network, development of the computer science workforce, societal needs, and to DOE ASCR's priorities.

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

Grain boundary structure engineering of resilient tungsten alloys for fusion applications

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In magnetic fusion energy systems, the temperature, strong fields and radiation from the burning plasma pose extreme demands for containment. Even though magnetic fields do much of the job of containing the charged particles of the plasma, ultimately it is engineering materials that provide the interface to the world. To face the harsh fusion conditions, tungsten has been proposed as a plasma-facing armor material to meet the needs for high thermal conductivity, high melting temperature, low sputtering rates and superior resistance to neutron damage. Despite these advantageous properties, tungsten is very brittle, which poses a major challenge for both performance and additive manufacturing of tungsten parts, with cycles of melting and rapid solidification creating high residual stresses that lead to cracking along grain boundaries. Solutes, impurities, and transmutation elements from neutron bombardment are also known to strongly affect grain boundary strength and fracture behavior. The aim of this research is to understand how different impurities change the structure and mechanical properties of grain boundaries and how these changes in turn affect the ductility of polycrystalline tungsten alloys. The project will use the state-of-the-art modeling tools to predict grain boundary phases at different concentrations of solutes, and massively parallel computing to model tensile deformation of tungsten grain boundaries to predict associated mechanical properties and failure mechanisms. This research will advance the fundamental understanding of how polycrystalline alloys deform and suggest new strategies for crack mitigation in additively manufactured refractory alloys, thus enabling the design of resilient tungsten alloys for fusion energy applications.

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

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Solutions for a more efficient and economical fusion fuel cycle

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The success of nuclear fusion as a future power source highly depends on power plant economics, ability to reach a significant energy gain factor, reliability, and overall safety. One of the major economic implications of a deuterium-tritium fueled power plant, whether it is based on magnetic or inertial confinement, is the efficiency of the fuel cycle infrastructure dedicated to capturing and reusing the unburned tritium from the reactor exhaust. The need for technology to reduce power plant tritium inventory has been apparent for decades, but its development was never funded at any appreciable level in the US. Several high-level reports on fusion have stressed this need with the most recent being the National Academy of Sciences (NAS) report, which was informed by the US fusion Community Planning Process. The NAS report outlines the need for a plant tritium inventory of <1 kg for public safety, licensing, and economic viability. One of the most effective methods of reducing overall tritium inventory is through the implementation of a continuous plasma exhaust separation loop, which results in a large fraction of the exhausted DT fuel bypassing the tritium exhaust reprocessing plant and being supplied directly back to the fueling systems. This concept of directly recirculating the machine exhaust gas to the fueling system to make fuel pellets has been termed Direct Internal Recycling (DIR). In this approach, the fusion fuel in the plasma exhaust stream is separated from impurities locally on a fast time scale and diverted directly back to the fueling systems, bypassing the slower acting tritium plant isotope separation and other processing equipment, and therefore significantly reducing its size and overall power plant tritium inventory. The objective of this research is to develop scientific understanding through modeling and experiments to design and demonstrate proof-of-principal cryogenic pump-based technology that will efficiently recirculate the DT fuel from the plasma exhaust to the fueling injectors using the expertise and infrastructure available at Oak Ridge National Laboratory.

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

Urban Resilience across the Terrestrial-Aquatic Continuum: Mechanisms to Mass Balance

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Over 70% of the world's population is predicted to live in urban areas by the end of the century, yet the impacts of urbanization on coastal ecosystems are poorly understood. These systems disproportionately impact the global carbon (C) cycle, and in turn, are key to understanding climate change. My vision is to develop a process-based understanding of urban C cycling and its response to disturbances from land to sea.

Across the urban terrestrial-aquatic continuum, a plethora of land uses and associated anthropogenic activities contribute excess C and nutrients (nitrogen [N] and phosphorous [P]) to soils and waterways, which in turn generate distinct biogeochemical processes. Extreme precipitation events heighten these impacts by flushing materials into aquatic ecosystems and ultimately into the coastal ocean. However, despite the common selective pressures imposed by these factors, each urban system is uniquely designed and managed, so deriving generalized knowledge remains challenging. Here, I focus on unraveling the interplay of molecular controls, nutrient supply, and hydrologic factors that drive microbial metabolism of organic matter (OM), the primary constituent of organic C in most ecosystems, in urban coastal systems. I hypothesize that commonalities in urban microbial community function create generalizable mechanisms regulating OM decomposition in the context of anthropogenic activities.

I specifically seek to (1) identify specific locations (control points) most critical to C flux into urban coastal zones; (2) determine the impact of anthropogenic activities on microbial organic matter (OM) decomposition under ambient conditions and extreme precipitation; and (3) uncover generalizable processes across urban centers. To do so, I am teaming with 16 collaborators that routinely collect hydrologic and biogeochemical measurements in three coastal urban centers with different population densities, land uses, and climates. This team includes a mixture of federally funded, university, and nonprofit groups to create a one-of-a-kind network while also supporting place-based learning and inclusivity of underrepresented groups in science. We will use field surveys and a model-experiment workflow to discover hydrologic and biogeochemical processes that regulate C cycling from source to sink across urban ecosystems.

Collectively, this research will generate a mechanistic framework of coastal urban C cycles that incorporates molecular-scale responses to precipitation. It provides a basis for alleviating key uncertainties in the Office of Science, Biological and Environmental Research's existing multiscale models that will enable enhanced predictions of the global climate system.

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

Multidimensional Parameter-Space Feature Tracking, Analysis, and Visualization

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Computational science, machine learning, and data analysis constantly advance and accelerate scientific discovery. Scientific simulations, models, and analyses for such advances usually depend on parameters whose exact values require tuning. A key challenge in such tuning is understanding how the outcome of a model changes with varying parameters and the sensitivity of each parameter. This research aims to establish a novel paradigm to help visualize and understand the outcomes of parameter changes by multidimensional parameter-space feature tracking. A generalization of traditional spacetime feature tracking, parameter-space feature tracking associates essential features such as extrema, vortex core lines, and boundary surfaces across multiple data instances induced by different input parameters.

Specifically, we will research the tracking, analysis, and visualization of features across multidimensional parameter spaces. First, we will research mesh- and density-based methods for feature tracking in continuous and discrete parameter spaces. Second, we will research analysis algorithms to derive insights directly from multidimensional features. Third, we will investigate visualization methods to help enable parameter space exploration and understand multidimensional features. The proposed methodology will be applied to help understand ensemble simulations and machine learning models in Earth systems, fusion energy, and X-ray tomography applications.

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

Connecting Molecular Electronic Structure and Electron Spin Decoherence Mechanisms for Quantum Information Science

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The next generation of information processing devices will rely upon detailed understanding of quantum phenomena at the single atom and molecule level. While the electron spin relaxation processes inherently important for applications in quantum information science have been rationalized on the basis of the Debye model, the assumptions behind this model are incompatible with the structure of molecular materials and, thus, this approach does not yield meaningful insights or predictions for slowly relaxing, highly coherent molecules. A new approach rooted in molecular structure is therefore required to fully understand high temperature decoherence mechanisms. Our lack of current understanding further stems from a dearth of experimental studies and approaches aimed at probing the key spin-phonon coupling and chemical bonding contributions to decoherence mechanisms. To address these issues, this research employs and develops new lines of spectroscopic inquiry to quantitatively evaluate the critical spin-phonon coupling processes that control high temperature quantum coherence/decoherence in molecular systems, thus integrating advances in spectroscopy with an impactful scientific research directive. The research aims to provide firm experimental grounding for theoretical models of spin relaxation, enabling a rational path to high temperature, highly coherent molecular quantum technologies. More generally, this research ties together new experimental and theoretical approaches to study the structural and dynamic electronic properties of molecular systems, as the models developed here can be translated directly to other critical molecular processes such as intersystem crossing and single-ion magnetism. As in high temperature decoherence mechanisms, these dynamical processes are governed by the coupling between electronic spin states and ultrafast atomic motions.

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

Density Profile Control for Improved Performance in Wendelstein 7-X

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This project seeks to improve the attainable performance parameters of plasmas in the Wendelstein 7-X (W7-X) stellarator and sustain these improved parameters for extended periods of time (up to 30 minutes). One of the main factors limiting plasma performance is thought to be turbulent transport, which can prevent the plasma from retaining enough input energy to attain the conditions for fusion burn. Since the density profile can heavily influence turbulent transport, the project will develop the capability to control the density profile in real time to minimize turbulence. This will be accomplished through three main project objectives. First, a system will be deployed for real-time evaluation of electron temperature and density profiles from Thomson scattering signals, which will serve as key inputs to profile control algorithms. Second, feedback algorithms will be developed for controlling the density profile that employ the W7-X Continuous Pellet Fueling System (CFPS), foreseen to be installed later this year, as an actuator. Third, these profile control schemes will be used to design experiments that improve plasma performance through turbulence reduction and discharge length extension. The choice of target profile parameters will be informed by gyrokinetic simulations to determine stability to turbulent fluctuations. If successful, the methods developed in this project to establish profile control and sustained turbulence reduction could serve as a model for attaining similar outcomes on next-step stellarator devices and stellarator-based fusion reactors.

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

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Main Ion Transport and Fueling in the DIII-D Pedestal: From Formation to Sustainment

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Plasmas on ITER and in future fusion power plants (FPPs) are expected to rely on an edge transport barrier, known as the H-mode pedestal, to reach the core parameters required to achieve significant fusion gain. Improved understanding of the mechanisms behind the formation and sustainment of the H-mode pedestal is a critical gap for developing accurate predictive models required to optimize future magnetic fusion devices. The structure of the H-mode pedestal is determined by the complex interplay of several processes including atomic physics interactions that couple the confined plasma to the edge neutral population. These effects are poorly characterized with existing measurements and the understanding of their impact on plasma fueling and pedestal structure remain inadequate for robust predictive capabilities. The objectives of this research are to address key outstanding physics issues related to plasma fueling and how the density and temperature profiles can affect plasma turbulence and achievable pedestal parameters. The research will be carried out at the DIII-D National Fusion Facility and will be enabled through major upgrades to the main-ion CER (MICER) diagnostic system to provide measurements of the density and energy of the neutrals from inside the pedestal top to the scrape off layer of fusion grade tokamak plasmas. These new measurements will be used to uncover the extent that higher energy 'thermal' neutrals, which are born through charge exchange with confined ions, may be capable of fueling the plasma in the conditions expected at reactor scale. The combination of these new measurements and the extensive capabilities of the DIII-D tokamak will allow this research to test state of the art theoretical models of pedestal transport and provide insight into the complex interplay of physical processes that govern the pedestal structure in current and future fusion devices.

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

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Reusable Molecular Platforms for On-Demand Photochemical Dihydrogen Production

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Hydrogen has the potential to revolutionize the world's energy production, storage, and distribution infrastructures. But while hydrogen stores more energy by mass than any other chemical fuel, it stores very little energy by volume, even as a cryogenic liquid. Thus, reusable solid or liquid materials that store hydrogen indefinitely at ambient temperature and pressure and release it on demand are critical to facilitate the expansion of the renewable hydrogen economy. The overall aims of this research are 1) to investigate the mechanisms of a newly discovered photochemical reaction in which hydroxymethyl groups appended to dye molecules undergo photooxidative dihydrogen elimination to give their corresponding aldehydes and 2) to develop molecular materials that take advantage of this reaction to store and release hydrogen on demand using visible light as a trigger. Hydroxymethyl derivatives of three common organic dyes – anthracene, acridine, and proflavine – have been found to undergo this transformation following illumination with light-emitting diodes and even sunlight, and regeneration of the hydrogen-storing materials may then be accomplished through catalytic hydrogenation. The trajectory of the hydrogen elimination reaction will be investigated at the atomic level using a combination of isotope labeling experiments, ultrafast transient absorption spectroscopy, and quantum chemistry calculations. Insights from these studies will then be used to design new molecular species with increased hydrogen storage capacity, higher quantum yields, and stronger absorption of the terrestrial solar spectrum. In addition to application in hydrogen storage, this work will provide fundamental insights into the excited state dynamics in a new class of photochemical reactions with important implications for molecular solar energy conversion processes.

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

AI-ACCELERATED DISCOVERY OF DARK ENERGY PHYSICS WITH LSST, DESI, AND CMB-S4 CROSS-CORRELATIONS

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The expansion of the universe is accelerating. This phenomenon defies expectations based on ordinary gravitating matter and indicates that contemporary theories of cosmology are either incomplete or fundamentally incorrect. Many of the premier DOE cosmology experiments of the 2020s have been specially designed to measure the cosmic acceleration with unprecedented precision, such as the Rubin Observatory Legacy Survey of Space and Time (LSST), the Dark Energy Spectroscopic Instrument (DESI), and Cosmic Microwave Background Stage 4 (CMB-S4). This proposal provides a critical tool in the quest to understand the physics of the "dark energy" driving the cosmic acceleration. Historically, studies of dark energy are carried out using a single galaxy sample observed by an individual survey, but the character of our data is changing: multi-survey information from thousands of square degrees of overlapping sky will soon become available for the first time, which opens up the exciting prospect of a new era of multi-wavelength cosmological analyses that use multiple datasets simultaneously. This proposal focuses on developing a new generation of models that have the capability to make multi-wavelength predictions with an accuracy that matches the quality of cosmological survey data in the 2020s. The linchpin of this program is a ground-up reformulation of present-day techniques that leverages the computational gains of Artificial Intelligence (AI) algorithms. Our program will lay the foundation for a novel approach to cosmological inference that unlocks the predictive power of the world's largest simulations through targeted application of AI and will help propel the field of cosmology into the era of exascale computing.

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

Biogeochemical Controls on Phosphorus in Urban-influenced Coastal Ecosystems

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Coastal river deltas are home to hundreds of millions of people worldwide and provide trillions of dollars of economic and ecosystem services each year. However, deltas are being degraded by human activities that cutoff their supply of sediments and remove protective ecosystems. As a consequence, low-lying coastal areas are vulnerable to flooding and landward migration of ocean water. Coastal degradation driven in part by urban flood control measures has resulted in substantial land loss along the Louisiana Gulf Coast. A 50-year effort is underway to preserve existing land through projects that include water and sediment diversions and marsh creation. Efforts to maintain or even rebuild the coast are expected to preserve habitats, support coastal industries, and buffer urban areas against hurricane damage and flooding; however, ecosystems that receive diverted river water may be impaired by excess nutrients from urban and agricultural runoff. To predict the future evolution of the Gulf Coast and its resilience to disturbance, it is critical to evaluate how nutrients are stored and processed across flooding and salinity gradients that represent current and future coastal ecosystems.

Phosphorus is a critical nutrient that influences plant growth and decomposition of organic matter by microorganisms; however, phosphorus binds strongly to soil minerals and can become limiting to ecosystem growth and function. Phosphorus binding to soil minerals and its release into solution are regulated by oxygen levels and salinity within soils, which are particularly dynamic in coastal ecosystems subject to tides and flooding. This project will evaluate phosphorus storage and mobilization in contrasting deltas on the Louisiana Gulf Coast where water management strategies have resulted in either growing or shrinking deltas. This work will explore the conceptual framework that urban flood control measures influence oxygen and salinity levels in coastal wetlands by altering sediment and freshwater inputs. These shifting regimes, which vary seasonally and are sensitive to sea level rise and storm surges, in turn regulate phosphorus binding to soil minerals. Findings from this research will inform Earth system models being developed to simulate coastal systems and will be particularly beneficial to efforts to improve model representation of phosphorus cycling.

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

Expanding Sensitivity to New Physics at the Large Hadron Collider Through Unconventional Track Signatures

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The Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) was built with two primary goals. The first was to complete the exploration of all known particles of the Standard Model (SM) of particle physics, which was accomplished in 2012 with the discovery of the Higgs Boson. The second was to break it: to find direct evidence that the SM disagreed with experimental observations; to find signs of something new. The measurement of a low-mass Higgs boson provided a theoretical indication that additional new particles should exist at the energy scales accessed at the LHC, but so far, nothing definitive has been observed. The overarching goal of this research program is to identify well-motivated new phenomena that could have been produced at the LHC but were missed due to their unconventional particle decay signatures. Thus far, the effort has been fundamentally limited by the trigger filtering systems developed for the LHC experimental detectors, which are responsible for discarding more than 99.99% of collision data before they can be recorded while capturing only those processes that match a pre-defined set of selection criteria. Unconventional signatures, such as diffuse decays and long-lived particles, rarely pass current filtering requirements. Using the large datasets collected by the CMS (Compact Muon Solenoid) experiment at the LHC, this project will leverage expertise in Field Programmable Gate Array (FPGA)-based fast tracking technologies and long-lived particle searches to expand the trigger menu, with a particular focus on recording the extremely challenging but well-motivated signature of a displaced tau lepton in the CMS detector. With the new data acquired during LHC's next running period, the research group will design and execute new search strategies that rely on advanced machine learning techniques to disentangle signs of new physics from the significant background processes expected from LHC collisions. Complementing these searches, a real-time FPGA-based tracker will be developed to advance CMS's High-Luminosity LHC detector upgrade and thereby further expand the sensitivity to unconventional signatures during the initial stages of the real-time trigger process. Ultimately, the research will allow for the exploration of new territory at the LHC thereby creating new opportunities for scientific discoveries.

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

INTELYTICS: An Efficient Data-Driven Decision-Making Engine for Performance in the Era of Heterogeneity

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Simulations leverage High Performance Computing (HPC) systems to evaluate numerous what-if scenarios of otherwise experimentally intractable phenomena quickly. However, HPC ecosystems consist of diverse components, e.g., architectures, programming models, and system software. Failure to consider how parameters at the user-, software-, and facility-level interact when running these simulations can delay the scientific return or leave these billion-dollar systems underutilized. Worse yet, the best parameter combination changes as resource availability evolves in these heterogeneous environments, making it difficult for users to respond to the dynamism in real-time. Machine-learning-based (ML) performance modeling and tuning can automate this decision-making process. However, off-the-shelf ML techniques assume that parameters are independent, thus failing to exploit their correlations during performance prediction. Consequently, the current approaches need to retrain models as the environment changes, requiring substantial training data and a long time to adjust their predictions.

This project will overcome the gaps mentioned above by transforming performance data into a graph structure to capture the parameter relationships and leverage the recent advancements in graph-based learning methods to accelerate real-time decision-making in HPC. Specifically, this project will build generalizable and interpretable ML techniques for recommending parameter settings to users, software, and facilities so that simulations can finish faster by efficiently utilizing the computing resources. The resulting engine, INTELYTICS, will fill gaps identified by ASCR experts toward an automated workflow management system in heterogeneous computing environments.

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

Understanding the Spatiotemporal Spectra of Transport-Inducing Instabilities in Low Temperature Plasmas

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The goal of this research effort is to develop a new experimental method to investigate instabilities that induce particle and energy transport in low temperature plasma (LTP) ion sources. LTP ion sources are among the most widely used types of man-made plasmas. Notable applications include water treatment, plasma medicine, materials processing, and in-space propulsion. In all these sources, understanding instability-driven particle and energy flux, known as anomalous transport, is important because these processes often dominate the fundamental plasma state, leading to undesirable effects such as poor confinement, efficiency loss, and reduced ion beam quality. However, there is currently a capability gap in experimental techniques to measure the key length scale and growth processes that govern transport-inducing instabilities in LTPs. This is the result of several factors including limited probe accessibility, limited spectral bandwidth, and the influence of random noise. The objective of this research is to address this capability gap by developing a novel probing technique based on bispectral analysis combined with Bayesian inference. This experimental method will be applied to assess instabilities in a range of LTP ion sources including a crossed-field discharge, an arc discharge, and a radiofrequency ion source. The project will address several key questions: what length scale do instabilities extract energy from the plasma and at what rate? how is the energy re-distributed across the instability spectra and can it lead to self-organization? what are the mechanisms that lead to the shape and saturation of the instability spectra? and how much ultimately do the instabilities contribute to anomalous transport?

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

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Understanding Enhanced Isotope Sieving Through Defects in 2D Membranes

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Atomically thin two-dimensional (2D) materials present new opportunities for advancing separation of isotopes and light elements with minor atomic number (Z) differences. The pristine lattice of graphene and h-BN is impermeable to Helium atoms but allows for permeation of sub-atomic species *i.e.* electrons, protons and its isotopes. The introduction of precise sub-nanometer defects/pores into the 2D lattice can significantly enhance transport of sub-atomic species and enable practical separations of interest to national security, energy generation and conversion, as well as environmental remediation/de-contamination efforts. A detailed fundamental understanding of the transport characteristics of isotopes and light elements with minor Z differences through sub-nanometer defects/pores in 2D materials is hence imperative but remains elusive. The proposed research aims to develop new experimental approaches to study and elucidate transport characteristics of isotopes and light elements with minor Z differences through sub-nanometer pores in the 2D lattice. Outcomes of the proposed research are anticipated to include ***i)*** fundamental insights into transport characteristics of isotopes and light elements with minor Z differences, ***ii)*** novel approaches to increase isotope selectivity of 2D membranes, and ***iii)*** new knowledge on the development of atomically thin membranes for isotope separations, furthering the Department of Energy Isotope Program mission to "*conduct R&D on new and improved isotope production and processing technologies that can make available isotopes for essential research and applications."*

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

Designing Chemical Disorder in Solid-State Superionic Conductors

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Phenomenological coupling between physical properties arises in crystalline solids, as dictated by symmetry and the chemistry of materials. This coupling however often hinders materials innovation by limiting materials design degree, for example, the well-known tradeoff between lithium (Li) conductivity and voltage stability in crystalline Li superionic conductors. Chemical disorder present in non-crystalline solids can offer new functionalities to materials properties that are restricted in crystalline solids. Non-crystalline solids, through flexibility in composition, have the potential to shift the paradigm of functional materials design. However, how non-crystalline solids form, transform, and function remains unclarified due to the lack of long-range structural descriptors, making it extremely challenging to rationalize materials development. In light of this clear motivation, the goal of this project is to establish unified materials design principles and synthesis guidelines for non-crystalline solids. Specifically, we will investigate non-crystalline Li superionic conductors for electrochemical solid-state energy storage by 1) elucidating how short-range structures and chemistry govern macroscopic Li transport and electrochemical stability and 2) monitoring how chemical disorder evolves under mechano-chemical activation. To achieve this goal, we will combine solid-state chemistry, synchrotron experiments, and electrochemistry to synthesize, characterize, and assess non-crystalline Li superionic conductors. Successful outcomes of this project will allow a transformational step forward in designing complex non-crystalline materials, providing pivotal solutions to discover non-crystalline Li superionic conductors and expand the frontiers of materials chemistry.

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

Heavy Flavor at RHIC

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In the first few microseconds after the Big Bang, the universe consisted of a hot and dense state of matter called the quark-gluon plasma (QGP). This state of matter is essentially a "soup" of quarks and gluons, the subatomic particles which make up protons and neutrons, which in turn are the building blocks of atomic nuclei. Scientists at modern collider facilities accelerate nuclei to very high energies and smash them into each other, which “melts” them into their constituent quarks and gluons and recreates the QGP. The plasma expands and cools during its short lifetime (~10-23 seconds) before making the transition back to regular matter. Physicists use a wide variety of probes to characterize the properties of the QGP in detail. This work will use heavy quarkonia, which are bound charm-anticharm or bottom-antibottom mesons, as probes of the quark-gluon plasma. The presence of a QGP will inhibit the formation of heavy quarkonia in a way that depends on both the temperature of the plasma and how tightly bound the quarkonium state is. Measurements of the abundances of different types of quarkonia in heavy-ion collisions, compared to a proton-proton collision baseline, will allow us to probe the properties of the QGP, including its temperature evolution. In this work, we will measure the yields of charm-anticharm and bottom-antibottom quarkonia in small (proton-proton) and large (heavy-ion) collision systems to shed light on how the suppression of these bound states evolves with system size. Furthermore, the quark-gluon plasma has been observed to behave as a liquid with a very low viscosity. We will conduct measurements of the flow parameters of bottom-antibottom quarkonia to characterize the extent to which bottom quarks participate in the collective motion of the system. This work will make use of the excellent particle identification and tracking capabilities of the STAR detector and the newly upgraded sPHENIX detector, both at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory. Our use of heavy, rare particles to probe the quark-gluon plasma will shed light on the behavior of this unique state of matter and help us better understand the strong nuclear force, one of the fundamental forces of nature.

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

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Fundamental Mechanisms of Newtonian Diffusional Creep in Structural Alloys

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Heat engines generate more than 70% of the world's electricity. To meet growing energy demands, advanced generation concepts will require significantly higher operating temperatures while addressing the need to limit CO_2 emissions and enable energy-intensive processes like hydrogen production. In these extreme environments, creep deformation (a type of deformation seen at high temperatures and relatively low stress) becomes a critical performance degradation process in structural alloys. Knowledge of fundamental mechanisms governing the creep deformation rate in materials under a broad spectrum of stresses and temperatures is crucial for creep-resistant materials design and service life prediction. There are several theories of the creep deformation mechanisms. In the Newtonian diffusional creep process, it is premised that vacancies flow between grain boundaries subjected to different stress conditions, giving rise to plastic deformation. Theories of diffusional creep provide a compelling picture for materials scientists to design microstructures that improve creep resistance. However, these theories remain vigorously debated due to a lack of experimental evidence and poor prediction of creep rates.

To isolate the fundamental mechanisms controlling Newtonian diffusional creep, it is hypothesized that stress-assisted flow of vacancies to specific interfaces in multicomponent materials will cause elemental segregation. This hypothesis will be investigated by studying the influence of composition and soluble hydrogen on diffusional creep mechanisms in structural alloys. Advanced research tools available at Idaho National Laboratory and U.S. Department of Energy user facilities, including advanced testing and multiscale characterization techniques (i.e., in situ /ex-situ - secondary ion mass spectrometry, transmission electron microscopy, and atom probe tomography) and mesoscale phase-field modeling tools will be brought to bear to test this hypothesis. The mechanistic understanding of the diffusional creep mechanisms will enable new pathways for designing advanced creep-resistant materials for extreme temperature, stress, and corrosion environments.

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

Superconducting Qubit-Based Sensors for meV-Scale Particle Detection

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Many of the most pressing topics facing particle physics over the next decade will require detectors sensitive to much smaller energies than we have been able to probe in the past. Searches for dark matter below the electron mass, new physics with neutrinos, and deeper cosmological probes, all require innovations in sensor technology to see energy deposits one thousand times smaller than the current state of the art in detector technology. Quantum bits, or qubits, developed for quantum computers, are macroscopic devices which behave as quantum objects, and have already demonstrated sensitivity to events on these energy scales – to the point that interactions with radiation is the limiting factor for one class of qubits comprised of superconducting thin films. For these qubits, the amount of time they can remain in their quantum state, also called coherence time, is severely limited by the interaction of the superconducting qubits with their environment. Recent work has shown that qubits are sensitive to many of the same types of signatures we typically search for using scientific cameras and dark matter detectors. This project will work to broaden our understanding of how different types of radiation affect the qubit state, and work to improve coherence times to enable more complex quantum computations, a major priority of DOE science and industry partners. It will simultaneously design novel devices, based on the opposite optimization, to enable light-, heat-, and charge-sensitive detectors needed to address a wide range of scientific priorities in high energy physics. This research will thus help bring together the quantum information science and high energy physics communities in a highly synergistic area and improve our understanding of superconducting devices and their interaction with their environment, enabling major advances in both fields.

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

The Role of Strain Localization at Interfaces on Fatigue Crack Initiation in Highly Textured Magnesium Alloys

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New and novel materials with extraordinary properties, from superior fatigue resistance to excellent high temperature performance, enable a shift from energy-expensive materials to sustainable materials with a positive impact on communities and the environment. Though these material systems provide many advantages, the underlying meso- and micro-scale structures are complex and as a result, the mechanical behavior is very different than that of traditional metallic alloys. Of the properties, fatigue – the repeated cycling of stress on a material – is the most critical form of damage in load bearing structures. In fact, fatigue accounts for 80 to 90% of failures in structural components and is still a major problem in many industries. Though fatigue has been studied for over 180 years there are still gaps in our understanding of the processes controlling fatigue crack initiation and growth. This project will directly address these challenges using a specifically designed and multimodal systematic study that combines electron microscopy, digital image correlation, and high energy X-ray based techniques to understand the mechanisms of damage accumulation at interfaces in complex microstructures leading to crack initiation and growth. A fundamental understanding of the complex interactions at the meso- and micro scale that influence fatigue behavior and crack initiation will provide the underpinning knowledge needed to: 1). inform physically based models that accurately predict fatigue lifetime in complex systems and 2). develop fatigue resistant, microstructurally, and compositionally complex alloy systems.

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

Revealing Sensitive Battery Liquid-Solid Interfaces via Cryogenic-Electron Microscopy

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One of the most important global challenges of our time is the development of clean energy technologies. Batteries that can store more energy without compromising stability play a critical role in this transition. Although a metallic lithium anode enables batteries with more than double the energy densities of the current state-of-the-art, large-scale deployment remains absent due to poor cycling efficiency, short lifetime, and significant safety concerns. These drawbacks are fundamentally linked to the nanoscale liquid-solid interfaces that govern electronic and ionic pathways during battery operation. This research project will develop innovative cryogenic electron microscopy (cryo-EM) techniques to reveal and understand the liquid-solid interfaces in lithium metal batteries. Specifically, the goal is to investigate how swelling, reactions, and wetting proceed at the liquid-solid interface and correlate their nanoscale features with macroscale battery performance. New insights from this research will fill an important unmet need for identifying guiding principles to engineer longer lasting and safer batteries. More broadly, the technical innovations in cryo-EM developed in this project have broad implications for diverse research fields beyond energy storage, where liquid-solid interfaces play a critical role in governing the nanoscale processes in systems spanning biology and chemistry.

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

Probing the Coordination in Confinement for Electrochemical Separation among Rare Earth Elements

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Rare earth elements are a group of seventeen elements of enormous importance to clean energy production and storage. Their separation relies on the construction of optimal coordination environments to differentiate the slight differences in their ionic radii and Lewis acidity. This research aims to understand and control rare earth separations by modulating their coordination in confinement using electrochemistry. Electrochemical separation has the potential to reduce environmental pollution, promote electrification of chemical production, and reduce the carbon footprint. The electrode crystal structure determines the termination atom position, atom-atom distance, lattice spacing, and crystal water amount. These parameters determine each rare earth ion's equilibrium coordination configuration and strength. In competition, the rigid framework induces a significant energy penalty to unfavorable coordination configurations and kinetic pathways to promote the separation among rare earth elements. Coordination in confinement represents a similar strategy to the use of size and binding but in an inorganic framework for selective separation. Additional physical and chemical processes (such as solid transport and material morphology) are explored to enhance selectivity. Synthetic methods are developed to modulate the compositional and structural factors of the host materials and correlative characterization tools are used to resolve their effects on rare earth coordination and separation, thus probing the fundamental limit in separating individual rare earth elements.

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

Physics-informed neural operators for fast prediction of multiscale systems

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High-fidelity simulations like direct numerical simulation (DNS) of turbulence and molecular dynamics (MD) of atomistic systems are computationally very expensive and data-intensive, and most of the outputs produced are permanently lost. Furthermore, for multiscale problems, the microscale component is so expensive that it has stalled progress in simulating time-dependent atomistic-continuum systems. These open issues, in turn, have delayed progress in the forecasting of real-time dynamics in critical applications such as astronomy, extreme weather patterns, and designing efficiently new functional materials. Scientific machine learning (SciML) has the potential to totally reverse this rather inefficient paradigm and significantly accelerate scientific discovery with direct impact on technology in the next few decades, if it can be used creatively.

We propose to develop a new generation of neural operators, universal approximators for operators, by extending the deep operator network (DeepONet) and Fourier neural operator (FNO) that can learn explicit and implicit operators from data only. While preliminary results are promising in diverse settings, we need to extend the predictability of neural operators for unseen out-of-distribution inputs and to speed-up the training process via high performance and multi-GPU computing. To this end, we will endow neural operators with physics, multifidelity data, and equivariant principles (e.g., geometric equivariance and conservation laws) for continuum systems and with seamless coupling for hybrid continuum-molecular systems, where neural operators will replace the expensive molecular component. We have formulated a research program in three research areas, and we have designed a set of large-scale simulations (active control of turbulence, learning constitutive laws, and crack propagation) in order to demonstrate the effectiveness of the proposed developments.

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

Searching for New Physics with
Advanced Liquid Argon Detector Capabilities at Neutrino Experiments

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The Liquid Argon Time Projection Chamber (LArTPC) has been chosen as the main detector technology for both short and long baseline neutrino oscillation projects in the US. In addition to delivering the precision measurements of neutrino oscillation parameters, the large-scale detectors combined with intense neutrino beams from the Fermilab accelerator complex also provide a unique platform to search for physics Beyond the Standard Model (BSM). These neutrino experiments are particularly advantageous in searching for new long-lived particles with MeV - GeV masses, covering a parameter space complementary to collider or low energy experiments. Significant advancement in detection technology is however needed to transform these LArTPCs from measuring neutrino interactions to catching sub-GeV new particles. Specifically, neutrino background suppression is the primary challenge for any rare new physics search. Leveraging the fine time structure of the pulsed neutrino beam, this research program addresses background rejection first through nanosecond timing measurement of a particle's time of flight. One nanosecond resolution can effectively separate the early arrival neutrinos from heavier BSM particles, presenting a new method to dramatically boost sensitivity to new physics. Another focus of this program is the development of a low threshold, low background, scintillation-light based trigger system dedicated for new physics searches. This work is centered around photon detector R&D to increase signal light yield and the investigation of puzzling high rates of single photoelectron backgrounds. The software component of this research lies in the development of novel reconstruction and analysis techniques targeting electron-positron pairs -- a common final state signature predicted by numerous BSM models. Machine-learning based techniques will be developed to suppress photon background induced from standard neutrino interactions without compromising the signal efficiency. Although aimed for new physics searches, the advances in liquid argon technology that this research program envisions will also enhance the precision of neutrino oscillation measurements, strengthening these experiments' designed goals.

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

Practical Tensor Hypercontraction Coupled Cluster Methods for Excited State Dynamics

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The interaction of light with matter is a critical process which must be understood in order to explain and control microscopic phenomena encountered in many different DOE BES program areas. For example, a detailed microscopic understanding of energy and charge transport between molecules is important for designing inorganic and organic semiconductor materials, coherent control of photocatalytic reactions, and obtaining a detailed understanding of photosynthetic energy transfer mechanisms. The combination of experimental measurements and computational modeling is necessary to fully elucidate these complex problems, but one major obstacle is the rapid increase of computational cost (computer time) with the size of the molecule or system studied. The goal of this research is to break this barrier by developing the tensor hypercontraction coupled cluster (THC-CC) approximation into an accurate, efficient, and practical tool for simulating the structure and dynamics of molecular excited states. As a reduced-scaling method, the decrease in computer time for THC-CC compared to traditional approaches improves rapidly with molecular size and will enable entirely new application areas. This research will combine a number of approaches and techniques including orbital localization, reduced-scaling tensor factorization, data compression via H-matrices, and analytic gradient theory to produce a practical THC-CC implementation which can calculate energetic, geometric, and electrical properties of both ultra-violet/visible and x-ray excited states. In particular, the dynamics of excited states will be addressed by developing exact analytic gradients for both ground and excited states. Additionally, this research will include pilot applications to the photostability properties of both natural and artificial/modified nucleobases and environmental effects thereon, and to the study of singlet and triplet dynamics in organic photovoltaic materials, including microscopic singlet fission/triplet fusion dynamics.

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

Ultrafast Control of Spin Fluctuations in Light-Driven Quantum Materials

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Quantum materials feature subtly interacting lattice, orbital, charge, and spin degrees of freedom. The delicate balance among these interactions makes quantum solids extremely susceptible to external stimuli and is key to the appearance of emergent collective phases such as superconductivity, magnetism, and charge order. Manipulating spins via ultrafast light-matter interaction is a promising route to dynamically control quantum materials' properties and induce novel light-matter hybrid states. However, understanding how lasers modify the microscopic spin dynamics in quantum materials is still a challenge, mainly due to the lack of momentum sensitivity of ultrafast optical probes. This project will address this fundamental problem by tightly integrating advanced ultrafast optical spectroscopy and time-resolved Resonant Inelastic X-ray Scattering methods. The main goal is to provide a comprehensive understanding of the microscopic physics of light-driven spin fluctuations in quantum materials. We will map these phenomena in paradigmatic examples of quasi-one-dimensional, quasi-two-dimensional, and frustrated interacting spin systems. This research will make use of transformative new spectroscopic capabilities at x-ray free electron laser facilities and is poised to advance our understanding of light-matter interaction processes in interacting electron systems. The results of these studies will define a strategy to synthesize light-driven states of matter without equilibrium analogues and to establish protocols for the realization of next-generation quantum technologies based on ultrafast light-matter interactions.

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

The three-dimensional structure of the proton

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Protons and neutrons are the basic building blocks of almost all visible matter, and account for 95% of the mass of the visible universe. Protons and neutrons are composed of smaller particles, quarks, bound together by the strong nuclear force, which is carried by gluons and is responsible for all nuclear matter, from hydrogen ions to neutron stars. The exact arrangement of quarks and gluons inside protons and neutrons is not well known. This project helps understand the three-dimensional arrangement of quarks and gluons within protons and neutrons, using large-scale supercomputing facilities to calculate the properties of protons and neutrons directly from the strong nuclear force. These calculations complement data on proton and neutron structure obtained from experiments performed at Thomas Jefferson National Accelerator Facility and the planned electron-ion collider at Brookhaven National Laboratory and provide a basis for combining experimental and theoretical data in a consistent framework.

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

Isotropic Microstructure and Defect Tolerance in Additive Manufacturing by Leveraging Metastability in Alloy Design

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Anisotropic properties and scatter in mechanical performance of printed parts are major challenges impeding greater adoption of additive manufacturing (AM) technology. The former is due to formation of columnar grains along build direction and the latter is due to the stochastic nature of process-induced defects. It is hypothesized that a single alloy design criterion - metastability alloy design - could address the above-mentioned challenges concurrently. In particular, metastable alloys could undergo multiple phase transformations during layer-wise AM process and develop fine-grained microstructures with reduced anisotropy. Such metastable alloys could also be defect-tolerant as they can trigger phase transformations or other deformation mechanisms in the vicinity of defects upon loading and retard their growth. While metastable alloys have been successfully processed using AM, there is currently no fundamental knowledge about the effect of various degrees of metastability on 1) solidification pathways, 2) grain morphology and 3) defect tolerance in AM parts. This gap will be addressed by systematic studies of metastable alloys under AM processing conditions and their microstructure and deformation mechanisms. To conduct these studies, advanced characterization techniques including operando synchrotron X-ray diffraction and in-situ mechanical testing will be adopted. This research is in line with the Priority Research Direction 5: Co-Design Materials, Processes, and Products to Revolutionize Manufacturing highlighted in the “Basic Research Needs for Transformative Manufacturing” report. While the initial focus will be on a FeMnCoCr complex concentrated alloy system, the findings will be extended to other phase-changing materials like titanium and ferrous alloys, broadening the use of this alloy design concept to a wider range of applications.

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

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Topological Phases Unraveled by Spin Noise Magnetometry with a Single Spin Qubit

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Insulating magnetic van der Waals materials (MvdW) are an emergent class of low-dimensional materials that can be mechanically exfoliated down to the monolayer limit, providing a unique opportunity to access magnetic topological phases. These topological phases are insensitive to disorder and are therefore promising candidates for next-generation energy relevant applications such as spintronic microelectronic devices and fault tolerant quantum computation. Topological phases are challenging to probe because they do not spontaneously break lattice symmetries and, since there is no static order, the spectrum of magnetic fluctuations (i.e., the spin noise) is often detected to characterize topological phases. However, traditional, bulk probes of spin noise are insufficiently sensitive to characterize emergent topological phases in few- to single-layer MvdW and new approaches for detecting topological phases in low-dimensional materials are required. Nitrogen-vacancies (NV) in diamond are an emergent single spin qubit probe with the sufficient sensitivity to detect magnetism in these nano-scale quantum materials. This project will utilize NVs to unravel the magnetic properties of topological phases in MvdW down to the monolayer limit using NV spin noise magnetometry. This investigation will, for the first time, characterize archetypes of the dynamic characteristics of topological phases in 2D magnetic materials. In addition to discovering new insights into topological phases, this project will also advance the NV quantum sensing user program at the Center for Integrated Nanotechnologies by developing new capabilities to further access topological phases in quantum materials.

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

Allowing Collider Data to Tell Their Own Story with Deep Learning

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High Energy Physics at the energy frontier has transitioned back from a theory-driven to a data-driven era. For decades, there has been clear theoretical guidance driving the field, culminating about ten years ago with the discovery of the Higgs boson at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN). While all particles of the Standard Model of particle physics have now been detected, there are key experimental observations such as the astrophysical evidence for dark matter that compel the field to expand search efforts for new particles. Theory has traditionally played a central role in these searches at the LHC, but it is essential that a new data-driven paradigm complement the existing one given that present models cannot explain dark matter and other phenomena. To truly explore the unknown, we must allow the data to speak for themselves through model-agnostic methods using features that are as close to individual particle properties as possible. Due to the data complexity, artificial intelligence (AI) and machine learning (ML) are the most promising media for the data to tell their story. The research will extend the physics program of the LHC into uncharted regions of new particle parameter space by designing and deploying novel AI and ML methods that automatically identify anomalies in collider data. In order to be reproducible and reusable, the anomaly detection must be automated, accessible, and deployable at scale. This in turn will rely critically on studies at Berkeley Lab's Perlmutter supercomputer facility and use the large datasets from the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC, which is designed to capture nearly every particle produced from LHC collisions. AI and ML techniques will be applied to address deficits in the reconstruction of high energy particles so that the anomaly detection can be as effective as possible. In particular, deep learning methods will be used to combine inputs from multiple detector components to disentangle regions with high particle densities. Computing challenges have become as critical as detector challenges and thus motivate enhancing the existing computational infrastructure to ensure such computing-heavy approaches are ready in time for the future high-luminosity running era of the LHC. Therefore, advances in AI/ML under this project will not only have broader implications for employing data-driven techniques for the longer-term LHC program but will also enable scientific discoveries across all areas of fundamental physics and beyond.

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

Network-based simulations of coupled multi-physics systems

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Numerical simulations of complex real-world phenomena involve the interactions among multiple different physical systems. The knowledge of these interactions is crucial to enable accuracy, robustness, and scalability in high-performance simulation environments associated with critical DOE mission areas. This project will establish a network-based framework that models the coupling between interacting physical systems as a graph dynamical system of nodes connected to each other by weighted edges. The edge weights will inform the numerical implementation of discretization at the interfaces of the individual physics to improve the accuracy and robustness of the simulations. The network-based interactions will adaptively tune the spatial resolution of the meshes and the coupling tightness of the time integration schemes, leading to significant scalability in high-performance computing technology. Although our framework will be generally applicable to various multi-physics systems, we will focus our efforts on coupled fluid-structure-thermal interaction systems. The research insights from this project will facilitate an accurate characterization of the cross-physics sensitivities, automate the algorithmic selection process for high-performance computing, and enable energy-efficient functioning of multi-physics systems.

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

Photo-Induced Conformational Gating for Long-Lived Charge Separation

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The conversion of solar energy into chemical fuel represents a capstone goal of the 21st century and has the potential to supply terawatts of power in a globally distributed manner. However, the disparate time scales of photodriven charge separation (~fs) and steps in chemical reactions (~µs) represent an inherent bottleneck in solar-to-fuels technology. To solve this problem, copper complexes that undergo light-induced conformational changes are being employed to speed up charge separation, and slow down the reverse process, charge recombination. These dynamics create a charge separated state that lives long enough to facilitate chemical catalysis. This design approach is inspired by nature where conformational control underpins nearly all bioenergy conversion processes. Indeed, bioenergy conversion processes that rely on metalloproteins use triggered conformational changes to reversibly control the timing and direction of electron transfer reactions. The planned research mimics this mechanistic paradigm. Ultimately, this work will establish a new strategy for gating photochemical processes and providing molecular-level control over energetic excited states. These elements of molecular design are adaptable for incorporation into a wide range of assemblies for direct solar energy conversion and storage.

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

Trapped-Ion Quantum Simulation for Nuclear Physics

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Quantum Field Theories play a central role in our understanding of nature providing a framework for understanding the interactions between elementary particles and for studying the real-time dynamics of matter after the Big Bang. However, despite significant progress in classical computational techniques, there are a number of roadblocks that prevent us from simulating these theories at large scale and in their real-time dynamics using conventional approaches. A fundamental challenge is related to the

computational cost that grows exponentially with the number of particles, making large-scale simulations classically intractable. One promising approach to overcome these challenges is the use of quantum processors for directly simulating field theories. Recent advances in quantum-computing hardware have allowed access to regimes on the verge of surpassing classical computers. The overarching goal of this project is to use one of the most promising quantum platforms, trapped atomic ions, to directly map and simulate field theories and nuclear physics models. However, these theories are not readily mappable in existing quantum platforms. Therefore, the focus of this project is to study and experimentally realize new analog and hybrid analog-digital quantum simulation protocols that can directly realize quantum field theories in trapped-ion systems. The new experimental tools developed in this project will provide a foundation for the simulation of quantum matter in the Standard Model, approaching a regime that cannot be efficiently accessed with conventional computing techniques.

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

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Scalable Reconfigurable Computing Circuit Using Emerging Device Technologies

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As traditional complementary metal–oxide–semiconductor (CMOS) technology scaling is approaching its physical limit, new computing paradigm, such as reconfigurable computing circuits, has been proposed as a promising candidate to substantially improve circuit energy- and area-efficiency. Reconfigurable circuits are made of logic devices whose input-output mapping can be transformed in real-time, which means that the same circuit can be used to implement various logic functions with small device usage. It enables a higher computation density and lower cost and area, which is excellent for a wide range of applications from the high-performance data center to low-power portable devices. The rapid discovery of emerging reconfigurable device technologies also opens a new path towards an energy-efficient reconfigurable hardware paradigm to facilitate low-power logic circuits thanks to the unique device-level physics behavior. However, there is still a big question of "how to fully utilize reconfigurable devices to enable efficient reconfigurable circuits?" Limited research has been performed to take advantage of these emerging devices to realize large-scale reconfigurable circuits. A fundamental rethinking is needed to establish a comprehensive design methodology to efficiently obtain the true potential of emerging reconfigurable technologies in the early design and exploration stage.

The goal of this proposal is to use a synergistic device-circuit-synthesis co-optimization approach to (i) develop novel synthesis solutions to enable large-scale reconfigurable circuits and (ii) adapt the synthesizer to leverage emerging compact and energy-efficient reconfigurable logic devices. We will propose a novel Boolean Satisfiability (SAT)-based synthesis method and algorithm to realize large-scale area-efficient reconfigurable circuits. At the device/cell level, we will develop compact device-level models and generate cell library for several representative emerging technologies that will enable efficient reconfigurable synthesis and optimization. Furthermore, we will develop and validate a fast cross-layer co-optimization methodology to maximize the potential of proposed reconfigurable circuits with emerging technologies. Finally, we will explore several circuit applications that will fully utilize the proposed reconfigurable design method, and a comprehensive benchmarking will be carried out for a variety of promising technologies against the traditional CMOS counterparts to identify the most promising reconfigurable devices and their potential advantage and requirements.

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

Elucidating the Electrochemically Enhanced Surface Diffusion Mechanism in Materials for Clean Energy

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The goal of this Early Career Research Program is to explore, understand, and control the phenomenon of electrochemically enhanced surface diffusion in materials with potential applications in electrochemical energy conversion and storage technologies (electrolyzers, fuel cells, and batteries). Electrochemically enhanced surface diffusion is characterized by faster surface atom mobility observed on a given material when immersed in an electrochemical medium in relation to the same surface exposed to vacuum or gas phase environments. As the origins of this phenomenon are still not well understood, unraveling its mechanism will provide the means to quantitatively describe the kinetic pathways responsible for changes to surface structure and composition, and thus to the surface's functional sites. The central hypothesis of this work is that the mechanism of electrochemically enhanced surface diffusion involves nanoscale dissolution-redeposition events governed by the electrode and electrolyte properties. This work will use well-defined surfaces and electrolytes as blank canvases that will be studied by a suite of *in situ* multi-scale characterization tools that include ultra-high-sensitivity atomic mass spectrometry, scanning, electron, and X-ray microscopy tools enhanced with machine learning algorithms, and atomistic theory and simulations to uncover the relationships between electrochemically enhanced surface diffusion and dissolution-redeposition events. By elucidating the mechanism of surface mobility in the electrochemical medium, we will expand our ability to control surface dynamics on many materials used in electrochemistry, impacting how we understand materials stability and also how we can open the path towards the regeneration of materials for clean energy applications.

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

The Mathematical Foundations of Holography

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The holographic principle is a profound equivalence between two dramatically different-looking physical systems. It relates a gravitational theory in some spacetime to a non-gravitational theory in a different spacetime, with the latter spacetime possessing fewer dimensions than the former. In particular, a universe well-described by Einstein's general theory of relativity is encoded in a non-gravitational many-body quantum system that is often said to live "on the boundary" of the gravitational theory, analogous to a hologram. The so-called AdS/CFT correspondence from string theory is the most concrete instantiation of the holographic principle, and it posits that spacetime is an emergent notion, encoded nontrivially in the dynamics of the "boundary" theory. In this context, the AdS stands for anti de-Sitter, a spacetime geometry with negative curvature analogous to an M.C. Escher painting, and the CFT stands for the "boundary" conformal field theory, a special type of (typically very strongly interacting) quantum system. However, many aspects of the holographic principle remain implicit and poorly understood, which obscures fundamental questions about quantum gravity such as the nature of the black hole interior or the emergence of spacetime. Furthermore, holography has not been as well-understood in spacetimes outside of asymptotically anti de-Sitter space. This includes ordinary flat spacetime which is a good approximation, for many purposes, to the real world, and is the setting for a rapidly developing holographic dictionary called celestial holography. This research project leverages recent developments at the intersection of string theory, algebra, and geometry to develop new mathematical frameworks for both AdS/CFT and celestial holographic systems. This approach aims to help clarify and compute basic observables in the holographic dictionary from a novel perspective, and to work towards a mathematical proof of aspects of holography.

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

Spacetime from Information

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The question of how to reconcile quantum mechanics with gravity is the most important remaining mystery about the fundamental laws of nature. In recent years, we have begun to understand more and more that a crucial role in this reconciliation is played by ideas from information theory. In particular, we have seen dramatic progress on the Black Hole Information Problem -- the question of how and if information that falls into a black hole ever escapes -- that reveals how the shape of spacetime itself encodes the distribution of information. This research project uses ideas from general relativity, quantum error correction, quantum complexity theory and quantum field theory to investigate the fundamental origins of space and time. With these powerful interdisciplinary tools, we can attack some of the central mysteries in quantum gravity. How can a black hole contain more information on the inside than from the outside? How do quantum fluctuations change the classical structure of spacetime found by Einstein? What makes the universe appear “local” such that the physics here on Earth is independent of the state of a distant galaxy?

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

Mechanistic Understanding of the Criegee Intermediates Reaction Network in Atmospheric and Combustion Systems

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Criegee intermediates (CIs) are highly reactive key species with zwitterionic character that are formed in the ozonolysis of unsaturated organic compounds. Uni- and bi-molecular reactions involving CIs play an important role in atmospheric, combustion, and synthetic organic chemistry. A detailed mechanistic understanding of the CIs reaction network is currently lacking in part due to limitations in detecting intermediate species that usually occur in small concentrations. In particular, the pathways by which CIs can drive the formation of higher molecular weight, lower volatility secondary organic aerosols (SOA) precursors, via the formation of functionalized hydrocarbons are currently not understood. Identification and quantification of these reactive species within complex reactive mixtures is essential for the development of a fundamental, chemically accurate description of complex atmospheric and combustion systems.

This research aims to generate new mechanistic understanding of the CIs reaction network, and to find the pathways by which CIs can drive the formation of higher molecular weight, lower volatility precursors that can lead to SOA formation, and eventually detect and identify the size and composition of SOA. The reaction network of CIs formed in the ozone-assisted oxidation reactions of selected acyclic and endocyclic alkenes, which are analogues of important species found in atmospheric and combustion systems, will be investigated as a function of alkene structure and carbon number to understand the role of resonance stabilization induced by the competition between collisional stabilization and unimolecular reaction of the energy-rich CIs. In particular, the role of resonance-stabilized intermediates in the balance between oxidation and molecular weight growth will be investigated. The outcome of this research will represent a critical contribution to current and future atmospheric and combustion models, which currently do not include the effect of resonance stabilization. It will help connect our current understanding of the role and reactivity of CIs in the gas-phase to heterogeneous environments.

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

Quantum Capability Learning

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Quantum computers are rapidly advancing and they may soon realize scientific and economic breakthroughs. But quantum computing hardware experiences errors that cause real-world computations to fail. Those errors limit the power of a quantum computer, preventing it from executing some computations. Today, there is no way to accurately predict a quantum computer's capability or which quantum computations it will be able to run successfully. Experimentally verifying that a specific quantum computer has correctly executed a specific computation is challenging even with today's relatively small quantum processors; it will be practically impossible for quantum computers large enough to have a practical advantage over classical computers. Researchers and end users urgently need ways to (a) measure how well a quantum computer runs specific programs, and (b) predict what novel programs it will or won't be able to run. This research will address these problems, by: (1) designing methods to measure indirectly how well a quantum computer executes a computation; (2) creating techniques to learn which quantum computations a specific quantum computer can run, using machine learning and multi-scale modelling; and (3) leveraging these methods to implement quantum algorithms with the highest possible success rates. This research will make it possible to understand the capabilities of quantum computing hardware, and to make best use of each particular quantum computer's strengths. The techniques developed by this project will immediately provide a significant boost to DOE's entire quantum computing program, and will accelerate scientific discovery using quantum computers.

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

Developing TES with Sensitivity to meV Scale Excitations for Light Mass Dark Matter Searches and other Applications

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Dark matter is the one form of matter that humanity knows must exist beyond the Standard Model of particle physics because of its gravitational effects on the universe. However, essentially none of its properties (mass, spin, under what forces it interacts) have been directly measured yet. If dark matter particles have a mass between 10^{-3} and 10^{-11} that of a proton, the interactions between dark matter and detectors cannot been seen with currently available technology because they produce vibrational and photon excitations that are simply too small to be measured. This research will attempt to improve the sensitivity of the superconducting Transition Edge Sensor (TES) so that these excitations can be detected. A TES is a small volume superconducting film that has been stabilized at a temperature within its transition from a superconducting to a normal conducting state. Energy deposited in the TES will thermalize, increasing its temperature, resulting in a sharp increase in the resistance of the TES that is then measured. To increase the TES sensitivity, this project will develop new superconducting films with transition temperatures near absolute zero which will have both significantly reduced thermal fluctuation noise and heat capacity. This project will also develop improved electro-magnetic isolation techniques to isolate these extremely sensitive sensors from the environment. Using this new more sensitive sensor technology, prototype devices for dark matter searches will be developed.

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

Unraveling the Ultrafast Chemical Dynamics Governing Non-Equilibrium Molecule-Nanoparticle Interactions

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Photoinduced charge transfer is fundamental to processes such as photocatalysis, photosynthesis and photovoltaic activity, but the combination of strong electron correlation, and non-adiabatic and relativistic effects pose significant challenges to the development of a detailed description of charge transfer, particularly in systems containing transition metals. These challenges are exemplified in plasmonic photocatalysis, where electronic interactions across nano- and molecular length scales govern charge and energy transfer between photoexcited plasmonic nanoparticles and adsorbed molecules, ultimately driving chemical reactions. However, due to the complexity in theoretically treating and experimentally probing plasmonic nanoparticle-molecule interactions with sensitivity to both nanoparticle and molecular responses to photoexcitation, open questions remain regarding the principal mechanisms that underlie plasmonic photocatalysis. Deciphering which mechanisms are active requires investigations of non-equilibrium electronic interactions between plasmonic nanoparticles and molecules using advanced time-resolved and element-specific probes, which constitutes the primary objective of this research.

This project will systematically investigate non-equilibrium molecule-nanoparticle electronic interactions by studying how ultrafast electronic and vibrational dynamics vary as a function of the electronic properties of the adsorbed molecules, the mode of nanoparticle electronic excitation (i.e., intraband *vs.* interband), and the chemical composition of the nanoparticle itself. The first part of this project will investigate electronic and vibrational dynamics in gold nanoparticle-molecule systems, with the goal of unraveling the dependence of molecule-nanoparticle energy and charge transfer mechanisms on adsorbate electronic structure and the mode of nanoparticle excitation. The second part of the project will study the influence of catalytic metals on nanoparticle-molecule electronic interactions by probing ultrafast electronic dynamics in functionalized core-shell nanoparticles containing plasmonic and catalytic metals. Experiments will use ultrafast core-level spectroscopy as element-specific probes of electronic dynamics, providing sensitivity to both nanoparticle and adsorbate electronic structure evolution. Ultrafast broadband infrared spectroscopy, in turn, will monitor vibrational dynamics across all adsorbate infrared-active vibrations in the mid-infrared region following electronic excitation.

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

Structural Tuning of Photosynthetic Light Harvesting

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Biological photosynthesis – the biological conversion of solar energy into chemical fuel – has long served as an inspiration for light-harvesting technologies. Fascination with this fundamental process has driven a century-long effort to uncover its mechanistic details. Despite dramatic advances, our understanding of photosynthesis at the atomic and molecular level remains limited by uncertainty over the "structure-spectrum relationship", i.e., how protein structure tunes optical properties of the pigment protein complexes (PPCs) that capture light to drive photosynthetic chemistry. From the examples nature has provided us, it is evident that pigment-protein interactions offer a wide degree of control over the optical properties of bound pigments, enabling the same chemical pigment (e.g., chlorophyll *a*) to be used in different PPCs for many different purposes (e.g., optical antenna, electron donor, photoprotective energy sink). The specific mechanisms by which such optical tuning occurs, are poorly understood, leaving significant gaps in our ability both to understand native PPC function and, potentially, to tune PPC function for new or optimized light-harvesting applications. To overcome this challenge, this project aims to develop a transferable "toolkit" for identifying and controlling structure based optical tuning in photosynthetic PPCs. The three core components of this toolkit – robust site energy prediction methods, structure-dependent vibronic mixing models, and experimentally calibrated quantum dynamics simulations – will be parameterized directly against an experimental library of mutagenesis data on model PPCs, establishing a quantitative connection between theory and experiment. Finally, these methods will be applied to resolve the long-standing question of the structural origins and functional significance of low-energy trap states in Photosystem II of cyanobacteria through a combination of structure-based spectroscopic simulations and toolkit-guided mutagenesis. A key goal is to produce a strain of the cyanobacterium *Synechocystis* PCC6803 that lacks low-energy trap states in Photosystem II, allowing the functional role of these states to be directly assessed. The successful completion of this work will both provide definitive answers to long-standing mechanistic questions in photosystem II energy funneling and pave the way toward rational mutation-based optimization of photosynthetic light harvesting.

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

Unraveling the Physics of Earthquake Precursors
Using Ultrasonic Imaging and Physics-Informed Machine Learning

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Improving our understanding of earthquakes is critical to help assess seismic hazard and has broad implications for numerous subsurface activities related to energy extraction (oil/gas, geothermal), CO_2 sequestration and waste repositories. The heterogeneous nature of Earth's crust, which leads to non-uniform stress states and complex fault systems, is often cited as a major impediment in interpreting field results, assessing seismic risk, or even one day, predicting the occurrence of earthquakes. Despite these challenges, recent work at the laboratory scale shows that machine learning (ML) algorithms can successfully predict the timing and magnitude of laboratory quakes using radiated ultrasonic waves that emanate from the faults (equivalent to seismic waves in nature). Existing studies show that laboratory quakes are preceded by systematic changes in wave properties. Inspired by these new developments, the first objective of the proposed work is to reveal the underlying physics that allows ML-based prediction of laboratory quakes. In the long term, advanced ML models – if generalizable – could provide a pathway to improving seismic risk assessment (or even predicting earthquakes) in nature. In the short- to medium-term, the use of advanced ML models in laboratory settings – where large datasets under well-constrained conditions are readily available – represents a unique opportunity to improve our understanding of earthquake physics and in turn, better understand why/how the reported predictions work. Here, I propose to build a ML framework informed by current knowledge on constitutive laws governing frictional instability. If successful, the proposed physics-informed ML framework would require less training data for equally good predictions, and make predictions more generalizable, for instance when tested outside the bounds of the training set (e.g., for real earthquakes). The second objective of the proposed work is to illuminate the role of fault heterogeneity and off-fault rock damage. High-resolution imaging of laboratory-scale faults, through the use of dense arrays of ultrasonic sensors and in combination with the physics-informed ML framework, will allow us to visualize the mechanics of earthquake nucleation and to build process-based models that connect pre-seismic activity (or lack of) to the precursory changes in wave velocity/attenuation occurring on the fault plane and surrounding host rock, in relation with heterogeneity on the fault plane. In sum, the combination of physics-informed ML models with high resolution imaging of laboratory faults will provide a physical basis that can in turn improve our interpretation of field observations as well as inform future use of ML approaches in the field.

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

Characterizing the Limits of Nonequilibrium Control for Dissipative Self-Assembly

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Biological systems produce molecular components that assemble into complex, multiscale structures. The process by which these components spontaneously come together is known as self-assembly. Self-assembled biomolecular materials are highly dynamic and adaptive. This research focuses on two such materials 1) self-healing networks that consist of proteins that demonstrate exotic elastic properties and 2) nanoscale capsids that robustly assemble to specifically encapsulate well-defined target cargoes. While both classes of materials have important technological applications, we continue to have a limited fundamental understanding of the properties of these complex materials. Our ability to design and control these materials would be greatly enhanced by synergistic developments in computational and theoretical techniques that enable an improved understanding of how to control the assembly process of such systems. This project seeks to develop theoretical and computational methods for characterizing the self-assembly dynamics of biomolecular materials when the dynamics is modulated by external control variables. We aim to address theoretical questions of 1) how to control assembly dynamics by changing external conditions affecting growth and 2) how to characterize the limits and thermodynamic costs of controlled growth to understand which nonequilibrium structures are realizable given a fixed set of control parameters. This research aims to expand our theoretical toolkit to understand the behavior and properties of these nonequilibrium biomolecular materials. Alongside the proposed theoretical developments we aim to build computational tools using physics-informed machine learning techniques and reinforcement learning, both of which will allow us to study the properties of complex systems.

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

Polymeric chelators for rare-earth element extraction and separation

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Rare-earth elements (REEs) are crucial to many modern technologies including wind turbines (Nd, Dy), electric vehicle motors (Nd, Dy), and lighting phosphors (Eu, Tb, Y). However, in 2015 the U.S. produced only 3.3% of the REEs mined globally. This lack of domestic REE production necessitates importing REEs into the United States. As world demand for these metals outpaces supply, new and sustainable sources are needed, as well as more efficient methods of extraction and purification. Metal-chelating polymers exhibit potential in these applications due to their relatively low cost and high affinity for target elements. Developing materials capable of selectively adsorbing individual REEs would enable the efficient separation of these critical components from REE-containing waste streams. This research focuses on studying and ultimately controlling the interaction between polymers and REEs to improve extraction and purification processes. The approach includes measurements of metal-binding thermodynamics, specifically elucidating the connections among ligand structure, linear polymer parameters, and polymer topology in the context of metal chelation. Synthesis and characterization of a series of structurally-related polymers enables determination of precise structure–property relationships, thereby uncovering design principles for producing more effective metal-binding materials.

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

The interplay of reconnection and turbulence in relativistic plasmas: the case of black hole accretion flows and coronae

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Massive black holes provide a unique environment for studying physical processes that cannot be investigated in the laboratory. A novel view of the black hole surroundings has recently been made available by the Event Horizon Telescope (EHT). EHT has provided images of the immediate vicinity of the supermassive black hole of the galaxy M87 and soon will deliver observations of Sagittarius A* at the center of our Milky Way galaxy. A large number of general relativistic magnetohydrodynamic (MHD) simulations have been performed to model the EHT data with different (but arbitrary) assumptions for the properties of the emitting electrons. Even though these models are very elaborate, they are unable to probe the physics of the emitting particles from first principles. This is the realm of particle-in-cell (PIC) simulations. The planned research project will deploy PIC simulations and analytical tools to study the role of two fundamental plasma physical processes: (i) magnetic reconnection - the annihilation of oppositely directed magnetic fields, and (ii) turbulence. These processes are responsible for powering the emission from the accretion flows feeding massive black holes.

This research plan will tackle two aspects of the physics of plasmas near black holes: (i) determine the origin of the observed hard X-ray emission and test whether coronae are likely sources of Ultra High Energy Cosmic Rays (UHECRs), the most energetic particles in the Universe. This will be done by studying the self-consistent interplay of reconnection and radiation in the most magnetized regions (“coronae”) around a luminous black hole; (ii) study the development of turbulence and reconnection in low-luminosity accretion flows feeding a supermassive black hole. The project is expected to help better understand the properties of ions and electrons. Since electrons dominate the emission, this will be of paramount importance to produce more accurate models to compare with EHT observations.

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

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Integration of in situ Monitoring and Artificial Intelligence in the Synthesis of Uranium Alloys and Compounds to inform Performance Following Melt Fabrication Processes

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High temperature stability is a hallmark property of many materials required for technological advancements in the energy sector, from steam turbine blades to oil/gas tooling to nuclear reactor materials. However, the material design and discovery process can be painstaking, requiring enormous time and effort to develop and test novel systems. The objective of this project is to develop and test a methodology to rapidly provide high quality, performance indicating data during the fabrication of uranium-based alloys and compounds. These data will be leveraged in the development of an artificial intelligence (AI) algorithm aimed to reduce time-to- and cost-of-discovery for high temperature materials. In turn, this matures a capability with the potential to predict performance for a broad set of materials and fabrication methods, including melt-pool based technologies like welding and additive manufacturing. Thermal and optical imaging as well as pyrometry facilitate *in situ* monitoring of the melting, solidification and rapid/quenched cooling of melt-synthesized compounds with temporal and spatial accuracy to the 10's of microns (approximately the thickness of a human hair). The principal investigator hypothesizes that by correlating the temperature, visual spectrum, and thermal (infrared) image data collected during part fabrication, several key performance-predicting phenomena will be identified. In essence, the research effort would employ fundamental materials science and AI to understand, predict, and ultimately control the synthesis and fabrication of novel material systems focusing on Uranium alloys as a test case to enable transformation of advanced manufacturing processes.

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

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Electrocatalytic Nitrate Reduction: Controlling Adsorbate Affinity to Tailor Reaction Products

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Every year, Haber-Bosch nitrogen fixation to form ammonia releases immense volumes of CO_2. At the same time, nitrate contamination from untreated wastewater threatens human health across the US. Development of circular processes to efficiently upgrade waste nitrate for reuse is critical to sustainably address this growing environmental hazard. Electrochemical reduction of nitrate operates at ambient temperatures and pressures, and can leverage distributed renewable energy sources and water as a hydrogen source for ammonia production. However, current catalysts lack electron efficiency in reducing nitrate versus water, lack selectivity in forming ammonia as a product, or rely on expensive rare metals, making widespread implementation unfeasible. To overcome these limitations, this proposal seeks a mechanistic understanding of nitrate electrochemical reduction on earth abundant metals and their alloys, with the goal of identifying active-site properties that improve both Faradaic efficiency and product selectivity. This insight will extend to other electrocatalytic reductive process that compete with water reduction.

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

Stable Hydrogen Isotopes as Tracers of H_2 Reactivity during Geological Storage

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Geologic systems such as confined aquifers, depleted oil and gas reservoirs, and salt caverns have been proposed to be suitable for H_2 storage at scale. A fundamental question in storing H_2 in these geologic systems is how well it is retained in the reservoir — i.e., is any H_2 being lost due to reaction or leakage.

The project will study the basic chemistry of the stable hydrogen isotopic composition of H_2 as a potential means for measuring the reactivity of H_2 in the subsurface. Specifically, the two stable isotopes of hydrogen, protium (^1H) and deuterium (^2H or D), lead to three different stable forms (isotopologues) of molecular hydrogen: H_2, HD, and D_2. These species react at different rates and their equilibrium isotopic compositions vary as a function of temperature both internally and with other hydrogen-bearing phases. The relative abundances of HD/H_2 (i.e., D/H ratios) have long been used to study the sources and sinks of molecular hydrogen in the environment. D_2 has not been utilized as a tracer previously given its exceeding rarity (~25 ppb relative abundance) and the difficulty of measuring it via mass spectrometry due to common interferences. D_2 is only now measurable using state-of-the-art high-resolution mass spectrometers.

One consequence of the storage of molecular hydrogen in the subsurface is that it will inevitably be brought into contact with water. H_2 will then be able to react with the liquid water, dissolved chemical species, or microorganisms. Such reactions may lead to the destruction of H_2 while others may lead to isotope exchange reactions (or both). As the H_2 dissolves in the fluids, it will exchange its hydrogen isotopes, changing composition in both its HD and D_2 abundances in an attempt to reach isotopic equilibrium. The kinetics of these reactions and the ultimate final equilibrium isotopic compositions dictate the overall rate and trajectory of changes in H_2, HD, and D_2 abundances during storage. Knowledge of these fundamental chemical properties could thus provide a way to measure in real time if H_2 is reacting during storage and the rate of that reaction.

This project will employ both methodological developments and experiments to use the full suite of molecular hydrogen isotopologues in order study the reactivity of hydrogen gas in geological settings. Specifically, the research will experimentally determine abiotic rates of hydrogen isotope exchange and final equilibrium compositions between molecular hydrogen and water with and without minerals present for all stable isotopologues of H_2 (i.e. HD and D_2 as well) from 25-100°C. These constraints will provide a basic scientific framework that will allow for the establishment at the molecular level of whether H_2 is reacting with other substances during geologic storage.

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

Efficient and Accessible Interactive Visual Analytics of Exascale Scientific Data

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The need to accurately model and measure complex phenomena is driving a continual increase in the size of scientific data. In practically all disciplines, multi-gigabyte, terabyte, or even petabyte-sized datasets are becoming more common. While advances have accelerated our ability to create large data, the ability to share and analyze these datasets has struggled to keep pace. Through the technological advances of this project, the simple, intuitive, and wide-reaching use of large scientific data will be possible.

First, this project will develop technologies allowing scientists to search repositories of scientific data using intuitive examples. Specifically, it will create new machine learning approaches to map scientific data to a concise representation, a hash, that will allow similarity calculations between datasets to scale massively. These fast, scalable comparisons will allow scientists to interactively search vast databases to find similar or dissimilar datasets. This project will develop learned hashes that define similarity between datasets either directly through labels created by domain experts or indirectly via features that describe the fundamental structure of data. In addition, these new hashing methods will ignore the noise in data and allow large data to be fully queried, comparing features at all scales.

Next, this project will explore innovative data reduction and post-transfer reconstruction approaches that provide both efficient data transfer and accurate analyses. Large data are usually sent initially at a reduced size, with data fidelity increased over time through progressive data transfers. This project will design novel data structures that will provide accurate analytics at all points of this progression. In addition, the project will develop new approaches to skip this additional data transfer, using machine learning to reconstruct datasets locally.

Finally, this work will develop formal models that describe interactive computer systems for the visual analysis of large data. Current systems in this space must leverage many algorithmic accelerators for performance and handle the variability of distributed processing and storage while maintaining the strict feedback times required for interactivity. This complexity often leads to complicated system deployments using ad-hoc configurations. This project will develop the first models that formally describe the complexities of these systems. Using these models in a formal design will result in large-data systems that are maintainable, testable, predictable, scalable and - ultimately - simple to deploy.

In addition to its research objectives, this project will develop new systems for large image segmentation and anomaly detection in simulations. By incorporating the developed research advances, these systems will directly support ongoing efforts at Department of Energy laboratories.

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

Understanding the 10 seconds neutron lifetime discrepancy

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The Standard Model of particle physics describes the way that all known elementary particles behave under three of the four known forces of the universe, the electromagnetic, weak, and strong interactions. Under this theory, the free neutron decays 100% of the time into a proton, electron, and antineutrino, with a lifetime of about 15 minutes. In combination with other experiments, the neutron lifetime can provide constraints on many extensions of the Standard Model. Also, knowledge of the neutron lifetime at the 1 second level is necessary to improve predictions of the elements generated from the Big Bang. There are primarily two different methods to measure the neutron lifetime: experiments based on cold neutron beams and experiments using ultracold neutron bottles. The results of these two methods differ by 9.6 seconds, which corresponds to a chance of 1 in 3.5 million that the two results are compatible with each other. There are two possible explanations for this large discrepancy: unaccounted effects in the interpretation of data (systematic error) in one or both of the methods, or a new mode of decay of the neutron that produces thus far unknown and undetected particles. This research plans to measure the neutron lifetime to the 1 second level using an alternative method with completely different systematic errors compared to previous measurements. A result that agrees with the bottle experiments will suggest that there are unaccounted systematic errors in the beam measurements, and a result that agrees with the beam experiments can be interpreted as a discovery of a new hidden decay mode of the neutron.

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

Energy Recycling for a Green Plasma-Based Collider

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High energy physics particle colliders enable scientific discoveries and allow us to probe the fundamental building blocks of the universe. However, one of the limits on their scientific reach is the tremendous electrical power needed to operate them. This project develops a path to decreasing the energy consumption of a future collider by a large fraction, translating to tens of millions of dollars of cost savings per year. Savings are achieved by developing compact, plasma-based energy recycling and taking full advantage of the enormous accelerating gradients possible with plasma-based accelerators. This project will demonstrate experimentally that residual energy in a collider-relevant plasma wakefield acceleration structure can be absorbed by trailing laser pulses, which can then be reused or their energy recycled. Plasma-based energy recycling provides two additional advantages. First, as energy is extracted from wakefields, the plasma cooling time decreases, which may enable higher collider luminosity and increase discovery potential. Second, radioactive material production in the beam dump decreases because beam energy is extracted after the collision and upstream of the beam dump. In a society sensitive to both cost and environmental issues, plasma-based energy recycling may be the key to obtaining support for the construction of a lepton collider at and above the Terra-electron-Volt (TeV) scale. Experiments will be performed on the petawatt laser system of the Berkeley Lab Laser Accelerator (BELLA) Center at Lawrence Berkeley National Laboratory (LBNL) and are enabled by the facility's new Second Beamline.

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

Assessing Greenhouse Gas Structural and Functional Resilience of Freshwater Coastal Wetlands Subject to Persistent Saltwater Intrusion Events

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Greenhouse gas production and fluxes in coastal wetlands are controlled by complex interacting hydrological and ecological processes whose dynamics are, in turn, modified by saltwater intrusion (SWI) events. In suburban and urban transition zones, the floodwalls and levee systems built to protect infrastructure and urban development intensify the SWI events resulting from floods during storm surges. When the flood waves travel inland, they meet these barriers, and saltwater can remain stagnant for prolonged periods, increasing the exposure of adjacent coastal wetlands to salt stress (i.e., persistent SWI events). These stress conditions induced by SWI are rarely represented in biogeochemical models, limiting our capacity to predict and assess the long-term effects of SWI on coastal greenhouse gas production and fluxes. Moreover, significant knowledge gaps exist in how the ecosystem reorganizes after SWI disturbance. Specifically, what trajectories do biological components (ecosystem structure) and greenhouse gas production and emission (ecosystem function) follow after SWI? Also, it is not clear what the relevant scales to evaluate these trajectories are. Using an ecohydrological patch approach defined by plant functional types and water levels, this early-career proposal aims to understand better how ecosystem structure and function linked to greenhouse gas fluxes in freshwater coastal wetlands affected by the built environment are influenced by SWI in the short- (days to weeks) and long- (years to decades) term. This project will evaluate carbon dioxide and methane pools and fluxes before, during, and after simulated SWI events covering a wide range of salt exposure (salinity concentration, duration, and frequency). The measurements will be conducted on a multi-setting sampling approach composed of controlled mesocosm in greenhouses and experimental wetland ecosystem units and will be complemented with time-for-space replacements in coastal wetlands with a history of persistent SWI. Data collected will be used to produce and incorporate an explicit salinity-dependent function to the methane biogeochemistry module integrated into the E3SM Land Model (ELM v1). The improved module will then be used to assess the sensitivity of methane emissions to different scenarios of SWI, accounting for increased storm magnitude and frequency expected from climate change and sea-level rise and exacerbated by current and projected build environments.

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

CASPT2 Geometries, Spectra, and Relativistic Electronic Structures of Actinide Species

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The pairing of electron spin in molecules can be tuned through the interactions between the metal center and its coordination environment. For molecules that can access multiple spin states, these spin properties can be exploited for use as sensors or molecular switches. The spin-coupling in the heaviest elements, the *f*-block, are among the most challenging to model due to the prevalence of such interactions. In addition to using modeling to design new molecules, results from the state-of-the-art computational methods used in this work can be used to assess the reliability of more affordable methods. Through comparisons with experiment, this work can assist with the development of the next generation of theoretical tools by quantifying if and when today's methods breakdown. Since the 5*f*-elements often present with multiconfigurational electronic structures and large spin–orbit effects, modeling the electronic structure, molecular geometries, and vibrational spectra of larger systems containing actinides with more accurate methods than commonly used will provide new insights into spin properties and bonding. Improved descriptions of the behavior of *f*-electrons will be achieved by 1) computing structural properties, 2) predicting spectra, and 3) and accounting for strong correlation and spin–orbit coupling using methods based on the complete active space approach. Modeling will include optimizing geometries and performing vibrational analysis with second-order multireference methods followed by relativistic electronic structure studies using analogous methods based on the Dirac equation. This work will be performed in close collaboration with experimental groups and, when feasible, in both the absence and presence of a magnetic field.

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

Analog Quantum Simulation for Solid-State Spectroscopies

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Quantum materials are materials in which many electrons behave collectively through quantum entanglement in ways that are incongruous with classical models. Understanding, controlling, and designing quantum materials with particular functionalities, such as superconductors and batteries, comprise a large part of the innovative landscape at the frontier of energy science. These innovative applications rely on the accurate and efficient characterization of electrons' collective properties using advanced spectroscopies. However, due to non-negligible quantum entanglement in these materials, simulations based on classical computers cannot efficiently capture the underlying physics of the materials' spectroscopies, leaving a gap between predictable theories and practical experiments. The objective of this project is to develop analog quantum simulation protocols for certain classes of solid-state spectroscopies, including linear and nonlinear x-ray and neutron scattering spectroscopies. The objective also includes extending the theory and simulations of these spectroscopies to laser-engineered nonequilibrium matter. The protocols developed in this project can be realized by near-term quantum machines and will exceed the reach of any classical computer. The simulated spectroscopies generated by this project will then provide spectral fingerprints for exotic properties and enable efficient control of designed phases. This project will lead to transformative discoveries in the field of superconductors, energy materials, and quantum devices. The tight connection to DOE-operated, advanced spectral experiments will also enhance the scientific impact of world-class user facilities.

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

Polariton Reaction Dynamics: Exploiting Strong Light-Matter Interactions for New Chemistry

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The development of novel methods to break and form specific chemical bonds will overcome major barriers to innovation in chemistry, revolutionizing our capabilities in chemical synthesis and energy technologies. A programmable reactor environment – where a researcher might "turn a knob" in the laboratory to activate or protect a selected bond – would enable a new level of rational chemical control. The emerging field of polariton chemistry inspires a means to develop exactly such devices for directing chemical reactions. Polaritons are hybrid light-matter states with unusual properties arising from strong interactions between a molecular ensemble and the confined electromagnetic field of an optical cavity. Polaritons inherit the wave-like nature of light while maintaining local molecular structure. It should perhaps not come as a surprise that polaritons can demonstrate energetics, reactivity, and photochemistry dramatically distinct from ordinary molecules. Polaritons formed from molecular vibrational states have recently been shown to impact the reactivity of specific chemical functional groups, but the mechanisms and scope of this phenomenon remain open questions that define the leading edge of the field. The fundamental physics underlying molecular polariton reactivity must be understood before we can engineer practical devices. This goal necessitates a new body of experimental work directly surveying cavity-coupled reaction trajectories on clean, easily-modeled reactive surfaces, working in close partnership with theory.

In this research project, we aim to decipher the ground rules of polariton reactivity through experimental spectroscopic studies of a library of foundational chemical transformations carried out under strong light-matter coupling. Our primary aim is to survey cavity-altered reactivity in elementary reactions, harnessing radical hydrogen abstraction reactions in particular as probes of polariton dynamics. These reactions have well-characterized single-barrier reactive surfaces; they can be initiated with photolysis and tracked directly on ultrafast timescales; they are exothermic and proceed rapidly so dynamical signatures are not washed out; and they are accessible to theory, enabling detailed interpretation of reaction pathways. We will use direct time-resolved spectroscopic methods to measure intracavity reaction rates and the quantum state distribution of nascent products, aiming to pinpoint precisely how reactive trajectories are influenced by strong light-matter interactions. Examples of both significant and insignificant changes in intracavity reactivity will elucidate the experimental parameters crucial for achieving cavity-altered chemistry and validate or eliminate emerging theories. Our results will provide fertile ground for mechanistic interpretation and a toehold for future efforts to harness polaritonics to direct increasingly complex chemistry.

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

Dream Beam: Diffraction-limited Radiation Enhancement with Adaptive Mirrors for X-ray Coherent Beamlines

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DOE x-ray light sources facilities such as the Advanced Photon Source, the LINAC Coherent Light Source and the Advanced Light Source are undergoing major upgrades to increase the source brightness and enable groundbreaking science, based on laser-like high coherent flux. The Diffraction-limited Radiation Enhancement with Adaptive Mirrors (DREAM) project takes advantage of recent technological developments in the field of x-ray adaptive optics to shape and control coherent x-ray wavefronts at the nanometer level, tuning their properties in novel ways. This work will develop automated beamline alignment procedures using adaptive optics to achieve optimal performance during routine user operation, using machine learning procedures. It will also seek the tighter integration of beamlines with their experimental end stations, demonstrating dynamic x-ray sample illumination for high-throughput data collection and autonomous experiments. The project will explore the use of adaptive optics to engineer wavefronts to give rise to new contrast mechanisms and higher sensitivity in experiments, tuning the phase of the light when it interacts with the sample. The DREAM beam project represents a critical, collaborative step forward toward enabling high-speed experiments for in-operando studies of new micro-electronics, quantum devices, or batteries.

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

Disentangling Quantum Electronic States Layer-by-layer via Space-Frequency Lock-in

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Layer-by-layer material engineering has led to an enormous testbed for energy and quantum applications due to the flexibilities to manipulate many-body interactions. In particular, it is poised to launch the next wave of topological quantum materials based on the precise control of topology, which enables the flow of electrical currents with quantized conductance, nontrivial statistics, and maximum protection. However, the understanding of the distribution of electronic wavefunctions across different layers, which is key to the realization of topological quantum phases, has remained experimentally intractable. The goal of this research program is to establish and utilize a space-frequency lock-in scheme enabled by time- and angle-resolved photoemission spectroscopy to address this challenge. In this program, we will "see" the layer origins of electronic states by "listening" to the characteristic lattice mode frequencies: femtosecond laser pulses launch coherent lattice vibrations with layer-specific frequencies; photoemission spectroscopy tracks the electronic responses. Through decomposition of the electronic structure dynamics in the lattice frequency domain, we will be able to deduce the layer origins of different electronic states. Furthermore, we will connect time-resolved photoemission with time-resolved X-ray diffraction to quantify the electron-phonon coupling strengths, which will in turn quantify the weights of electronic wavefunctions in each layer. In digital superlattices Manganese Bismuth Tellurides, we will reveal the layer origin of the topological surface state, which is critical to the realization of quantized edge conduction. In Iron-Tellurium-Selenium ultrathin films, we will unveil the layer origins of the Dirac electronic states to establish the topological superconducting phase. This space-frequency lock-in regime will be broadly applicable to other heterostructural materials such as transition metal dichalcogenides and oxide superlattices. The layer-by-layer deciphering of electronic structures will provide direct feedback to layer-by-layer engineering, leading to a rapid optimization of new digital superlattices to enable future quantum and energy applications.

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

Investigation of Encapsulin Nanocompartment Systems as a Scaffold for Biomaterials Synthesis in *Rhodococcus jostii*

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With recent innovations in synthetic biology, genetically engineered microorganisms can now produce a wide variety of bioproducts, including fuels, commodity chemicals, plastics, and inorganic materials, to support a robust bioeconomy. However, challenges such as poor reaction efficiencies and toxicity often limit yields and prevent the production of desired chemicals. One strategy to overcome these challenges is to isolate biosynthetic reactions into protein compartments or cages within engineered microorganisms. Confining biochemical reactions into such cages may help increase reaction yields by bringing the reaction components closer together. At the same time, keeping the desired bioproducts inside these cages can prevent any potential toxic effects of the products, or the conversion of those products into undesired molecules. Some bacteria, such as the emerging model bioproduction bacterium *Rhodococcus jostii*, naturally produce protein cages, called encapsulin nanocompartments. The goal of this research is to identify mechanisms for engineering compartmentalized biosynthesis in this bacterial strain. This project will develop approaches to control encapsulin production by investigating the native regulation, biosynthesis, and maintenance of the encapsulin system. Gene-editing methods will be used to engineer encapsulins with novel structural properties for expanded bioproduction capabilities. As a case study, the encapsulin system will be used to biosynthesize cadmium sulfate (CdS) nanoparticles, which are semi-conducting materials used in many important optical and electronic applications. Ultimately, this work will establish encapsulin compartmentalization systems as a means of improving yields and enabling new biosynthetic routes toward next generation bioproducts and biomaterials in support of DOE's mission to build a strong bioeconomy and thus enhance our energy security.

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

Quantum Simulation and State Preparation for Two-Dimensional Materials

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Many of the proposed uses for quantum computers require them both to be large, operating on many thousands of quantum bits, and to manipulate these "qubits" with near-perfect fidelity. While steadily improving, existing quantum hardware is not yet at the threshold required for running generic algorithms, making it important to find new approaches which can run on existing hardware. One of the most promising routes is "quantum simulation": Given the chemical composition for a material of interest, can we use quantum hardware to predict its low-temperature properties such as electrical conductivity and magnetism? The objective of this research is to develop and deploy quantum simulation algorithms applicable to near-term quantum hardware, focusing on both gate-based quantum computers and Rydberg atom "quantum simulators." The first approach will pursue efficient algorithms for studying two-dimensional materials like graphene using small gate-based quantum computers. By using the quantum computer to encode the correlations between any two halves of the material, simulations can be performed with resources that scale only with the size of the material's surface, rather than its volume, greatly reducing the required hardware resources. The second approach will provide a roadmap for using the intrinsic dynamics of arrays of atoms trapped by optical tweezers to simulate the physics of several magnetic compounds whose properties have remained enigmatic for decades. The research will combine analytic methods, large-scale computational modeling, algorithm validation on quantum hardware, and close collaboration with experiments.

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

Exploring the Role of TOR kinase in the Regulation of Central Metabolism and Lipid Synthesis

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Triacylglycerol (TAG), is one of the highest energy forms of stored carbon in living systems having an energy density similar to that of petrochemicals, making it an ideal target for the development of net-zero carbon fuels. TAG principally accumulates in plant seeds where it fuels post-germinative seedling establishment. Oil yield from seeds is limited by seed biomass, so there is increasing interest in engineering the accumulation of TAG in vegetative tissues of high-yielding biomass crops. This approach requires a detailed understanding of the regulatory network that controls carbon conversion and of the factors that limit TAG accumulation in vegetative tissues. Two key components of this network are the sucrose non-fermenting 1-related protein kinase1 and the target of rapamycin (TOR) sensor kinase. These sensor kinases act antagonistically to modulate central metabolism by integrating information about the availability of energy and nutrients and phosphorylating target proteins that control the synthesis or breakdown of cellular components. When mammalian TOR is activated by growth factors and nutrients, it promotes TAG accumulation by upregulating lipid synthesis and downregulating its breakdown. However, the regulatory role of plant TOR is poorly understood. Planned research will focus on how carbon signals interact with, and modulate the activity of plant TOR. Key plant lipid regulating targets of TOR kinase will also be investigated. Foundational knowledge from this work will inform on energy flow and conversion and provide a new perspective on the mechanisms that plants use to control those processes.

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Optical Manipulation of Magnetic Order in van der Waals Heterostructures

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Controlling the electronic spin plays a critical role in the development of modern technology. Most established methods rely on electrical transport. Developing an all-optical approach will enable a non-invasive and potentially ultrafast method to initiate, control, and read the spin states, which will greatly advance the spintronics and quantum information device research. Although a circularly polarized photon carries a spin of ±h, direct magnet domain manipulation with light helicity has been challenging due to the weak angular momentum transfer between photons and magnetic ions. The recently discovered atomically thin, two-dimensional (2D) magnets offer new possibilities with their rich electric and optical properties. In particular, novel interfacial effects within such 2D magnetic heterostructures can lead to new control capabilities of magnetic states. This proposal uses optical pump-probe spectroscopy to investigate the photon-induced magnetization modulation in 2D magnetic crystals and magnetic heterostructures. The project will develop a fundamental understanding of the non-equilibrium spin dynamics in 2D systems, and aims to achieve a full spin-flip and further coherent spin control with ultrafast laser pulses. The results will provide insights into emergent phenomena between different physical systems and stimulate 2D device development for high-speed spintronics and quantum operations.

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Advanced Uncertainty Quantification Methods for Scientific Inverse Problems

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We will develop a new array of mathematical methods for accurately and efficiently sampling high-dimensional Bayesian posterior distributions to quantify uncertainties in solving scientific inverse problems. Scientific inverse problems seek to infer unobservable parameters of a physical model from quantities that can be measured in scientific experiments. Measurements obtained from scientific experiments are often subject to data noise or lack of important information, i.e., data uncertainty; the forward model could miss a critical physics phenomenon, which is interpreted as model uncertainty. Solving a scientific inverse problem in the Bayesian context is equivalent to sampling from the posterior distribution that encapsulates all sorts of uncertainties. Because the posterior distribution could have arbitrarily complex geometry, it is impossible for any method to overcome all challenges in inverse sampling. In this project, we will develop a level-set learning based inverse sampling method for multimodal posterior distributions to overcome the challenge of mode mixing intractability in existing sampling methods. The level sets of the posterior distribution will be learned by deep neural networks. The developed inverse sampling method will be combined with a neural-network based dimension reduction approach to handle high-dimensional ill-conditioned posterior distributions. Additionally, sampling the posterior requires many forward model simulations. When the forward model is computationally intensive, a surrogate posterior is needed to accelerate time to solution. Recent advancement of neural networks has naturally led to neural network-based surrogates for Bayesian inference. However, a neural network model usually requires time-consuming hyperparameter tuning. To address this issue, we will develop a generalized deep neural network model with continuum architecture, where the standard fully connected network becomes a special case of our model. We will derive theoretical results on the expressive power of our model to explain its superior performance. The outcome of this project will significantly improve the accuracy and efficiency in solving scientific inverse problems that arise from the U.S. Department of Energy's mission space.

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Probing and Controlling Novel Electronic and Magnetic Ordering in Electron-Hole Wigner Crystals

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Understanding and controlling the competition between electron correlation and quantum fluctuations are central to the studies of correlated electronic materials, which may enable novel materials functionalities. However, it is often challenging to understand such a competition in solids since there is usually a strong interplay between electronic and other degrees of freedom, such as lattice. Van der Waals heterostructures, made of atomically thin two-dimensional materials, have recently emerged as a new platform for investigating correlated electron physics, where electronic behaviors can be controlled by electrostatic perturbations. For example, in a coupled bilayer of two-dimensional semiconductors, the electronic behaviors of one layer can become highly dependent on the other layer, leading to the formation of correlated phases, including Wigner crystals and excitonic insulators. This research program will explore how the interlayer Coulomb interactions between atomically thin materials could lead to new correlated states, such as electron-hole Wigner crystals. In addition, the project will develop techniques to probe charge orderings in such heterostructures. The program will further leverage the control of charge states to engineer novel magnetic states. The ability to control charge and magnetic ordering will impact our understanding of a broad range of quantum materials.

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Understanding Thermal Oxidation of Tungsten and the Impact of Radiation under Fusion Extremes

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Fusion energy holds great promise for replacing fossil fuels for baseload electrical power, however, harnessing such energy is a demanding process and requires materials that can cope in extreme environments including hush off-normal conditions. This project addresses a well-known fusion safety hazard concerning aggressive high-temperature oxidation of tungsten plasma-facing materials (PFMs) in case of air-ingress accident scenarios, which could generate highly volatile radioactive oxide dust and lead to uncontrollable first-wall decomposition. Currently, there is not a complete understanding of the fundamental nanoscale processes of tungsten oxidation in either pristine or irradiated conditions. To fill these key gaps, this project leverages novel in-situ environmental microscopy methods combined with dedicated computer vision models to unveil the dynamic evolution of passivating tungsten oxide layers at the nanoscale and in real-time, including in the presence of radiation-induced defects. These in-situ insights will then be correlated with tungsten oxidation rate kinetics providing a coupled experimental and theoretical framework for predicting tungsten performance under off-normal conditions. This new mechanistic understanding will provide the knowledge basis for developing creative strategies to improve tungsten oxidation resistance, and will impact the designing criteria for next-generation tungsten-based PFMs that will have to balance between radiation tolerance and oxidation resistance, both of which are essential for the safe and reliable operation of fusion energy systems.

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

Upcycling of All-Carbon Polymer Backbones into Value-Added Amines via Skeletal Rearrangement

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During the past century, development of polymers—large molecules formed by repeated linking of smaller units—has enabled unparalleled global technological progress. However, this progress has come at the cost of a global plastics pollution crisis. Among the most abundant polymers that contribute to this pollution are vinyl polymers and polyolefins. At the heart of their accumulation is the fact that cleavage of strong carbon-carbon bonds in the polymer chains is a daunting process. These bonds typically require such high temperatures (≥350 °C) to be cleaved, that mixtures of products form during pyrolysis, which further compounds the recycling problem. New strategies toward controlled breakdown of such polymers are urgently needed. To address this demand, the objectives of this project are (1) to develop catalytic installation of nitrogen atoms along all-carbon polymer backbones and (2) to utilize skeletal rearrangements to enable polymer upcycling—i.e., conversion to add value—into nitrogen-containing small molecules. This project particularly focuses on diene polymers, which makes up a large proportion of commodity rubber materials and plastics but whose recycling remains an unsolved challenge. If successful, the proposed research will transform rubber waste into building blocks for functional materials. More broadly, it will advance plastic sustainability by introducing a new strategy—namely, skeletal rearrangements—for the upcycling of waste polymers.

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