**Development of High-Density Microwave-Multiplexed Transition Edge Sensor Bolometers for Next-Generation CMB Cameras**

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The infrared glow of the hot, dense, infant universe from more than 13.8 billion years ago is still around today, although the expansion of the universe has redshifted it into the microwave spectrum. This redshifted light is called the Cosmic Microwave Background (CMB). Studying it provides key insights in cosmology as well as into the high-energy physics that was dominant in the early universe but inaccessible in laboratories now. The CMB is imaged using microwave-sensitive cameras that contain arrays of cryogenic superconducting sensors. This research effort aims to enable the next-generation of CMB cameras with 50 to 100 times more sensor pixels than current cameras. The desired leap in sensor count must overcome scaling limitations of the various cryogenic signal-multiplexing readout schemes used in CMB cameras today. The planned work will optimize and combine in a single package Transition-Edge Sensor (TES) Bolometers, a reliable CMB sensing technology, with superconducting electrical resonators, which naturally support signal multiplexing in far greater numbers than currently achieved. The coupling between these elements will be made using optimized Radio-frequency Superconducting Quantum Interference Devices (RF-SQUIDs). A scalable readout electronics system suitable to this signal transduction scheme will also be designed and implemented. This work will benefit the proposed next-generation ground-based CMB experiment called CMB-S4, which aims to probe the early-stage expansion of the universe called inflation, search for hints of undiscovered sterile particles, and constrain the mass of neutrinos. Additionally, CMB-S4's data will provide further insights into dark energy and the large-scale structure of the universe when combined with complementary data from optical and x-ray surveys. Finally, this work will enable the scaling of many other ultrasensitive photon- and particle-sensing applications that use TES arrays.

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

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**Investigation of Short-Range Ordering in Transition Metal Compounds by Diffuse Scattering**

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Future energy needs and sustainability require new materials with novel properties for such applications as energy production, storage and transport and microelectronics. Quantum materials with several competing interactions at the electronic level offer tremendous opportunity to discover, design and tune properties for such applications. Although it has been recognized that small deviations in atomic positions, driven by the competing electronic interactions, in crystalline materials can have significant impact on properties, it remains a challenge to accurately characterize such deviations (short-range order) due to the lack of advanced instruments and analysis tools to characterize them. Recently, powerful neutron and x-ray scattering instruments have been developed at the DOE user facilities to address this challenge, and new methodologies and efficient analysis tools are being developed to accurately measure such short-range order. The planned project will conduct research on transition metal compounds whose properties can be tuned by strategically substituting some atoms. High-purity single crystals will be grown, and diffuse scattering will be measured using the newly available capabilities. Theory-based computational tools will be developed to accurately analyze the short-range order to understand its effects on material properties. This understanding can then be used to design materials with improved properties. The project thus will unveil new insights on a class of quantum materials and concurrently develop new methodologies and tools that can be augmented with the tools being developed at the scattering facilities.

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

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**Microbial Environmental Feedbacks and the Evolution of Soil Organic Matter**

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The vast majority of Earth's organic matter is stored in soil. The products of microbial metabolism as well as dead microbes (necromass), along with residues from plants and other organisms at different stages of decomposition, constitute a large fraction of that soil organic matter (SOM). The ability of microbes to modify and degrade SOM depends on physicochemical characteristics of the soil, affecting SOM stability and persistence. While the contributions of microbes to the decomposition and loss of SOM have been intensively studied, their role in maintaining the terrestrial SOM is poorly understood. Specifically, how fungi, bacteria, and archaea participate in the production of SOM, the interaction between SOM and minerals, and the formation of soil aggregates remains a significant gap in our understanding of the terrestrial nutrient cycle. The chemical composition of SOM is in large measure determined by soil bacterial metabolism, which is impacted by changes in rainfall patterns. This research will conduct field and laboratory experiments and computational modeling to understand the role of microbial communities in stabilizing SOM under different water availability conditions in tropical soils. The results of this project will increase our understanding of the effects that microbes have on the global geochemical and nutrient cycles, addressing DOE's mission in energy and the environment.

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

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**Next-Generation Particle Spectroscopy at FRIB: A Gas Jet Target for Solenoidal Spectrometers**

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Nuclear reaction studies with radioactive beams can provide crucial information on the structure of exotic nuclei, the mechanisms by which they interact and self-organize, and how strongly they participate in the reactions that drive explosive and quiescent astrophysical scenarios. A powerful tool for studying transfer reactions is the solenoidal spectrometer, such as the HELIcal Orbit Spectrometer (HELIOS) device at Argonne National Laboratory. By applying a large external magnetic field, a simple relationship between the position of a detected particle and its energy is obtained, and experiments do not suffer from the kinematic compression and worsened energy resolution of typical transfer reaction measurements with radioactive beams. However, with increasingly exotic beams such as those anticipated from the flagship Facility for Rare Isotope Beams (FRIB), target effects play a larger and larger role in the best achievable resolution of solenoidal spectrometers. A gas jet provides a dense, localized, uniform, and robust target for radioactive beam reaction studies with many significant advantages over traditional target materials. For light-ion-induced nucleon transfer reactions, a gas jet provides a pure target of hydrogen, deuterium, or helium, without window materials or contaminants. The target is also robust against radiation and heat damage. By providing a gas target that is localized, reaction products can be precisely measured, and coincidence measurements are improved. Transfer reaction measurements made with gas jet targets can be cleaner, can display better resolution than those made with traditional targets, and can overcome the current bottleneck in the best achievable resolution of HELIOS-like devices. This research program will undertake a unique technical approach, implementing a pure and localized gas jet target with HELIOS and exploiting the hybrid system to better understand exotic nuclei and their astrophysical reactions. Such a device could then act as a blueprint for a next-generation solenoidal spectrometer at FRIB. With the availability of a pure and localized gas jet target in combination with developments in exotic radioactive beams and next-generation solenoidal spectrometers, the range of reaction studies that are experimentally possible with FRIB is vastly expanded.

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

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**Polarized Resonant X-ray Scattering to Measure Molecular Orientation and Conformation in Organic Nanostructures**

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The ordering of organic (carbon-based) molecules into nanostructures drives useful materials properties for applications such as organic light emitting diodes, polymer batteries, and flexible transistor circuits. However, there is a current lack of techniques to measure this ordering. Recently, X-ray scattering techniques involving molecular resonances have shown promise in distinguishing molecules and their orientation. Such a resonance occurs when an atom absorbs an X-ray precisely tuned in energy to excite a core electron into a bound molecular orbital associated with a local bond. Each resonance is bond selective, and the X-ray polarization is, furthermore, sensitive to the orientation of that bond. The objective of this research is to develop methods, models, and analysis techniques that harness these resonant phenomena in X-ray scattering measurements to quantitatively probe ordering of organic molecules within nanostructures. New physical models for polarized resonant X-ray scattering that accurately describe these complex molecular resonances will enable measurements of how molecules assemble, orient and conform at the nanometer scale. The work will test the sensitivity of the technique in terms of both spatial resolution for molecular position and orientation for molecular ordering. This new measurement capability will enable characterization of structure-property relationships that lead to disruptive technologies of printable, stretchable, and biocompatible devices based on organic materials.

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

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**Flow-Through Neutron Reflectometry - An *In Operando* Sample Environment for Active Polymer Interface Studies**

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Polymers play a key role in numerous energy storage and conversion devices (such as fuel cells and batteries), which will enable electric vehicles to mitigate the environmental impacts linked to conventional fuel use. Despite the importance of these polymers, there are several unanswered questions about their properties in actual operating devices. These limit the development of cost-effective energy storage solutions. Neutron reflectometry (NR) is a powerful technique for material analysis at layered thin-film interfaces in relevant chemical environments, but the technique's need for very flat samples currently limits NR measurements relevant to operating devices. Because devices such as lithium-air batteries and polymer electrolyte membrane fuel cells (PEMFCs) require stable materials that provide fast chemical reactions and species transport, measurement of active polymers – during chemical reactions or while species move through the polymer – is essential to understand and address the limitations of polymers in these devices. This work will enable first-of-their-kind "flow-through" NR measurements in the presence of reactions and species transport to advance the understanding of polymers for lithium-air batteries and PEMFCs. In this work, flow-through NR measurements at Oak Ridge National Lab will be combined with other experimental results to provide heretofore-unavailable fundamental insight into the role of polymers in operating energy storage devices. Computer simulations validated against the multiple measurements will be used to correlate, interpret, and understand the information for a consistent description of polymer and device function. Fundamental insights about material properties will be scaled up via device-level simulations, which will be validated against real-world devices to provide a scientifically guided design tool for next-generation energy storage and conversion devices. These activities represent a unique integration of *in operando* measurements and multi-scale numerical models, which will enable efficient iteration between theory, experiment, and simulation for advances in the understanding and design of advanced energy devices. The work will have a significant positive impact on the US energy economy, enabling efficient electrochemical energy storage and conversion for electric vehicles powered by clean energy. Moreover, this work will lay the foundation for fundamental insights in a number of other important systems, including sodium-air batteries, water purification systems, sensors, biological membranes, and chemical separators.

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

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**Multi-scale Modeling of Extreme Events and Impact Information**

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The simultaneous occurrence and persistence of multiple extremes can be associated with large-scale surface temperature gradients, regional forcings, and intermediate atmospheric variables such as the potential vorticity (i.e., a measure of cyclone generation), regional blocking frequency, and frequency and intensity of persistent meteorological high and low pressure systems. This research will adopt a novel methodology for identifying the causality and predictability of hydrometeorological (i.e., the water cycle and the transfer of water and energy between the land surface and the lower atmosphere) extreme events. The hydrometeorological extreme events that are the primary focus in this context are extreme precipitation, and the resulting floods due to compounding rainfall events. The two research objectives include: (1) investigation of the physical causality of regional to continental scale hydrometeorological extreme events using Information Theory-based causality tests in a Bayesian learning framework; and (2) development of stochastic simulation and predictive models using these drivers for the occurrence of extreme precipitation and floods of varying duration. For the first objective, statistical learning frameworks using causality tests, model checking, and hypothesis generation will be designed with both reverse causal inference (what causes an outcome) and forward causal inference (effects of the causes) to verify dependence of the above-identified hydrometeorological extreme events on the earth system and atmospheric controls. The second objective will employ a stochastic modeling strategy that integrates the above factors and accounts for correlations across multiple events and multiple locations under dynamic earth system conditions at different time scales. Bayesian network models will be used with full uncertainty analysis along the causal chain.

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

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**Future Directions in the Hunt for the Electric Dipole Moment of Radium**

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One great mystery is how our universe came to be dominated by matter when our current understanding suggests that a nearly perfect symmetry should exist between matter and antimatter. The Big Bang should have yielded a universe with nearly equal parts matter and anti-matter, with subsequent matter-antimatter annihilation leading to a universe almost devoid of either. These considerations imply there must be some significant, undiscovered violation of time-reversal (T) symmetry. Under Time-reversal symmetry, physics should behave identically if time runs forward or backwards. The discovery of any new fundamental process or property that violates T-symmetry would therefore provide a powerful clue toward solving the matter-antimatter mystery. One such property is an Electric Dipole Moment (EDM). This research will look for the EDM of a radium atom, which is believed to have remarkable sensitivity to T-symmetry violating forces due to the unusual "egg-like," asymmetric shape of the radium nucleus. To measure the EDM of this rare atom, lasers are used to cool and trap radium at a temperature less than one thousandth of a degree above absolute zero, and its rotation in an intense electric field is observed. At present, radium's EDM is known to be less than $1.4\times10^{-23}$ e-cm, about 300 trillion times smaller than that of a water molecule. This work will improve experimental sensitivity more than 1000-fold, thereby breaking new ground into the origins of T violation beyond the Standard Model that could explain matter's dominance in the universe. This research will also study the possibility of performing a similar experiment on the molecule radium monofluoride, which could further improve the experiment's sensitivity by a factor of hundreds due to the enormous electric fields that exist within a radium monofluoride molecule.

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

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**Scalable Control of Multidimensional Coherent Pulse Addition for High Average Power Ultrafast Lasers**

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High average power (kilowatt range) ultrafast lasers are essential tools that support fundamental science and applications that include, for example, laser-driven plasma wakefield acceleration toward a future high energy collider; high harmonic generation sources for attosecond science; high repetition rate pump-probe experiments at modern X-ray Free Electron Laser facilities and synchrotron light sources; medical proton accelerators and ion beam generation; and electromagnetic radiation ranging from terahertz radiation to gamma rays. One promising path for creating such lasers that also meets stringent requirements for ultrashort pulses and high repetition rate involves combining many low energy parallel pulses coherently in the dimensions of time, space and wavelength into a single, high-energy pulse. Turning that concept into working lasers involves sophisticated, real-time control systems that depend on models that incorporate the physics of the relevant processes. This research addresses the control needs associated with such novel laser architectures, leveraging the world-renowned Berkeley Lab engineering expertise on high precision digital radio frequency feedback control systems and femtosecond optical synchronization. The objectives of this research are to design, build and demonstrate a scalable distributed digital stabilization control system for robust multidimensional coherent combining of ultrafast fiber lasers and to make the control system available as a general toolbox for ultrafast optics control.

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

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**Understanding Severe Thunderstorms in the Central United States**

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Severe thunderstorms (STs) are an extreme form of storm clouds that produce large hail, damaging winds and/or tornadoes, and torrential rainfall. There is increasing concern about how these "deep convective" clouds are changing in occurrence and intensity. Earth system models (ESMs) are used to understand these ST systems, yet two significant problems persist with the previous research: (1) coarse resolution ESM simulations only account for the large-scale environments, thus ignoring the smaller, storm-scale physical processes and how they feed back to the storm's dynamics; and (2) there is a built-in assumption that the mechanisms controlling ST initiation will not significantly vary across different Earth system states. This research addresses the two issues by answering major overarching science questions: Q1. What are the significant interactions of storm dynamics with the specific environmental factors of land surface, atmospheric particles, and extreme precipitation that affect ST occurrence and intensity? How do urbanization and wildfires affect ST characteristics over the central United States (CUS)? Q2. What are the overall effects of the compounding extremes on ST characteristics over the CUS? The objective of this research is to improve the foundational understanding of key physical processes that impact ST characteristics. First, the research will (a) focus on the impacts of urbanization and wildfires and (b) explore the feedback of soil moisture resulting from extreme precipitation to subsequent ST formation and intensity. Second, the research will provide a comprehensive performance assessment of ST characteristics in a new, regionally refined ESM with advanced formulations of dynamics, urbanization, and wildfire. Third, this research will provide a robust understanding of how ST characteristics change in the CUS by considering the compounding extreme events of droughts, extreme precipitation/flash floods, and urbanization. The grand deliverable of this research is advanced understanding of ST activities in the past and future by investigating previously unexplored links between STs and the evolving Earth system, which is affected by wildfires and urbanization. The research will fill a significant gap in understanding the important physical and dynamical interactions involving microphysics, atmospheric particles, the land surface, and precipitation that affect ST characteristics.

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

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**Particle Acceleration in High-Energy-Density Plasmas: from Astrophysics to the Laboratory**

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Astrophysical plasmas, from solar flares to gamma-ray bursts, are known to be good particle accelerators. In spite of a wealth of observations and proposed models, clarifying the various acceleration mechanisms in these extreme environments remains a long-standing scientific challenge. This arises from the complexity of the kinetic and highly nonlinear interplay between the plasma flows, magnetic fields, and high-energy particles, which operate at different scales. A transformative advance in the understanding of the acceleration processes requires a combination of first principles simulations and controlled experiments where numerical findings and theoretical models can be tested. This project will use massively parallel kinetic simulations to explore the physics of particle acceleration and magnetic field dynamics in plasmas, focusing on collisionless shocks and magnetic reconnection. It will identify the processes responsible for the onset of particle acceleration and characterize in detail the efficiency and spectral signatures of the particles. This understanding will then be used to design and guide the interpretation of high-energy-density plasma experiments, where these processes can be directly probed and connected, through appropriate scaling laws, with astrophysical and laboratory plasma models.

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

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**Imaging Nanoscale Energy Transport and Conversion with Ultrafast Electron Microscopy**

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Light-matter interactions are central to innumerable fundamental phenomena and technologies. These include charge-carrier photoexcitation in semiconductors, molecular rearrangements during photocatalytic reactions, and electromagnetic-field enhancement in nanoscale materials. At the most basic level, such interactions drive electron and nuclear motions, with the ultrafast coupling of photons, charge carriers (electrons and holes), and atoms in the lattice often giving rise to unexpected and hard-to-predict behaviors. The objective of this research is to elucidate how coherent, photo-excited charge-carrier dynamics lead to the generation of initially commensurate atomic-to-nanoscale motions in both semiconducting and metallic materials. Critical new insight into such behaviors will be generated using the emerging technique of ultrafast electron microscopy. By combining a femtosecond laser with a conventional transmission electron microscope, and by operating at unprecedentedly low instrument repetition rates with maximum photoelectron-collection efficiencies, behaviors occurring in previously inaccessible experimental parameter space will be uncovered.

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

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**Determination of Vibrational Motions Driving Photoinduced Electron Transfer Reactions in Molecular Crystals and Organic Thin Films**

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The objective of this research is to develop an understanding of how molecular motions can be used to control photoinduced chemical processes. The research aims to determine what interplay of nuclear coordinates is most efficient in driving photoinduced charge transfers, a necessary first step in most photovoltaic and photocatalytic devices. Systems such as molecular crystals or polycrystalline films are promising for solar energy conversion, but the role that specific molecular structural features play in driving charge transfer is currently unknown. To determine the mechanism of processes such as ultrafast charge transfer, singlet fission, and long-range transport, a structurally sensitive technique with high time resolution is needed to monitor molecular structures along the reactive multidimensional potential energy surfaces. This work will utilize femtosecond stimulated Raman microscopy to track the nuclear dynamics driving charge transfer and to probe the effects of localized environments on long-range charge transport. By following the structural evolution of photoreactive molecular solids on the timescale of their nuclear motion, this work will provide multidimensional reaction coordinates and uncover molecular structure-function relationships. This fundamental knowledge should ultimately guide rational design of highly efficient photovoltaic and photocatalytic systems by determining how, when, and where energy is lost during charge generation and transport.

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

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**Surface Ligand Effects on Energetics, Charge Transfer, and Stability at Interfaces Between Metal Halide Perovskites and Organic Semiconductors**

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The chemistry at organic-inorganic interfaces plays a major role in determining the performance of electronic and optoelectronic devices and the electronic and optical properties of organic-inorganic composite materials. Understanding, developing, and using surface chemistry is thus essential for creating improved and novel materials and devices. Two families of materials that will benefit tremendously from an improved fundamental understanding of the surface chemistry are organometal halide perovskites and metal halide perovskites, abbreviated as (O)MHPs. These perovskites are emerging as inexpensive materials that can be printed from solution to make efficient photovoltaic cells for harvesting solar energy; light emitting diodes for energy efficient solid-state lighting applications; solid-state lasers; and transistors. To realize the full potential of (O)MHPs, their surface chemistry and interfacial properties must be better understood and utilized. This research revolves around determining how the surface chemistry of (O)MHP thin films and nanoparticles influences optical properties, charge transfer processes, energetics, and stability. The objectives of this research include quantifying ligand binding strengths to (O)MHPs; determining how the ligands influence photoluminescence properties, energetics, and charge transfer processes; determining how ligands influence (O)MHP stability; developing strategies to stabilize (O)MHPs through surface ligands; and developing mixed surface ligands to systematically manipulate energetics, charge transfer, and stability at perovskite-organic interfaces. Overall, this research will establish key information regarding the surface chemistry of (O)MHPs that can be widely applied in both academics and industry to facilitate the development of this exciting material class.

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

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**Scale-Bridging Simulation of Magnetically Confined Fusion Plasmas**

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Magnetically confined nuclear fusion represents the potential of clean, safe, and virtually limitless power for the world. However, in contrast to nuclear fission, fusion has proven a far more complex problem to solve. The spatial scales of the relevant physical processes span more than six orders of magnitude, and the timescales span more than ten. Such multiscale processes, combined with the extreme environment within a fusion device, make the physics inherently difficult to diagnose in an experimental setting. As such, advancing our understanding of magnetically confined fusion plasmas has leant heavily on the use of computer simulation where the available information is limited only by the assumptions in the model, the uncertainty in the calculation, and the capabilities of the computer. With the rapid advances in high performance computing, exascale computing platforms are slated to be available in the US by 2024. With such a scale of computing capability comes the tremendous opportunity to simulate a fusion device in its entirety from its fundamental describing equations, possibly unraveling the essential fusion reactor physics we presently cannot predict from theory. However, the multiscale nature of fusion plasmas makes realizing this potential challenging, and significant research into computational methods that can effectively treat this wide range of scales is needed if we are to fully exploit the coming wave of computing power. To achieve this, we will develop a robust scale-bridging method for fusion simulation based on implicit projective integration, combined with online uncertainty quantification and sensitivity analysis and enabled by the massive on-node parallelism of modern supercomputers. Such a capability has the potential to significantly advance scientific discovery in fusion plasma science.

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

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**Advanced *Ab Initio* Methods for Nuclear Structure**

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Exotic neutron-rich nuclei have moved firmly into focus in nuclear physics research. The structure of these nuclei is governed by a complex interplay of nuclear forces, strong many-body correlations, and continuum effects. It challenges our present understanding and has far-reaching implications, ranging from the creation of elements in the cosmos to tests of fundamental symmetries of the Standard Model of Physics. The Department of Energy's Facility for Rare Isotope Beams (FRIB) will make it possible to produce and study many of these exotic nuclei for the first time under laboratory conditions. The experimental efforts at FRIB and similar facilities go hand in hand with theory efforts to develop a reliable description of exotic nuclei. The present project will develop advanced theoretical methods for that purpose, with an emphasis on renormalization group ideas. It will leverage state-of-the-art computational techniques to handle the enormous memory requirements of nuclear forces and the computational effort associated with the treatment of deformed, weakly bound nuclei. The goal is to create a framework that can scale from day-to-day applications in support of experimental data analysis to large-scale simulations on leadership-class computers.

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

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**Seeing Neutrinos: The Physics Potential of Photon Signals in DUNE**

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Discoveries in particle physics require state-of-the-art detectors, and, if the particle you want to study is the neutrino, those detectors must be built on an enormous scale. The flagship experiment of the US high energy physics community in the next decade, the Deep Underground Neutrino Experiment (DUNE), is just such an experiment. It will be made up of four gigantic tanks, each larger than a jumbo jet, filled with liquid argon. Even with these large detectors, catching a neutrino is rare, so we need to learn as much as we can about each neutrino using the signature it leaves behind in the argon. One of these signatures is the emission of particles of light (photons), and this research will build a foundation that enables precise measurements using this signature. The photons do not travel freely once emitted; they may scatter in a new direction or reflect off a wall in the detector, so the goal of this research is to understand and correct for such effects. New software algorithms will be developed that take these effects into account, and they will be tested in the prototype detectors now under construction. Then, the optical properties of liquid argon itself will be measured directly to enable even more precise understanding of the behavior of light in liquid argon detectors. The combination of these new techniques with the data from direct measurements will allow the full potential of the photon signals in DUNE to be realized.

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

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**Understanding the Chemical Complexity of Multi-Component Systems: Uranium Polyoxometalates as Nanosorbents**

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The actinide series consists of the fifteen elements with atomic numbers 89-103 (i.e., actinium through lawrencium) and carries great societal importance due to the elements' use in medicine, power generation, national security, and nuclear waste management. Due to the complex nature of the actinide elements and the relative difficulty of working with radioactive materials, research in actinide chemistry has lagged far behind that of most other elements on the periodic table. To address current knowledge gaps, this research will study the chemistry of the actinide elements uranium, neptunium, plutonium, and americium. The thermodynamics and kinetics of the interactions of neptunium, plutonium, and americium with nanometer-sized uranyl peroxide cage clusters will be used to describe bonding and structure (i.e., how electrons are shared in these unique complexes). This research represents the first study that uses actinide materials as nanosorbents for other actinide elements. The well-defined structure of the uranyl peroxide cage cluster allows it to serve as an experimental model for other metal oxide surfaces.

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

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**Probing Naturalness with Searches for Supersymmetric Higgs Partners at the Large Hadron Collider**

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The 2012 discovery of the Higgs boson at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland concluded the search for particles predicted by the standard model (SM) of particle physics, which describes our understanding of the basic building blocks of matter and their interactions at the most fundamental level. While the SM has been successful in describing a wide variety of observations with excellent numerical accuracy, it is nevertheless incomplete. It does not explain the nature of dark matter, which forms ~25% of the mass and energy of the universe. Nor does it explain the difference in strength of fundamental forces or whether they are different manifestations of a single force. To answer these questions, an extension to the SM incorporating a new space-time symmetry, Supersymmetry, has been proposed. We plan to search for signatures of Supersymmetry, specifically partners of the Higgs boson, in data collected by the ATLAS (A Toroidal LHC Apparatus) detector at the LHC. Upgrades to the ATLAS trigger system are pursued to enable fast hardware-based charged particle tracking, which will enhance the sensitivity of these searches. A discovery would transform our understanding of the composition and fundamental laws of the universe.

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

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**Proximity Effects and Topological Spin Currents in van der Waals Heterostructures**

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Solids have traditionally been categorized in terms of their electrical conduction: conductors such as aluminum conduct electricity; insulators such as wood and plastics do not; semiconductors such as silicon show an intermediate behavior. In the last decade, this simple picture has been upended. It is now well established that there is a class of solids in which the bulk of the solid is insulating yet the surface of the solid can behave as a special type of conductor. These materials are known as *topological insulators* (TIs), and the electronic states responsible for the conduction are known as *topological boundary modes*. These topological boundary modes can have special properties not generally present in other conductors such as a strong coupling between the spin and the charge current of electrons and a protection against scattering that means the electrons can flow without dissipation of energy. The scientific objective of this proposal is to investigate a new framework for the creation and manipulation of topological boundary modes using the *proximity effect* in solids, where certain properties of one solid can "leak" over a short distance into an adjacent solid. We will study proximity effects in vertical layered structures composed of graphene and other two-dimensional van der Waals crystals, known as "van der Waals heterostructures." These crystals exhibit magnetic order and strong spin-orbit coupling, and we will study the mechanisms by which these properties can be imprinted on the graphene layer and the conditions under which topological boundary modes can be realized in graphene as a consequence of these particular proximity effects.

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

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**Fundamental Study of Fatigue Crack Initiation at Grain Boundaries in Austenitic Stainless Steel**

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Fatigue damage under cyclic loading conditions accounts for the majority of failures in structural metals, yet the underlying mechanisms dictating when and where failure initiates remain poorly understood. This information is needed to guide the development of novel, fatigue resistant materials and to better predict the lifetime and reliability of materials currently in use. The objective of this project is to understand the evolution of the defect state leading to fatigue crack initiation. This includes determining what local mechanisms drive the crack initiation process and how damage accumulation/failure initiation is influenced by the surrounding microstructure. Defect accumulation/failure initiation is inherently a multiscale process, with defect interactions occurring across hundreds of microns but crack initiation occurring at the nanoscale. To access information across these length scales, novel *in situ* scanning and transmission electron microscopy deformation experiments capable of resolving the evolution of the local defect state and the accompanying stress fields will be developed. The primary material that will be investigated in this research is 316L stainless steel, a broadly-used structural steel alloy, though many of the observed mechanisms are expected to be applicable to a range of engineering alloys.

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

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**Large-scale Deep Learning for Intelligent Networks**

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This research project is focused on enabling the design of intelligent networks that allow improved response, utilization, and reliability for exascale scientific workflows. The research pursues building robust networks through the use of machine-learning-based approaches, cloud computing, and software-defined networks (SDN). For example, deep learning algorithms have recently been used to process real-time events and prevent accidents involving autonomous cars in highway traffic. Analogously, the proposed research couples deep learning methods with SDN for predicting real-time network behavior and avoiding data traffic congestion or degraded network performance. Distributed processing models such as cloud computing will be used to reduce learning time and improve real-time network reactions. As data demands from scientific communities rapidly increase, the proposed research is timely for ensuring the development of reliable and robust networks with guaranteed high-throughput data transfer and uninterrupted performance.

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

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**Vegetation Dynamical Responses to Multivariate Extremes in the Western US**

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The Western US is experiencing an increase in a particular multivariate extreme: high temperatures and reduced precipitation, which together combine to create hot droughts. At the same time, forests are dying throughout the region, and their elevated mortality is likely driven by these increasing extremes. This mortality will continue to drive changes to the composition of the Western US forests and others throughout the northern hemisphere. Because forest compositional changes may feed back to changes in the Earth system, both via biogeochemical and biophysical feedbacks, it is critical to include these processes within Earth system models (ESMs). Such dynamics are currently not permitted in most ESMs, including DOE's Energy Exascale Earth System Model (E3SM), which do not have active vegetation dynamics. The advent of new tools—such as the Functionally Assembled Terrestrial Ecosystem Simulator (FATES)—allows us to mechanistically represent both the individual-level physiological responses to drought as well as the ecological community assembly that governs long-term vegetation dynamics. Applying these tools to understand and predict feedbacks requires detailed testing against observations that span both physiological and vegetation dynamical processes. The overarching goal of this effort is to understand how long-term vegetation-dynamical processes interact with droughts in the Western US by using the recent California drought as a test case for examining multivariate droughts and by exploring how these dynamics are projected to occur at longer timescales and larger spatial scales in the future. Several sets of observations suggest that the forest structure in California is undergoing rapid change and make it an ideal test case for mortality-driven vegetation dynamics: the sizes, trait composition, and number of trees have shifted over the 20th century; tree mortality rates are increasing rapidly over recent decades; and the recent drought shows a particularly localized pattern of extremely high mortality that is suggestive of a biome shift. These observations will allow benchmarks of transient vegetation dynamics, which can be used to test dynamic vegetation models. We will use these events, as well as physiological measurements from a network of eddy-flux towers across an elevation transect in California's Sierra Nevada as well as airborne remote sensing data as tests of FATES, a modular, demographic, dynamic vegetation model for use in the E3SM model. Once tested for these ecosystems, we will then use FATES within the coupled land-atmosphere system to explore the role of vegetation dynamics in modulating land-atmosphere feedbacks on slow timescales. We will seek to understand the role of extremes versus mean-state changes in governing the rate of vegetation dynamical changes under changing climate and the roles of vegetation dynamics in driving feedbacks to both the mean state and extremes of the atmospheric state.

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

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**Unique Optical Excitations in Topological Insulators**

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The overall objective of this research is to understand how light interacts with topological insulator (TI) films and layered structures. Unlike normal materials, the electrons in TI films are trapped at the top and bottom surfaces of the film. These electrons have unusual properties, including low mass and high velocity. Light shining on these trapped electrons will excite electron density waves, called plasmons, which inherit the unusual properties of the electrons. This project aims to understand how these plasmons interact with each other and how the plasmon properties change as the film dimensions change. By controlling the physical properties of the films, the optical response of the film can also be controlled. In addition to single TI films, the project will also investigate the properties of stacks of TI films layered with normal insulating films. Stacking these materials results in multiple layers of trapped electrons whose plasmons can interact in ever more complex ways. After these interactions are understood, we can begin to engineer complex TI structures to obtain designer optical phenomena in the far-infrared and THz, wavelength ranges of interest for environmental monitoring and chemical sensing. This research directly addresses DOE Grand Challenges, including understanding how properties of matter emerge from complex electronic correlations and learning how to control these properties, as well as the mission of the Basic Energy Sciences program to understand and control matter at the electronic/atomic level.

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

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**Green's Function Methods for Multiphysics Simulations**

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Green's function methods are important tools in the numerical solution of partial differential equations. This research aims to establish Green's function methods that can enable multiphysics simulations such as crack propagation in materials and the design of next-generation batteries. This research will tackle the challenging question of how to couple the quantum and classical physics descriptions for the overall multiphysics system. The key mathematical difficulty is to properly formulate the boundary condition for the region described by quantum physics. In order to overcome such difficulty, this research will pursue the approach based on Dirichlet-to-Neumann maps, which in principle allows the quantum and classical regions to be coupled in an exact way. The key ingredient is to construct Dirichlet-to-Neumann maps in an efficient, accurate, and versatile manner. The proposed work will lead to the development of efficient Green's function methods that are ideally suited for predictive multiphysics simulations on massively parallel computers.

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

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**Advancing Polymeric Gas Separation Membranes through Molecular Engineering**

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The industrial scale separation and purification of chemical mixtures accounts for approximately 10-15% of the world's energy consumption. Because of this, methods by which these chemical separations can be accomplished in a more efficient and cost-effective manner are highly desired. One particular technology that has shown tremendous promise is the use of polymeric gas separation membranes, which have been targeted for a variety of applications including the separation of light-hydrocarbons, the purification of natural gas, and the separation of harmful greenhouse gases such as carbon dioxide. However, despite broad interest, the industrial-scale implementation of gas separation membranes has remained relatively limited due to a variety of scientific and practical challenges. One such scientific challenge is an overall lack of understanding regarding how molecular-level hierarchical controls may be harnessed to promote membrane performance. To bridge this scientific gap, this research project aims to synthesize and evaluate polymeric gas separation membranes possessing precisely defined structure at the monomeric, polymeric, and microphase levels. More specifically, detailed investigations will be conducted in an effort to 1) better understand how interactions between polymeric materials and penetrant gases may be systematically tailored, 2) develop a detailed relationship of how precise block copolymer composition and microphase separation dictate membrane performance, and 3) better understand how advanced molecular and polymer architectures may be used to influence gas transport. These membranes will be evaluated using a barrage of techniques, which will inform the systematic design of subsequent membrane generations. The information obtained herein will strengthen the scientific community's fundamental understanding and may facilitate the development of broadly applicable, highly efficient membranes for gaseous separations.

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

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**Measurements at the Facility for Experiments of Nuclear Reactions in Stars (FENRIS)**

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Nuclear reactions in stars have transformed the universe since the Big Bang, turning hydrogen and helium into the heavier elements we see around us today. These reactions fuel a star throughout its lifetime. These reactions fuel a star throughout its lifetime. When the star burns out, its ashes are ejected into space to enrich the next generation of stars. Thus, to understand the origin of the elements in the cosmos, we must learn how stars burn their fuel. In this stellar burning, the rates of nuclear reactions are key. The rates can, in principle, be determined by recreating the reactions in the laboratory. At the low energies characteristic of stellar burning, however, many of the reactions occur too rarely to be measured. Novel, indirect measurements must be used. A research program will be developed to perform such measurements, primarily using the Facility for Experiments of Nuclear Reactions in Stars (FENRIS), a charged-particle spectrometer at the Triangle Universities Nuclear Laboratory (TUNL). At FENRIS, high-energy nuclear reactions coupled with theoretical models will be used to ascertain the rate of the low-energy nuclear reactions occurring in stars. Detailed analysis of the data will reveal the structure of nuclei and how they affect stellar burning. High-energy photons will be used as a different lens with which to examine these nuclei at another facility - the High Intensity gamma-ray Source – to supplement the measurements at FENRIS. In parallel to these experimental efforts, theoretical tools will be developed to identify which nuclear reactions are most critical for understanding stars, helping set the priorities for future measurements. This complementary suite of experiments and theoretical calculations will be used to answer one of the key questions facing the physics community: How did visible matter come into being and how did it evolve?

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

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**First-Principles Tools for Nonadiabatic Attosecond Dynamics in Materials**

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Controlling materials at the level of electrons and characterizing and controlling matter far-from-equilibrium are two ongoing grand challenges in solid-state science. Successfully addressing these challenges has the potential to revolutionize fields ranging from energy storage to conversion of light into electrical and chemical energy. In particular, the mechanisms of ultrafast light-induced changes in solids are poorly understood at the atomic level. These dynamics occur at the attosecond (billionth of a billionth of a second) time scale and involve a complex interplay of electron motion coupled to the movement of the atoms in a crystal lattice. The objective of this research is to develop computer simulation tools for predicting the ultrafast response of materials subjected to intense pulses of light. These tools are crucial for understanding the underlying mechanisms and for interpreting and motivating attosecond experiments. First-principles approaches for this type of dynamics, especially for photochemistry-like processes near dopants and defects, are lacking. This project will develop density functional theory-based methods for attosecond electron/nuclear dynamics in semiconductors and insulators under the influence of high-intensity and/or high-energy (X-ray) laser pulses. These will be validated against experiments and will enable computation of optical breakdown, electron/lattice couplings, excited-state lifetimes, and the origins of non-thermal damage.

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

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**Discovering Dark Energy, Dark Matter, and Neutrino Properties with Cosmic Structure**

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Maps of the distribution of galaxies, or the cosmic large-scale structure, provide information about the past several billion years of cosmic history. These maps have the power to inform several of the largest scientific puzzles driving the Department of Energy's High Energy Physics program: the neutrino mass scale, properties of dark matter, the existence of new particles, and the mechanism responsible for cosmic acceleration. This research will develop the theory of structure formation in the presence of cosmic neutrinos and other novel types of matter. This work will ensure the exploitation of the full power of the cosmic-structure data. The primary goal is to ensure that modeling uncertainties are not an obstacle to detecting the neutrino mass scale and other cosmological parameters with next-generation experiments. A secondary goal is to anticipate the possibility of new physics by developing the astrophysical phenomenology of novel dark-matter and cosmic-acceleration scenarios. This research will produce new tools to study neutrinos, hidden components of dark matter, dynamical dark energy, and structure formation in the Universe.

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

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**Mechanistic Studies of a Primitive Homolog of Nitrogenase Involved in Coenzyme F430 Biosynthesis**

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Methyl-coenzyme M reductase (MCR) is the key enzyme in the biological formation and anaerobic oxidation of methane (AOM). Methane is the major component of natural gas. Given the abundance of natural gas reserves in remote areas, there is great current interest in a scalable bio-based process for the conversion of methane to liquid fuel and other high-value chemicals. MCR holds much promise for use in such a methane bioconversion strategy. However, MCR cannot currently be produced in an active form in an industrially viable strain due to the lack of genetic and biochemical information about the formation of its unique nickel-containing coenzyme, F430. The coenzyme F430 biosynthesis (Cfb) pathway was recently elucidated, and the key step was found to involve an unprecedented reductive cyclization reaction that converts the intermediate Ni-sirohydrochlorin a,c-diamide to the immediate precursor of F430, 15,173-seco-F430-173-acid. This remarkable transformation, which involves a six-electron ring reduction, cyclization of an acetamide side chain to form a ϒ-lactam ring, and the formation of seven stereocenters, is catalyzed by a primitive homolog of nitrogenase (CfbCD). Nitrogenase is a two-component metalloenzyme that catalyzes the adenosine triphosphate (ATP)-dependent reduction of nitrogen gas to ammonia and hydrogen gas (biological nitrogen fixation), a reaction of great industrial importance. Homologs of nitrogenase are also involved in the biosynthesis of the photosynthetic pigments chlorophyll and bacteriochlorophyll. Phylogenetic analysis of the CfbCD complex suggests that it is representative of a more ancient lineage of the nitrogenase superfamily, and a thorough investigation of its structure and function is likely to shed light on the mechanisms and evolution of these important metalloenzymes. Moreover, a detailed understanding of the mechanism of the CfbCD complex may be exploited for the production of MCR for use in methane bioconversion. Towards these goals, the objectives of this research are focused on 1) the identification of physiological electron donors and *in vivo* coenzyme F430 synthesis, 2) the analysis of the iron-sulfur centers, structure, and oligomerization state changes, and 3) the characterization of transient intermediates and the intercomponent electron transfer of the CfbCD complex.

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

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**Attosecond Light-Field Control of High-Density Plasmas**

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This project explores transient micro-sized high-energy-density plasmas formed in the interaction of focused multi-terawatt laser beams with solid targets. According to theoretical predictions, relativistic electrons in such plasmas may emit high-order-harmonic soft-x-ray radiation more powerful and of shorter durations than that of the current fourth-generation free-electron laser sources. This radiation may serve as an informative probe of nonlinear plasma dynamics with sub-femtosecond precision and open the path for high-temporal-resolution x-ray diagnostics with applications in plasma and atomic physics, material science, biology and medicine. This project aims at characterizing and controlling the properties of high-order-harmonic emission from dense plasmas driven by accurately tailored light waveforms.

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

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**High-Gradient Accelerators at THz Frequencies**

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Advanced particle accelerators are enabling technologies for the exploration of high energy physics. Successful accelerator technology for future particle colliders must efficiently accelerate beams and rapidly increase particle energy using intense electromagnetic fields to provide high accelerating gradients. One approach to achieving accelerating gradients orders of magnitude above present capabilities is to dramatically increase the operational frequency into the Terahertz (THz) range. This program will explore new accelerating structures designed to withstand high gradients, power them with the newest generation of THz sources, and lay the foundation for THz accelerator technology. This research aims to answer fundamental questions about the limits of accelerating gradients and to improve understanding for the role of frequency, pulse length and stored energy in plasma breakdown. This knowledge will also provide feedback to the design of lower frequency accelerators, potentially improving their performance. Compact, high-gradient THz accelerators also hold the promise of having an immediate broad impact with many potential applications of relevance to biologists, chemists and physicists investigating ultrafast processes and to physicians developing new tools for medical therapy.

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

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**Modeling Charge Transfer Excitation with Variation After Response Quantum Monte Carlo**

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Processes that move electrons between molecules play crucial roles in battery technology, light harvesting, liquid fuels production, and many other high-priority areas of energy science. This research will develop high-fidelity models for electron transfer by combining theoretical chemistry, the mathematics of random processes, and the Department of Energy's unparalleled infrastructure for high performance computing. Like custom-tailored suits, these models will optimize wave functions for individual processes with unprecedented precision. The resulting efficiency will permit reliable predictions to be made at technologically relevant length scales, a critical capability that is lacking in current models. In the same way that computational models of fluid dynamics have revolutionized the design of engines and aircraft, this research will help support a revolution in the rational design of molecular scale technologies for energy science.

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

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**Symmetric Convex Sets: Theory, Algorithms, and Application**

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The past few decades have seen rapid growth in the types of problems that can be solved using computers. Improved algorithms, combined with improved hardware, have allowed optimization to become a ubiquitous tool used in a range of areas such as transportation and power systems. Even though it is routine to solve extremely large optimization instances, one will occasionally come across a problem that is considerably difficult to solve, even if the instance is very small. A hypothesis of this work is that these difficult instances tend to be highly symmetric. By developing tools that exploit this symmetric structure, one will be able to easily solve optimization problems considered intractable and improve the computational speeds by orders of magnitude. The challenge of solving optimization problems will thus be transformed by changing a large part of the work to one of seeking symmetry and then exploiting it.

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

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**Searching for Parton Energy Loss in Quark-Gluon Plasma Droplets**

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Very high energy collisions of nuclei at the Relativistic Heavy Ion Collider (RHIC) and the Large Hadron Collider (LHC) create a Quark-Gluon Plasma (QGP), a high-temperature, high-density form of matter in which quarks and gluons, collectively called partons, are freed from their normal state of being bound in protons and neutrons. The formation of a QGP is understood to have several experimental indications, including: (1) correlations in how the particles produced in the collision are distributed in angle, attributed to a QGP that can "flow" with near perfect fluidity, and (2) the degradation of high-energy collections of particles, called "jet quenching", attributed to a QGP that attenuates any partons that attempt to pass through it. Remarkably, recent measurements of flow-like correlations in much smaller collisions of protons and deuterons with nuclei suggest that a droplet, or small region, of QGP is formed even in these systems. However, the expected accompanying signature of jet quenching has yet to be observed. Given the complications in applying traditional observables to these small systems, a search for jet quenching requires the examination of individual events, such as those with a produced photon and particle jet pair. In these events, the photon escapes the collision zone without interacting and provides an estimate for the energy of the balancing partons before they pass through the QGP. For this reason, photon-tagged measurements have long been recognized by the theoretical and experimental communities as a "golden channel" probe of these effects. Through the analysis of high-luminosity data recently collected by the ATLAS (A Toroidal LHC Apparatus) detector at the LHC and that to be collected with the sPHENIX (super Pioneering High Energy Nuclear Interaction eXperiment) detector at RHIC, this research seeks to determine how high-energy partons are affected by the varying shapes and sizes of QGP regions they encounter.

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

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**A Continuous Model of Discrete Scientific Data**

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The Advanced Scientific Computing Research (ASCR) mission to advance science through high-performance computing depends on managing, analyzing, and visualizing data. While our computational capability to generate more raw data grows, our ability to process the resulting quantity and diversity—to store, transform, and to draw scientific conclusions from scientific datasets—is lagging. Rethinking the way that scientific data are represented is one way to break out of this spiral. This project explores a fundamentally different kind of data model that will conserve resources while improving data understanding and sharing. The approach being taken recasts discrete scientific data with continuous, functional approximations that will be more efficient to communicate, store, and analyze than the original form. The new model, which can accommodate many types of scientific datasets on high-performance supercomputing architectures, provides for file size compression and facilitates analytical reasoning not possible before. Moreover, the accuracy of the data model will always be known and guaranteed. In addition, the new model preserves geometric, visual, and statistical properties, making it directly usable for analysis.

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

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**Probing Condensed Phase Structure and Dynamics in Hierarchical Zeolites and Nanosheets for Catalytic Upgradation of Biomass**

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A difficult scientific challenge is the understanding of complex reactions at the molecular level in systems characterized by multiscale collective coupling across time and space. In this project, an example of such systems will be considered by pursuing the hypothesis that interactions of oligomers, solvents, and active sites can be tailored by suitable choices of solvent and of solid-acid catalyst pore architecture to promote chemical transformations during catalytic conversion of biomass. The architecture is determined by the choice of hierarchical zeolites, which provide large channels for macromolecule diffusion and small pores for catalysis. A multiscale computational approach will be used to elucidate physical and chemical interactions across multiple spatial and temporal scales. We will use advanced first principles Monte Carlo and molecular dynamics simulations along with electronic structure calculations to answer fundamental scientific questions pertinent to acid-catalyzed hydrolysis and hydrogenolysis of cellulose and lignin in ordered mesoporous zeolitic structures. One outcome will be a better understanding of the interactions of reactant and solid acid catalysts in the presence of solvents, enabling rational design of catalytic systems that can upgrade biomass in a selective and energy efficient manner. Another outcome will be the development of sampling tools essential to detangle interactions in complex, reactive phenomena.

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

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**Fundamental QCD Theory and Transverse Momentum Dependent Physics**

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Quantum Chromodynamics (QCD) is the fundamental theory of the strong nuclear interaction. It lies at the root of the interactions between the elementary particles (quarks and gluons) that are ultimately responsible for the structure of particles like protons and neutrons that form ordinary matter. However, the precise mechanisms by which quarks and gluons interact to form the particles seen in nature remain mysterious and only partially understood. A major difficulty to forming a complete picture comes from the fact that QCD has dramatically different characteristics over large and small spacetime scales. Over small scales, quarks and gluons couple only loosely, so small-coupling theoretical techniques (called "perturbative") predict patterns of quark and gluon radiation with very high accuracy. By contrast, interactions over large scales involve a very strong coupling and are characterized by the types of QCD interactions (called "non-perturbative") responsible for binding quarks and gluons tightly together. In high-energy QCD experiments, an intricate combination of large-scale and small-scale interactions is responsible for physical observables like scattering cross-sections. Therefore, one of the keys to understanding how QCD gives rise to measured physical quantities in nature is the ability to disentangle these large-scale and small-scale interactions in theoretical calculations. A prescription for doing this is called a factorization theorem. A successful factorization theorem is the critical bridge between perturbative calculations of small-scale physics, non-perturbative calculations of large-scale physics, and experimental data. Experimental strategies continue to focus, with ever-greater detail, on the precise momentum and energy distributions of final states produced in high-energy particle collisions. At the same time, the associated factorization theorems necessary to interpret these data and extract meaningful information about fundamental QCD interactions become increasingly subtle. This project will improve existing factorization theorems to the point that they can be used most effectively in the future analysis and interpretation of transverse momentum dependent (TMD) observables. New theoretical techniques will be developed where needed, while incomplete aspects of established factorization theorems will be addressed. The outcome will be a unified factorization framework for combining non-perturbative theoretical calculations consistently with perturbative QCD calculations, such that descriptions of fundamental quark and gluon interactions can be meaningfully tested against TMD observables.

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

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**Program Generators for Exascale and Beyond**

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Program generators are an appealing solution to the problem of automatically producing high-performance libraries and applications for specific computational platforms from high-level descriptions of scientist intentions. When platforms are upgraded with new hardware architecture features to be supported, appropriate extensions to the generator should enable efficient code to be readily regenerated. Very few program generators currently exist because they are difficult to build. The main difficulty stems from the problem of designing an extensible approach to perform all the optimizations that compilers are unable to do. Furthermore, the actual implementation of the program generators often results in ad-hoc collections of stand-alone programs that are hard to extend, reuse, or further develop. The main research objective is to devise programming models and supporting tools that greatly simplify the development of specialized high-performance program generators. Success in this research direction will have a transformative impact on how exascale software is developed for DOE mission-critical science and engineering applications.

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

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**Dark Energy Constraints from Weak Gravitational Lensing in the Large Synoptic Survey Telescope (LSST)**

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The 2011 Nobel Prize in Physics was awarded for the discovery of the accelerating expansion of the universe, called "dark energy," that has no explanation by known physical phenomena. Measurements of weak gravitational lensing (i.e., the distortion of galaxy images by the gravity of cosmic structures) made with the Large Synoptic Survey Telescope (LSST) have the potential to distinguish the 'cosmological constant' hypothesis for dark energy from modified gravity hypotheses. However, the LSST measurements are limited by systematics rather than statistics because of the large data volume. Weak lensing is dominated by the noise from the unknown distribution of intrinsic galaxy shapes. We will advance our previously demonstrated 'hierarchical' Bayesian algorithms to significantly reduce this noise and simultaneously include more features of galaxy images (e.g., sizes, fluxes). The LSST will collect on the order of 1,000 distinct images for every source in the ten-year, 18,000 square degree survey. Combining these images for precision lensing measurements is an as-yet unsolved problem. We have demonstrated a massively parallelizable algorithm to optimally combine galaxy image measurements, including uncertainty propagation, for lensing shear inference. We will develop a pipeline for this algorithm with a goal of delivering a primary image reduction tool for the LSST survey.

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

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**Advancement of Hybrid Fluid-Kinetic Modeling Efforts for HEDP and ICF Science**

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Increasingly complex high-energy-density physics (HEDP) and inertial confinement fusion (ICF) experiments at the nation's three flagship HEDP facilities—the Omega Laser Facility, the National Ignition Facility, and the Z Pulsed Power Facility—are advancing the limits of our fundamental scientific understanding of matter at extreme conditions. Multi-physics radiation-hydrodynamics simulation capabilities are continuously developed and improved to help explain and predict the dynamics of matter in laser-driven and pulsed-power-driven experiments over a large range of temporal and spatial scales and from the solid to plasma states. In fact, scientists conducting these experiments increasingly rely on such simulations since they are useful and often necessary to help design and execute highly integrated experiments as well as to analyze and interpret the collected data. While progress has been made toward the development of robust and reliable models with predictive capability, more work remains since significant amounts of the data acquired at the facilities are not easily interpreted by radiation-hydrodynamics simulations alone. The science base in support of HEDP and ICF will be strengthened by the development of a particle-based hybrid fluid-kinetic code named *CHIMERA*, which will be benchmarked to a wide range of experimental data from lasers and pulsed-power accelerators. To self-consistently construct the model, particle-based fluid dynamics algorithms (macroscopic and short-range ensemble effects) are added to an electromagnetic and kinetic particle code (microscopic and long-range discrete particle effects) since interactions between dynamically co-existing fluid and kinetic particles can be treated straightforwardly. The combination of fluid and kinetic treatments into a single simulation framework with electromagnetic fields while using sophisticated material and laser interaction models is an area with significant innovative research opportunities. The hybrid method naturally allows the retention of many effects that are beyond either of the individual traditional modeling methods alone. Therefore, since the new hybrid paradigm wields the benefits of both approaches, it will either provide new physics insight into areas wherein confidence is low (for problems where the physics of both are important) or reinforce areas wherein confidence is higher (for problems where one or the other approach is valid).

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

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**Unraveling Catalytic Pathways for Low Temperature Oxidative Methanol Synthesis from Methane**

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There is a need for processes to convert abundant natural gas resources into higher value chemicals and fuels. Our objective is to study and improve catalysts for the direct catalytic conversion of methane ($CH_4$), the primary component of natural gas, into methanol ($CH_3OH$), a useful intermediate for chemicals and fuels production. This research builds on the recent discovery of a single step catalytic process for this reaction at low temperatures and pressures using inexpensive earth abundant catalysts. The reaction promises to be more economical than current multi-step processes, but improvements in performance are needed. We will study structures and reactions on well-defined model surfaces and powders, accompanied by theoretical modeling, to unravel surface reaction pathways. In particular, we will identify key catalyst features that activate the stable methane molecule through 'soft' oxidative activation of C-H bonds with oxygen ($O_2$) and water ($H_2O$) co-reactants in order to enable selective conversion to the desirable methanol product. The project will exploit unique capabilities to study catalysts in reaction environments (*in situ*) using X-ray spectroscopy, electron imaging, and other *in situ* methods at Brookhaven National Laboratory, particularly at the National Synchrotron Light Source II (NSLS-II). The goal is to establish and experimentally validate design principles for improved catalysts for single step conversion to methanol and, more broadly, to enable controlled oxidative activation of C-H bonds.

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

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**Bringing Inorganic Carbon to Life: Developing Model Metalloenzymes for C1 Conversion Reactions**

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A primordial metabolic pathway for the conversion of inorganic carbon into cellular biomass uses a large, nickel-containing enzyme called carbon monoxide dehydrogenase (CODH)/acetyl coenzyme A synthase (ACS). This system fixes carbon dioxide ($CO_2$) into carbon monoxide (CO) at the CODH site. The carbon monoxide is then used to generate acetyl coenzyme A, a biological building block, through a key carbon-carbon bond forming step at the nickel site in ACS. Despite the significance of these processes in the context of energy conversion, the fundamental chemistry underlying these transformations has remained elusive, in part due to the complexity of the natural enzyme. To better understand the principles governing these biological processes, which represent one-carbon (C1) activation reactions, this project will develop functional models of CODH and ACS based on modifications to a small metalloprotein scaffold. Comprehensive characterization of these systems using advanced spectroscopic and biophysical techniques will reveal key elements responsible for conferring high levels of activity to the model systems, and this then can provide us with key insights into the mechanisms of the natural enzymes. Moreover, the principles learned from this research can be used to guide design of robust catalysts for efficient conversion of $CO_2$ and CO into liquid fuels.

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

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**First-Principles Understanding of Optical Excitations within Low-Dimensional Materials**

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An important unanswered question for the design of new solar energy conversion materials is how to control the motion of bound electron and hole pairs (excitons) formed upon optical excitation. The objective of this project is to utilize first-principles computational approaches to understand excitons within two-dimensional monolayers and heterostructures with the ultimate goal of designing new materials by modifying the chemical and physical structure on the nanoscale. The PI will study the thinnest possible materials that can be assembled, one-atom thick layers. These are candidates for next-generation energy conversion devices. Controlling the nature and migration properties of excitons is a challenge because of the complex relationship between electrons, lattice vibrations, defects, disorder, and interfaces. Current theoretical models aimed at understanding these phenomena are elaborate and complex or highly empirical, hindering the ability to predict and design new materials. Performing highly accurate density functional theory and many-body perturbation theory calculations, the PI will determine how to decompose these complexities into simple, tunable parameters that explain the effect of electron-electron and electron-phonon interactions on excitons. These studies will reveal patterns in material structure that will be used to propose physically motivated rules for more efficient energy conversion mechanisms.

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

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**Hidden Sectors from Cosmos to Colliders**

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The existence of some kind of particle-like dark matter constituting the dominant form of matter in our universe has been solidly established through multiple lines of evidence based on gravitational interactions between dark and visible matter. There is no evidence - as yet - that dark matter interacts with the Standard Model in any other way. This research program investigates discovery strategies for a broad and general class of hidden-sector dark matter theories where the present-day abundance of dark matter is determined by interactions among multiple dark fields and is not directly related to its interactions with the Standard Model. However, the possible cosmological histories of these dark sectors still depend on the size and structure of their interactions with the Standard Model: for example, are the interactions between the dark sector and the Standard Model ever strong enough to bring the two sectors into thermal equilibrium in the early universe? Is the lightest dark state stable, or does it decay to Standard Model particles? This research will systematically address these and related questions, establishing links between dark sectors' cosmic history and their interactions with the Standard Model and thereby providing new avenues to search for dark matter and other dark fields. It will also explore the important and complementary role played by the Large Hadron Collider (LHC) in furthering the search for dark sectors at the energy frontier, particularly through measuring properties of the Higgs boson. As the LHC continues to take data, searches for exotic decays of the Higgs boson and particles with macroscopic lifetimes will provide some of the most exciting avenues for discovery. Combining new search strategies at the LHC with new cosmic motivations for signals of dark sectors, this research aims to substantially extend prospects for understanding the origin and nature of dark matter by leveraging results from intensity, cosmic, and energy frontiers.

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

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**Extreme-Scale Stochastic Optimization and Simulation via Learning-Enhanced Decomposition and Parallelization**

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Stochastic optimization and simulation models are common in designing and operating complex service and engineering systems. Significant computational challenges may arise due to the use of high-dimensional data and the sequential nature of decisions made in response to newly revealed data. The objective of this research is to develop an efficient and unified framework that integrates machine learning with discrete optimization and risk-averse modeling. The models we consider represent a broad class of complex decision-making problems, where 0-1 or continuous decisions are made before and/or after knowing multiple and potentially correlated sources of uncertainties. Machine learning will be used to dynamically decide and prioritize computational procedures such as cut generation, branching, and bounding of the optimal objective. Furthermore, the research will shed new light on the traditional decomposition algorithms for high-performance computing. Application examples include distributed computer server scheduling, sensor deployment for monitoring critical infrastructures, and other decision-making capabilities arising from DOE missions in energy, environment, and national security.

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

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**Strange Mesons and Gluonic Excitations**

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In the standard model of particle physics, the interactions between the fundamental constituents of nuclear matter, quarks and gluons, are governed by the theory of Quantum Chromodynamics (QCD). A central goal of nuclear physics is to understand how hadrons, such as protons and neutrons, are formed from these underlying quark and gluon degrees of freedom. A hadron is primarily constructed from three quarks or a quark-antiquark pair; however, the theory of QCD allows for much more exotic configurations. One of the predicted exotic configurations is known as a hybrid meson, which contains an excited gluonic field in addition to the usual quark-antiquark pair. This project aims to search for and study these gluonic excitations using the Gluonic Excitation (GlueX) experiment at Jefferson Lab in Newport News, VA. The discovery potential of the experiment will be significantly extended by studying the quark flavor composition of the meson spectrum through the completion and use of an enhanced detector to identify mesons containing strange quarks. The unprecedented statistical precision of the data collected at GlueX will allow us to search for a pattern of light-quark hybrid mesons, providing new insight into the interactions that bind the fundamental quarks and gluons into the hadrons we observe in nature.

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

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**Rational Selection of Transition-Metal Oxide Electrocatalysts from Structure-Electronic Structure-Activity Relations: The Role of Defects, Strain, and Sub-Surface Layering**

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Electrochemical reactions between carbon monoxide, water, and oxygen can produce electricity and create high-valued chemicals. A properly designed catalyst will increase the speed and selectivity of these electrochemical reactions, making them more efficient and cost effective. The objective of this research is to establish scientific principles to enable the design of top-performing electrochemical catalysts. This research focuses on transition-metal oxides, a class of proven high-performing catalysts, whose surface atomic arrangements that are responsible for performance ('active sites') are not well understood. This project uses single-crystalline transition-metal oxides, prepared through advanced thin-film deposition with atomic-level precision, to reveal the nature of the active sites. Oxygen reduction and carbon-monoxide oxidation, the efficiency-limiting electrochemical processes in reformate and syngas fuel cells, will be evaluated for their defects, strain, and sub-surface layering. By revealing how these structural variables affect performance, molecular-level mechanisms and scientific principles will emerge that enable the design of top-performing catalysts. The final aim is to connect structural variables and chemical functionalities to provide a convergence between the microscopic degrees of freedom and macroscopic catalytic properties in transition-metal oxides. This final component will establish a design route toward future high-performing catalysts for fuel and chemical production from both fossil and renewable feedstocks.

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

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**Awakening the Sleeping Giant: Multi-omics Enabled Quantification of Microbial Controls on Biogeochemical Cycles in Permafrost Ecosystems**

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Large expanses of permanently frozen soils, called permafrost, are found in the Earth's polar regions. Arctic soils store large amounts of biomass and water from warmer periods in the history of the Earth that became preserved in permafrost during cooling and glaciation events. Permafrost soils contain a broad diversity of cold-adapted microbes, whose metabolic activity depends on environmental factors such as temperature changes that cause cycles of freezing and thawing in the soil. Microbial metabolism leads to decomposition of soil organic matter, substantially impacting the cycling of nutrients and significantly affecting the arctic landscape. However, the relationship between permafrost microbial properties and biogeochemical cycles is poorly understood. This project will use field experiments, laboratory manipulations, and multi-omics approaches to examine how microbial processes, biogeochemical transformations, and hydrology interact during permafrost thaw in different sites in Alaska in order to determine how these factors drive biogeochemical cycles in different Arctic soils. This project will lead to an in-depth understanding of the underlying microbial processes governing biogeochemical cycles in an environment relevant to DOE's mission.

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

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**Enhancing the Performance of Plasma-facing Materials through Solute-stabilized Nanostructured Tungsten Alloys**

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Plasma-facing materials (PFMs) in future fusion devices will be exposed to demanding operating conditions involving high heat fluxes, aggressive particle and neutron fluxes, and high stresses. Although tungsten has emerged as a promising candidate, there are several outstanding issues yet to be resolved, including high temperature stability, mechanical performance, and radiation tolerance. The aim of this research is to address these limitations in tandem by precisely tailoring the volume fraction, chemistry, and structural state of grain boundaries in tungsten. These novel materials, known as solute-stabilized nanostructured tungsten alloys, will be designed and screened through thermodynamic modeling coupled with *in situ* electron microscopy experiments. Select alloys will then be scaled via powder metallurgy processes to synthesize bulk materials for mapping structure-property-performance correlations. The insights established through this research will markedly enhance the state of tungsten alloys for fusion applications and, in turn, provide opportunities to validate their performance under relevant PFM conditions.

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

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**Nonequilibrium Phenomena in Plasmas in Contact with Liquids**

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Plasmas in contact with liquids are found in diverse applications, both established (e.g. electric welding, metallurgy, confining walls of fusion reactors) and emerging (e.g. water treatment, nanoparticle synthesis, biomaterials and medicine). The advancement of these applications and, potentially, of unforeseen ones requires cohesive fundamental understanding of plasma-on-liquid interactions. These interactions present two distinct but interdependent types of nonequilibrium phenomena: (1) *kinetic* (microscopic, across the interface), involving complex multiphase physical and chemical kinetics; and (2) *dissipative* (macroscopic, along the interface), comprising superficial transport that is often conducive to instabilities and to the emergence of collective effects such as the spontaneous formation of spot patterns. Kinetic nonequilibrium is responsible for some of the remarkable characteristics of plasma processes such as high selectivity and energy efficiency. In contrast, dissipative nonequilibrium is often detrimental, limiting process uniformity and throughput. The project will establish a computational modeling and simulation method for the study of plasmas in contact with liquid electrodes. The method is based on a Heterogeneous Variational Multiscale approach that uses macroscale and microscale models consistently and complementarily: The macroscale model provides the backbone for the description of distributed fields, while the microscale model describes detailed kinetics locally. The approach is designed to achieve the high model fidelity *and* high numerical accuracy required to concurrently capture kinetic and dissipative nonequilibrium in application-relevant configurations. The method will be used to determine the parameters controlling stability and the emergence of collective behavior at the plasma-liquid interface and to characterize the role and interrelationship of these parameters with the rate of plasma-driven electrolysis.

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

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**Unveiling the electroweak symmetry breaking mechanism at ATLAS and at future experiments with novel silicon detectors**

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The discovery of the Higgs boson at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland has confirmed the mechanism for the origin of masses in the Standard Model (SM), providing key insights into electroweak symmetry breaking but, at the same time, posing several new questions. Despite direct searches, no compelling evidence for new physics signals at the LHC has yet been observed. Precision measurements of fundamental predictions of the SM are an effective way to identify signatures that may lead to a paradigm change in particle physics. This research program focuses on the analysis of data from the ATLAS experiment at the LHC to comprehensively study interactions between the Higgs and W and Z bosons. Any discovery of deviations from SM predictions in such vector boson fusion and scattering processes can signal new physics at very high energies not directly accessible by the LHC. This method of probing physics beyond the SM can become even more constraining through the high luminosity upgrade of ATLAS currently being carried out for longer-term operations at the LHC that are planned to begin in 2026. This project aims to advance the upgrade of the ATLAS silicon detectors using novel, state-of-the art technology capable of precision tracking and timing that will help distinguish primary collisions from background events. These developments can have profound impact for the design and development of future instrumentation for use in high radiation environments.

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

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**Towards Precision Cluster Cosmology with LSST**

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Only ~5% of the Universe is in a form of matter familiar to us - planets, stars, gas, photons, and neutrinos. The vast majority of the Universe is in the form of dark matter (~25%) and dark energy (~70%). While dark matter is a form of matter that does not interact with us apart from gravity, dark energy is even more mysterious - it describes the puzzling fact that the expansion of the Universe is accelerating rather than slowing down due to gravity. This is akin to throwing a ball up in the air and, after it initially slows down, seeing it accelerate upwards. Solving the puzzle of dark energy requires precision measurements of the expansion history and evolution of structure of the Universe. Clusters of galaxies provide particularly powerful measurements of the Universe. The number of clusters as a function of mass and evolution of this function with time are very sensitive to the details of the inner workings of the Universe: if there is more dark matter, clusters grow faster; if there is more dark energy, clusters grow slower; if our understanding of gravity is incorrect, clusters grow differently than expected. The challenge for cluster cosmology lies in relating cluster observables (such as the number of galaxies, the X-ray luminosity, or the shadow cast on the Cosmic Microwave Background) to the actual mass of the cluster. The most promising technique to determine the absolute mass calibration of clusters is through weak gravitational lensing. The Large Synoptic Survey Telescope (LSST) will revolutionize our understanding of many aspects of the Universe, and, in particular, it will be the definitive ground-based weak-lensing survey. The purpose of this project is to develop and test techniques necessary to utilize LSST weak-lensing capabilities for cluster cosmology and to apply these techniques to targeted pre-cursor and early LSST data. The results of this project will enable cluster surveys to harness their tremendous statistical potential and to be a leading probe of cosmology in the next decade.

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**Designing Metastability: Coercing Materials to Phase Boundaries**

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Transition metal oxides often possess metastable and non-equilibrium states that can interact across multiple length scales to give highly desirable emergent properties ranging from metal-insulator transitions to superconductivity to multiferroicity. Due to the strong coupling between the spin, charge, orbital, and lattice parameters in these materials, even small changes to the underlying crystal lattice can have dramatic impacts on behavior. Thus, effective control over lattice parameters not only facilitates the understanding of multiple interactions in strongly correlated systems, but it can also be used to create new phases and emergent behaviors. This project will apply low energy ion implantation as a means of strain doping transition metal oxides to create, understand, and utilize previously inaccessible structural distortions to obtain new and highly controllable functional properties. Central to this effort is the ability to apply these distortions across vastly different length scales, which will allow comparative studies on top-down and bottom-up approaches. This will give a deeper understanding of how global structural changes influence local competing phase stabilities and will provide much-needed insight into the role of local distortions on emergent meso- and macroscopic phenomena. The specific aims are to design new metastable ferroic states; to understand local inhomogeneity's role in the formation of emergent phases; and to understand the mechanisms of structural distortions under strain doping. This work will deliver insights into the structure-function relationship of transition metal oxides while providing a means of designing multiple coexisting but dissimilar properties at the nanoscale in single crystals.

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

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**Determining the Genetic and Environmental Factors Underlying Mutualism within a Plant-Microbiome System Driving Nutrient Acquisition and Exchange**

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The importance of symbiosis is highlighted in plant-microbe interactions where a microbe can acquire nitrogen from the air (nitrogen fixation) and provide it to the plant in exchange for sugars necessary for growth and metabolism. However, such beneficial interactions can shift to commensal (neutral) or even antagonistic, depending on genetic and environmental factors that are poorly understood. This project will provide a fundamental quantitative understanding on the role of plant host and microbial genetics on maintaining beneficial symbiosis during environmental perturbations. With that fundamental understanding, it will be possible to select host and microbes with the appropriate genetic makeup to manipulate symbiotic relationships adapted to different environmental conditions. The study systems will be a community composed of the moss Sphagnum and nitrogen-fixing cyanobacteria because of the genomic resources available for these organisms and their suitability for advanced genomic and imaging technologies. This effort will identify the genes and metabolic functions involved in nutrient exchange between the interacting plants and microbes and determine how symbiotic systems respond to environmental perturbations in laboratory and field settings. Ultimately, fundamental knowledge of the genetic and environmental factors driving plant and microbial nutrient exchange will enhance our understanding of nutrient cycling in natural systems and provide the foundation to improve bioenergy crop productivity in more complex biological communities.

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

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**Enabling Beyond Forward Simulation for Predictive Multiscale Modeling**

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This project is focused on the development of predictive modeling and simulation capabilities for the science and national security missions of the Department of Energy. Many problems in materials science, subsurface flow and mechanics, and magnetohydrodynamics are best described by multiphysics and multiscale models. These problems are challenging to simulate because they incorporate detailed physical interactions across a wide range of length and time scales. The proposed research will pursue mathematically rigorous and computationally efficient approaches for making accurate predictions about the properties and behavior of realistic, complex multiphysics applications. The proposed advances in numerical discretization, uncertainty quantification, data assimilation, and model adaptation will be integrated to enable greater predictive skill. In particular, these research developments will support high-consequence decision-making capabilities that benefit a wide range of DOE-mission applications.

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

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**Genomes to ecosystem function: Targeting critical knowledge gaps in methanogenesis and translation to updated global biogeochemical models**

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Natural freshwater temperate wetland systems currently represent the largest natural source of atmospheric methane but are relatively understudied using systems biology tools (e.g. meta-omics) compared to other high producing methane systems (e.g. peat, tropical, or reconstructed wetlands). Using field investigations at the NOAA operated sentinel site on Lake Erie, methane producing activities and responses to geochemical conditions will be determined along seasonal and spatial gradients (Objective 1). Here, a combination of high-throughput activity and gas measurements, combined with high-resolution systems biology and analytical methods, will provide in depth knowledge of the microbiological, chemical, and physical constraints on methane production in wetlands. Using laboratory microcosms, the formation of anoxic microsites and their capacity to facilitate methane production in wetland soils will be simulated (Objective 2). This objective will validate the findings from the field investigations, offering a more controlled environment for teasing out the role of different yet interrelated variables. Lastly, these field and laboratory data will be used for multi-scale, process-level evaluation of an ecosystem biogeochemical model that accommodates these newly identified processes and parameterizes representation of these processes along relevant environmental gradients (Objective 3). This research will identify multiple interacting geochemical, ecological, and metabolic constraints that are poorly understood, oversimplified, or missing in global biogeochemical methane models. This proposal targets the role of oxygen limitation on methane processes in soil domains, to improve reactive transport models of microbial carbon cycling across terrestrial-aquatic soils and generate data on nutrient cycling activities in Great Lake wetlands. This information could provide new insights into the microbial controllers of Lake Erie eutrophication.

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

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**Optimization of Liquid Argon TPCs for Nucleon Decay and Neutrino Physics**

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The question of why there's a predominance of matter over antimatter in our universe is one of the greatest unsolved mysteries of science. The US-hosted international Deep Underground Neutrino Experiment (DUNE), scheduled to start collecting data in the mid-2020s, aims to explore this mystery through the search for two rare but necessary conditions for the imbalance: evidence that some processes produce an excess of matter over antimatter and a sizeable difference in the way matter and antimatter behave. The DUNE experiment will look for signs of these conditions by studying proton decays and neutrino oscillations using four massive 10-kiloton detectors. The detectors, located 1.5 km underground in caverns excavated at the Sanford Underground Research Facility in Lead, South Dakota, will receive a high-intensity neutrino beam generated at Fermilab in Illinois, 1,300 km away. This project aims to optimize the performance of the Liquid Argon Time Projection Chambers (LArTPCs) that are at the heart of these detectors to fully realize their potential to track and identify particles in three dimensions, with a particular focus on sensitivity to proton decay. This research activity will establish a hardware calibration system to aid in the robust extraction of signals from low-noise cold electronics; develop software for 3D reconstruction of complex events; analyze data from the prototype experiment (ProtoDUNE) to verify the expected performance; and optimize the DUNE far detector design to enhance its sensitivity to proton decay and neutrino physics. The research will strengthen our understanding of the LArTPC technology and push the capabilities of LArTPC detectors beyond their current design goals.

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**Understanding and Controlling Aggregation Processes in Mixed-Molecular Solids**

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This project will develop structure-property relationships between molecular properties and nanometer-scale structure (i.e. morphology) of solid molecular mixtures and also between morphology and macroscopic material properties. Solids formed from mixtures of different molecules are important for a wide variety of applications including organic light emitting diodes (OLEDs), high-resolution photoresists, charge-carrier doping of organic electronics, and organic photovoltaics. In most cases, these molecular mixtures are expected to perform best when mixed perfectly to the molecular level; however, many blends exhibit significant phase segregation and clustering. Previously existing methods to measure morphology of molecular blends have either resolution or chemical discrimination capabilities insufficient to understand structure at nanometer length scales. Recently developed atom probe tomography techniques for analyzing organic molecular materials have an unparalleled combination of high-resolution three-dimensional imaging and sensitive molecular mass discrimination capabilities to measure morphology at the nanometer scale. This research will compare the nanometer-scale morphology of molecular solids to molecular cohesive forces to understand why materials phase-segregate and to learn how to prevent segregation by creating thermodynamically stable solid solutions. Morphologies of OLED materials will then be compared to their light emission properties to test and validate hypotheses on morphology-materials property relationships. The results will improve efficiency of OLED lighting and displays, reducing energy consumption in homes and mobile devices; conclusions will also be generalized for a broad impact to other molecular mixtures.

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