Diagonalization Solvers for Electronic Collective Phenomena in Nanoscience

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This project aims to advance theoretical modeling capabilities to understand collective phenomena at the nanoscale in strongly correlated electronic materials, including Mott insulators and high temperature superconductors, through the use of the density matrix renormalization group (DMRG). Studies will focus on (1) the time-dependent electron transport in Mott insulators (e.g., copper oxides), particularly on nano-patterned structures; (2) the temperature dependence of the collective orders, including charge, spin and orbital orders, of superconductors and correlation with critical temperature; and (3) combining dynamical mean-field theory with DMRG to study emergent phenomena at the nanoscale and nanoscale inhomogeneities in high-temperature superconductors. Fundamental understanding of both the correlated behavior of conduction electrons and the interaction between electrons and lattices in these materials, in which the "standard one-electron model" of metals breaks down, can provide insights for the development of new materials and structures with enhanced functionality for solar cells, solid-state lighting, and superconductor power transmission. Computer codes will be made accessible to the scientific community as part of the user-driven program at the Center for Nanophase Materials Sciences.

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

Templated Bottom-Up Synthesis of Semiconducting and Nanostructured Graphene Materials

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The objective of this project is to develop a fundamental understanding of how nanostructured graphene materials can be rationally synthesized from the bottom up with atomic precision and exceptional properties. The research will focus on studying the nucleation and kinetics of graphene growth in confined patterns and channels, controlling the crystallinity of the graphene materials, and learning the mechanisms that determine the atomic ordering at their edges. The understanding that is gained will result in novel high-performance materials that could impact a number of energy technologies of national importance including low-energy semiconductor electronics, the efficient generation of electricity from solar and infrared light, and the high-density storage of energy in batteries.

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

Spatially Resolved Ionic Diffusion and Electrochemical Reactions in Solids: A Biased View at Lithium Ion Batteries

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The overarching goal of this project is to understand the ionic diffusion and electrochemical reactions in Lithium-ion batteries from the length scale of single microstructural elements to the macroscopic device level. A novel Electrochemical Strain Microscopy (ESM) probe with 100 fold better resolution than other probes will be used along with electrical and structural battery characterization techniques for macroscopic devices in combination with advanced theoretical modeling. The research will shine light on the complex interplay of ionic and electronic transport in battery materials and their correlation with the structural material properties. This will result in new tools to characterize energy storage materials and enhance the fundamental understanding of the nanoscale processes that define a battery.

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

In situ Measurements of Heterogeneous Reactions on Ambient Aerosol Particles: Impacts on Atmospheric Chemistry and Climate

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Heterogeneous reactions, occurring between gases and aerosol particles, alter the climate-relevant properties of aerosols and catalyze reaction processes that are energetically unfavorable in the gas phase. The objective of this project is to identify the mechanistic drivers that control the variability in heterogeneous aerosol processes through direct in situ measurement of reaction kinetics on ambient aerosol particles. The heterogeneous reactivity of complex, *ambient* aerosol particles will be investigated to determine: (1) how laboratory investigations of heterogeneous processes conducted on model, simple systems represent the real atmosphere, (2) the impact of heterogeneous processes on ambient particle hygroscopicity and optical properties, and (3) the uptake kinetics for a host of atmospheric trace gases as a function of particle composition and phase. The results of these investigations will be used to directly improve the representation of heterogeneous processes in global climate models.

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

Towards Predictive Simulations of Soot Formation: From Surrogate to Turbulence

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The aim of this project is to fill the gap in the present understanding and modeling of soot formation both in laminar and turbulent flames. The project focuses on the combustion of surrogate fuels comprised of several chemical species in contrast to current single-species models. A current state-of-the-art chemical model will be extended with additional components often found in surrogates. The inner structure of soot particles will be investigated as a means to gain insight into soot inception, growth, and oxidation via the development of a nested hierarchy approach combining Quantum Chemistry, Molecular Dynamics, and Monte Carlo simulations. The newly improved chemical and soot models will be incorporated in Direct Numerical Simulations of turbulent sooting flames and validated in turbulent jet diffusion flames. The outcome is expected to be a major leap in the development of predictive models for the combustion of transportation fuels, the formation/oxidation of soot, and Large Eddy Simulations. The impact of the research goes far beyond soot formation. It is relevant to the formation of all other nanoparticles (SiO_2, TiO_2, and AlO_3) as well as other slowly evolving processes in turbulent flows (CO, NO_x).

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

Energetics of Radiation Tolerant Nanoceramics

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Nanostructured materials are likely to play a large role in future nuclear reactors and radioactive waste storage due to their strength and potential resistance to structural damage from radiation. However, this potential is hindered by significant gaps in the understanding of interfaces' properties and their role in the overall performance of the nanocrystalline structures. The lack of reliable thermodynamical data of nanomaterials makes it extremely difficult to predict and fully exploit nanomaterials' properties in high-radiation environments, which is one reason the stability of the nanomaterials is still a big unresolved question. The goal of this project is to investigate two nano-scale materials [the aluminate based spinels (MAl_2O_4, M = Mg, Ni, or Zn), and zirconia based materials (ZrO_2 doped with Mg, Y, or Ca)], and establish the link between composition, interface thermodynamics, and radiation resistance to enable a better understanding of the nature of enhanced performance in nanocrystalline ceramics. Thereafter, we will exploit the achieved knowledge as a foundation to design a new nanocomposite ceramic capable of withstanding high radiation exposition by using elements of interface engineering on a thermodynamic basis.

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

Rigid Biopolymer Nanocrystal Systems for Controlling Multicomponent Nanoparticle Assembly and Orientation in Thin Film Solar Cells

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This project seeks to direct the assembly of nanoparticles into three-dimensional crystals of any desired configuration and crystallographic orientation using tunable DNA interactions. Despite the wealth of nanoscale materials that may benefit many current and future solid state technologies, difficulties in controlling and directing their placement and orientation into desired architectures has led to significant impediments in their applicability. Biological systems can form such structures using their inherent molecular information as guides to assemble organic and inorganic materials into highly organized structures ordered at multiple length scales. Using bio-inspired strategies, the research will control the two- and three-dimensional arrangement of semiconductor nanocrystals into a seed layer that can nucleate successive layers of single nanocrystals with long-range order and tunable crystallographic orientations. This work will elucidate how particle-DNA interactions influence nanoparticle crystallographic orientation, how nanoparticles on patterned arrays of biomolecules can nucleate long-range order, and how to synthesize 2- and 3-D superlattice arrays of DNA conjugated semiconductor nanocrystals.

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

Prediction of Thermal Transport Properties of Materials with Microstructural Complexity

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This project will focus on overcoming the major obstacle standing in the way of progress in dynamic multiscale simulation, the lack of a concurrent multiscale method that allows elastic waves, heat and defects to pass through the atomistic-continuum interface. This project aims to (1) establish a concurrently coupled atomistic-continuum methodology that can overcome this obstacle and that can be used to design and optimize materials with microstructural complexity for desired properties and (2) demonstrate the methodology through predicting the mechanical and thermal transport properties of thermoelectric materials and comparing the predictions with experimental measurements.

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

Search for Holographic Noise from the Planck Scale

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This grant will enable the construction and operation of the Fermilab Holometer, the world's most sensitive microscope for detecting tiny spatial position jitter, correlated between neighboring objects. The holometer is a new, modest-scale double Michelson interferometer device, optimized to isolate and measure a recently predicted position noise spectrum arising from a Planck scale information bound implied by the holographic principle in black hole thermodynamics. Very few probes of quantum effects at the Planck scale are known, and the present search for holographic noise represents one of the most cost effective ways to probe this extremely high energy scale. Should the holometer successfully detect the predicted noise spectrum, this detection will represent a first glimpse of the microphysics controlling the fundamental structure of space and time. The nature of this new physics can be elucidated with reconfigurations of the holometer and eventually with more elaborate future devices. If no exotic noise is detected, even at levels well below the predicted magnitude, a set of theoretical ideas of Planck scale information encoding will have been put to rest. In either case, the holometer represents a rare and valuable probe of Planck scale microphysics and may answer some profound questions about our possibly holographic reality.

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

Natural and Primary Catalysts for Molten Cellulose Pyrolysis to Targeted Bio-oils

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The use of lignocellulosic biomass as an alternative reduced-carbon feedstock processed within high temperature thermo-chemical catalytic reactors is hindered by a limited fundamental understanding of the role of catalysts that naturally exist within biomass. The natural catalysts of biomass including the inorganic ions necessary for biological function as well as the oxides obtained from soils have been shown to exhibit significant influence during pyrolysis. The objective of this research is to study the catalytic chemistry of naturally occurring inorganic materials within high-temperature molten carbohydrates to understand their effect on the selection of volatile organics and gases produced during pyrolysis. The role of inorganic catalysts on biopolymer decomposition within the high temperature (> 400 °C), intermediate condensed phase will be interpreted through a targeted study of specific molten carbohydrate reactions including ether hydrolysis, retro-aldol condensation, and dehydration, which select for the competing catalytic pathways of product formation. The reaction intermediates and oxidation state of natural catalysts within the molten liquid will be characterized with the use of a new experimental liquid sampling technique capable of extracting and quenching molten carbohydrate/catalyst mixtures.

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

Taus and the Trigger for Discovery at ATLAS

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The Large Hadron Collider (LHC) at CERN brings a new energy frontier to collider physics with exciting opportunities for discovery. This work focuses on the search for the Higgs boson in the ATLAS (A Toroidal LHC ApparatuS) experiment and takes advantage of the channels with an enhanced coupling of Higgs to tau leptons. Tau leptons, as members of the least-explored 3rd generation and as the most massive leptons, play an important role in many new physics searches. The discovery of the Standard Model (SM) Higgs boson, the supersymmetric charged and neutral Higgs bosons, a theorized Z' boson, or a heavy 4th generation neutrino can depend primarily on decays involving tau leptons in many possible scenarios where the coupling of the new physics to tau leptons is enhanced over couplings to electrons and muons. This work will optimize the reach of the ATLAS experiment toward discovering new physics by taking full advantage of event signatures with hadronically decaying tau leptons and maximizing the efficiency of the tau lepton trigger.

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

In-Situ TEM Observations of Degradation Mechanisms in Next-Generation High-Energy Density Lithium-Ion Battery Systems

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This project seeks to characterize nanoscale processes associated with the degradation of next-generation high energy density lithium-ion battery electrodes via in-situ transmission electron microscopy. Dynamic processes active in the electrodes, electrolyte, and intervening interfaces, which are chemical, electrical, and mechanical in nature, have been correlated with capacity fade in lithium ion batteries. However, without direct in-situ observation of these degradation mechanisms with high spatial and temporal resolution, it remains difficult to understand and predict how these processes initiate, propagate, and interact. This research will develop the experimental techniques necessary for investigating electrochemical systems by in-situ transmission electron microscopy and will provide a framework for distinguishing and limiting electron-beam effects that could potentially influence experimental results. This project aims to develop a fundamental understanding of degradation mechanisms in representative environmental conditions using commercial electrolytes and electrode designs that mimic commercial electrodes and in idealized solid-state batteries that will enable in-situ atomic-resolution imaging.

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

Electronic and Ionic Conductors from Ordered Microporous Materials

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This project aims to develop rational pathways towards the synthesis of ordered microporous materials with tunable electron and ion transport properties. Two convergent approaches will be used. In one, research will be carried out to modulate the electronic structure of nonconductive but highly porous metal-organic frameworks (MOFs). By combining the synthesis of electronically active bridging ligands with rigorous topological design principles, a cluster-directed approach towards porous and conductive MOFs will be developed. In the same context, new topochemical ion metathesis reactions are proposed for the synthesis of MOF-based lithium and sodium ion conductors. The new MOF-derived materials will display unique, tunable multifunctional properties with potential impact in electrical energy storage, electrocatalysis, and ionic conductors, among others.

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

An Enabling Computational Framework for Uncertainty Assimilation and Propagation in Complex PDE Systems: Sparse and Low-Rank Techniques

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This project aims to develop a set of new theories, algorithms, and computational tools that enable ultra-scalable representation and propagation of high-dimensional uncertainties to circumvent the issue of curse-of-dimensionality. The research components are motivated by the fact that highly scalable algorithms are needed to achieve exascale performance for uncertainty quantification and predictive simulation at extreme scales. Although these developments are generic and applicable to a wide range of high-dimensional, complex, stochastic, partial-differential-equation (PDE) systems, this research effort will focus on predictive simulation of high-energy-density lithium batteries. To create knowledge about the precise failure mechanisms of these batteries and ultimately predict their performance and reliability, a truly data-driven, multi-scale, multi-physics framework is needed that allows studying (i) dominant sources of uncertainty in the governing physical models at all scales of relevance and (ii) the interface between the interchanging physics and scales. The impact of the planned mathematical and numerical advancements in prediction of high-dimensional uncertain systems will be broad across areas of engineering and science such as climate modeling, fusion energy, combustion, and nanoscience, among others.

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

Meson Spectroscopy from Quantum Chromodynamics

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The basic building blocks of the atomic nucleus, protons and neutrons, are constructed from quarks, bound together by gluons in such a way that they are never seen in isolation. Quarks and their anti-particles can also pair up in short-lived states called mesons; the goal of this project is to predict the theoretical properties of these mesons. Although we know the fundamental theory of quark and gluon dynamics to be solved, “Quantum Chromodynamics” (QCD), exact mathematical solution of the theory eludes us. Our best available tool for studying QCD is “Lattice QCD” (LQCD), a numerical solution of the theory with controllable approximations. This research project will use novel LQCD techniques to predict the masses and quantum numbers of mesons, their internal quark-gluon structure, their decays into other mesons, and their couplings to photons. A major emphasis will be the predicted properties of “hybrid mesons,” hypothetical exotic particles in which the usual quark-antiquark pair is accompanied by an excitation of the gluon field that binds them. This project will complement a planned search for hybrid mesons by the Gluonic Excitation Experiment (GlueX) at the Thomas Jefferson National Accelerator Facility.

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

Engineering Robust Hosts for Microbial Biofuel Production

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Microbes contain a vast diversity of metabolic pathways that can be subtly tweaked and redesigned for the conversion of biomass to biofuels compounds. Next-generation biofuels such as short-chain hydrocarbons are particularly attractive target molecules since they would be compatible with existing engines and infrastructure. However, high levels of these compounds are often toxic to the microbes synthesizing them, limiting the potential rate and yield of industrial biofuel production. The objective of this research is to understand hydrocarbon tolerance mechanisms used by microbes inhabiting natural hydrocarbon seeps or oil-contaminated sites, searching genome sequences of these organisms for efflux pumps and other molecular machines that microbes use to separate toxic hydrocarbons from their delicate biological systems. Promising candidates will be introduced into biofuel synthesizing strains of E. coli and tuned for optimal gene expression to determine if it is possible to engineer strains with enhanced tolerance to hydrocarbons and improved efficiency of overall synthesis.

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

Quantum Control of Spins in Diamond for Nanoscale Magnetic Sensing and Imaging

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The goal of this research is to develop a magnetic field imaging technique with nanoscale resolution that would allow for non-invasive, non-destructive probing of a variety of important physical phenomena such as quantum tunneling in single molecule magnets and quantum bits encoded into spins in quantum dots. Diamond single spin magnetic sensors are a highly promising material platform featuring high magnetic field sensitivity, nanometer spatial resolution and the important ability to operate under ambient or harsh environmental conditions required to study many material systems. The proposed work will take a multi-faceted approach toward improving the accuracy, sensitivity and robustness of this platform through a unique combination of fundamental investigations into quantum control and precision quantum metrology coupled tightly to innovative design, sophisticated nano-fabrication and advanced measurement techniques.

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

Large Dynamic Range Beam Diagnostics and Beam Dynamics Studies for HIgh Current Electron LINACs

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The goal of this project is to advance the development of large-scale LINAC (linear particle accelerator) based fourth-generation light sources with high average current by gaining an understanding of electron beam halo formation processes and developing methods to control the halo. The project aims to develop beam diagnostic techniques for characterization of the electron beam parameters with dynamic range much higher than used now. One goal is the measurement of the longitudinal and transverse phase space distribution with a dynamic range of about 10^6. Such measurements will be used for experimental investigation of halo formation and its evolution through the accelerator. Another goal is to develop beam optics solutions to control and manage the beam halo such that it would not be a limiting factor for the next-generation LINAC based light sources. The program also aims to benchmark machine design codes in terms of their ability to describe the beam halo evolution. It is envisioned that better understanding of halo formation and evolution will contribute significantly to the performance of future light sources.

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

Many-body effects in transport and energy transfer

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The goal of this project is development of theoretical approaches capable of treating open molecular systems that are far from equilibrium. These include radiatively driven molecular electronic devices, nanoscale motors, and molecular-scale systems for control of chemical reactivity and energy transfer. Many-body effects, induced by electron-electron, electron-vibron, and excitonic interactions, are essential in predicting the response of these systems to external stimuli (bias, gate voltage, light sources). Although quantum chemistry has developed methods for dealing with correlated many-electron effects within the context of isolated molecules, ab initio calculations on open molecular systems mostly employ methods formulated within an effective single-electron picture. Approaches developed within the project will introduce established methods of quantum chemistry into the realm of molecular-scale electron transfer. This will provide a solid background to treat molecular correlation with high rigor (inaccessible by standard techniques in use today), incorporate molecular spectroscopy and non-adiabatic dynamics into the consideration, and develop practical schemes to account for system-bath correlations (e.g. Kondo effect). Developed schemes will be validated on simple models and then developed into practical computational approaches for realistic simulations.

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

Precision Physics and Searches with Top and Bottom Quarks

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The aims of this project are (1) to measure with high precision how top quarks interact with bottom quarks in the Standard Model of particle physics and (2) to search for new heavy particles that decay into top and bottom quarks. We propose to use the large available data from Fermilab's Tevatron proton-antiproton collider and the high-statistics data from CERN's Large Hadron Collider (LHC) proton-proton collider to comprehensively exploit the different production mechanisms and conditions in the two colliders. Final states with top and bottom quarks provide a promising avenue to look for physics beyond the Standard Model because top quarks can couple easily with new heavier particles or exhibit anomalous couplings. Additionally, this project aims to develop new electronics to read out the light signals from the hadronic calorimeter detector in the Compact Muon Solenoid (CMS) experiment.

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

Optical Manipulation and Detection of Emergent Phenomena in Topological Insulators

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The goal of this project is to develop short-pulse laser-based experimental tools to probe the ultra-fast electron dynamics of topological insulators. Topological insulators exhibit a newly discovered property of matter where surface electrons have exceptional conducting properties distinct from the non-conductive nature of the bulk insulator material. This project will develop advanced optical spectroscopy along with electron spectroscopy and diffraction, all based on ultrafast laser pulses as the initial excitation source. The techniques will be developed with the goal to observe the time-resolved signature of quantum interactions and order in topological insulator materials.

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

Extended MHD Modeling of Nonlinear Instabilities in Fusion Plasmas

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The principal objective of this project is to computationally model global dynamics in fusion plasmas. Tokamaks are the most promising devices for achieving sustained magnetic confinement of fusion plasmas. Such plasmas are typically modeled using magnetohydrodynamics (MHD), which treats a plasma as an electrically conducting fluid interacting with a self-consistently generated magnetic field. The interesting and relevant plasma regimes in these devices are weakly collisional, so it is important to extend the resistive MHD model to take into account additional physics such as the effects of the Hall current and electron pressure tensor, including anisotropic and off-diagonal terms. This research will apply extended MHD computational models to complex three-dimensional geometries such as tokamak and reversed-field pinch (RFP) configurations. The goal is to investigate the nonlinear dynamics of plasma instabilities in tokamaks and RFPs. Examples are the impact of toroidal coupling on the nonlinear evolution of the m=1 Hall-resistive kink instability in a tokamak, with potential secondary ballooning instabilities, and the dynamo effects caused by Hall currents and vortical flows generated at multiple unstable rational surfaces in an RFP. This work also has potential applications to space plasma physics phenomena like, e.g., magnetospheric substorms. The project contains a substantial effort to verify and validate extended fluid models by benchmarking with analytic theory and other computational codes, as well as comparison to observations from fusion and magnetic reconnection plasma experiments.

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

Interfacial Electrocatalytic Processes from First Principles

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The objective of this research is to develop computational models for enhanced understanding of chemical and physical processes at electrode/fluid interfaces. Many present and future energy and environmental technologies, including electrocatalytic production of electricity, electrocatalytic synthesis of fuels, pollution abatement, and energy storage and corrosion in metal air batteries, are sensitively dependent on chemical and physical processes that occur at the boundary between solid electrodes and liquid electrolytes. To understand these processes at an atomic level and to improve the performance of the associated technologies, quantum chemical computational models are of tremendous value. To develop such models for the formidably complex environments near solid-electrolyte interfaces, this project exploits the significant insights that may be gained from first-principles studies on analogous catalytic and physical processes at solid/gas interfaces. By combining these models and insights with new descriptions of uniquely electrochemical effects, such as the interaction of solvated charges with adsorbed catalytic species, the work will advance fundamental understanding of chemical and physical processes at electrode surfaces. This understanding will ultimately contribute to the continued development of technologies, ranging from fuel cells to batteries, that depend on such fundamental knowledge.

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

Investigation of radiation damage tolerance in interface-containing metallic nano structures

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The objective of this research is to obtain a fundamental understanding of interfaces in their role as helium sinks in irradiated metallic microstructures. Radiation damage and the associated production of helium in metals lead to degradation of a material's strength during the lifetime of nuclear reactor components. The research will use a suite of nanoscale characterization and testing techniques, as well as computational tools, to isolate and understand the effects of specific tailored interfaces and deformation mechanisms on the degradation of material properties. The elucidation of these mechanisms will give insight into the requirements for advanced materials for current and next-generation nuclear reactors.

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

Understanding Photochemistry using Extreme Ultraviolet and Soft X-Ray Time Resolved Spectroscopy

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Chemical reactions can be described as changes in the electron distribution of a molecule leading to bond formation and cleavage. A complete understanding of a chemical reaction requires monitoring the time-evolving distribution of valence electrons and the complex interplay of the electrons with the nuclei on their natural time and length scales. The experimental method planned for this work will use ultrashort light pulses in the extreme ultraviolet and soft x-ray spectral range. These light probes deliver sub-nanometer spatial resolution, femtosecond temporal resolution, and element sensitivity. The experiments will be performed on organic molecules containing transition metals at laboratory-based laser high harmonic sources and at the Linac Coherent Light Source (LCLS). The results of this research program will enable a better understanding of, and possibly control of, photocatalytic reactions such as light-harvesting at the level of electrons.

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

Search for Weakly Interacting Dark Matter with Liquid Xenon

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The nature of the mysterious dark matter is one of the most fascinating questions in fundamental physics today. Although its existence is convincingly demonstrated by a host of cosmological and astrophysical studies, there is no known fundamental particle that can account for the properties of dark matter. Many new physics models, however, include stable, weakly interacting massive particles (WIMPs), which are promising dark matter candidates. If the dark matter is indeed composed of WIMPs, then it follows that the Milky Way's dark matter halo could be directly observed by searching for its extremely rare interactions with the atomic nuclei in a terrestrial detector. We will search for these interactions using liquid xenon as our target material. Our search will initially take place within the context of the Large Underground Xenon (LUX) experiment, which is currently being commissioned at the Sanford Laboratory in Lead, South Dakota. The LUX experiment is expected to be the most sensitive WIMP search ever performed and will improve upon current experiments by more than an order of magnitude. We will also develop new experimental techniques to reduce backgrounds and improve the reliability of liquid xenon technology in anticipation of the ambitious dark matter experiments which will supersede LUX in the next three to five years.

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

Molecular and Material Approaches to Overcome Kinetic and Energetic Constraints in Dye-Sensitized Solar Cells

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The aim of this project is to use a fundamental understanding of the kinetic processes within a dye-sensitized solar cell to move the design of this cell into newer and better regimes for assembly and performance. The efficiencies of present forms of this cell reached a plateau twenty years ago. This research intends to remove the limitations that have impeded progress since that time. In this project, concerted changes will be made in the active chemical elements of the cell through the study and control of the electron transfer kinetics of the reactant dyes and regenerating agents and through a reconstruction of the mesoscopic architecture of the substrate metal oxide electrode. Through a fundamental understanding of both homogeneous and heterogeneous electron transfer theory, new chromophores, solvents, and current carrying regenerating molecules will be selected and studied to define the limiting kinetic steps and processes within this complex system. As a perturbation upon these kinetics, novel designs for the nanometer-sized architectures of the metal oxide anode will be developed and synthesized, and their efficacy as a component in a dye sensitized system will be established and analyzed.

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

Crystallization-driven assembly of conjugated-polymer-based nanostructures

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The goal of this project is to use crystallization of electronically conducting (conjugated) polymers to fabricate well-defined crystalline building blocks of nanometer-scale dimensions. These materials will then be assembled into photovoltaic devices with optimized structures, and therefore improved efficiencies, in a cost-effective manner. It is well known that conjugated polymers often crystallize into nanowires or fibrils, i.e., one-dimensionally extended crystals with micrometer-scale lengths and nanometer-scale widths and thicknesses. The project will employ crystallization of a model conducting polymer, poly(3-hexyl thiophene), as a driving force for the organization of several types of materials including inorganic semiconductor nanoparticles, diblock copolymers, and segmented polymer nanowires. Research will examine how these nanoscale structures organize themselves into superstructures on larger length scales and how organization of material on each length scale influences the photophysical properties of the resulting devices. The proposed work will open new routes to simultaneously controlling the organization and electronic properties of matter on three different length scales, the molecular scale, the nanoscale, and the colloidal scale. It will also contribute to the critically important mission of improving efficiencies of low-cost, polymer-based photovoltaic devices.

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

Plant-Microbe Genomic Systems Optimization for Energy

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To evolve from promise to practice, essential optimization of each step of an advanced biofuel industry based on cellulosic biomass is already underway. For the present research, the bioassay will be used to measure rates of ethanol production in various accessions of the energy crop model Bd and then assess genetic diversity for this trait in this species. In doing so, the research will seek to resolve the mechanisms underlying plant feedstock quality through genetic analysis with a focus on energy crop improvement. As a second phase, to determine the plausibility of specific positive interactions between plant and microbial genotypes, pairwise comparisons will be made, varying both plant and microbial genotypes. Similar to adapting crop varieties to different environments, these experiments will link the need for specific feedstock properties to biomass conversion processes. Importantly, the development and optimization of unified plant-microbe genomic systems will advance the concept of "plant-microbe co-development" within the industry, thus improving the efficiency of cellulosic biofuels production from ecologically and economically sustainable resources without affecting food supply.

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

Cosmological Probes of Fundamental Physics

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This project will investigate the theoretical aspects of cosmological probes of dark energy, dark matter, and inflation. The specific objectives are (1) to investigate nonlinear structure formation effects at high redshift, including the suppression of power due to the relative velocity of baryons and dark matter that has recently been identified; to explore its consequences for tests of dark matter and inflation (via the small scale power spectrum) and dark energy (via the effect on baryon-acoustic oscillations); and to search for other such nonlinear processes; (2) to explore the use of higher-order correlation functions of the cosmic microwave background polarization and galaxy surveys to measure primordial gravitational waves and constrain inflationary physics; and to critically examine the systematic uncertainties that may arise; and (3) to continue the search for new physical effects in the standard Lambda cold dark matter (CDM) cosmology that could contaminate the currently used cosmological probes, or be useful to reduce statistical or systematic errors.

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

Nanoscale Mercury Sulfide-Organic Matter Interactions and Implications for Solubility and Biomethylation

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Effective solutions for remediation of mercury contamination remain elusive because of our poor understanding of biogeochemical processes that control mobilization of mercury and biomethylation in sediments. This research seeks to characterize the geochemical forms of mercury that persist in polluted sediments and link this knowledge to their bioavailability toward microbes. The fate of mercury in these settings involves a complex series of transformations including HgS mineral dissolution, colloid formation and transport, oxidation/reduction, and methylation by anaerobic sediment bacteria. In all of these steps, natural organic matter (NOM) plays a critical role for reaction rates. This research aims to elucidate the nanoscale interactions between mercury, sulfide, and NOM that are critical drivers of mercury geochemistry. This information will ultimately be used to establish a new geochemical framework for predicting mercury methylation potential in contaminated sediments.

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

Quantum Transport in Topological Insulator Nanoelectronic Devices

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The goal of this research project is to investigate novel quantum electronic transport phenomena in a recently discovered class of materials known as topological insulators. Topological insulators (TIs) are materials with a bulk band gap but which have a conducting surface state. The unique geometry, band structure and topological characteristics of the TI surface states have generated extraordinary interest in the physics community and have led, together with graphene, to the emergence of a new paradigm of “relativistic” condensed matter physics. Ultimately, these studies in TIs may lead to new types of quantum devices based on the electron spin (rather than its charge) and, more fundamentally, to new information processing based on topological quantum computation.

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

Systems Level Investigation of Uranium Resistance and Regulation by *Caulobacter Crescentus*

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Microbes are known to play a major role in influencing the movement of uranium and other environmental contaminants. In addition to simply surviving exposure to radionuclides, some microbes are capable of using these compounds to promote their growth, altering their chemical state to restrict their movement in the environment. However, understanding of the basic mechanisms that microbes use to perform these metabolic reactions is limited, especially in environments exposed to oxygen. In this research project, the biological systems of the bacterium *Caulobacter crescentus* that allow it to detect uranium in the environment, accumulate the metal at the cell's surface, and use it to generate energy via respiratory metabolism (essentially "breathing" uranium) will be examined. The long term goal of the project is to develop a conceptual model of uranium cycling that could be used to understand processes occurring at contaminated sites and inform potential bioremediation strategies.

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

Efficient Graph Kernels for Extreme Scale Analysis of Environmental Community Data

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The goal of this research is to develop novel parallel algorithms for graph-theoretic analysis of biological data on next-generation supercomputing platforms. Graph methods have an immense potential to transform the information space in bioinformatics and computational biology. The growing sizes of data repositories have ensured that such potential cannot be realized without a comprehensive embrace of high performance computing. The methods developed in this project will allow scientists to discover community structures hidden within very large graphs built out of high-throughput biological data. The specific aims of the project are to (1) develop scalable graph-theoretic parallel algorithms for clustering biological data; (2) build new inter-database analytical capabilities using novel multi-graph representations of biological data; and (3) apply graph-theoretic algorithms on the clustering components of three large-scale applications in metaproteomics and phylogenetics.

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

The Neutrino: A Better Understanding Through Astrophysics

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Over the past decade the evidence for neutrino flavor mixing has passed from tentative to compelling. This remarkable phenomenon has widely recognized implications for astrophysics because neutrinos are so very important in the hot and dense environments, such as core-collapse supernovae, that one only finds in the cosmos. The hints of successful explosions seen in the latest supernova simulations mean we need to confront them with the observations that neutrinos can provide but, unfortunately, our current understanding of the neutrino is incomplete and the signal from the next Galactic supernova is uncertain. But by studying the behavior of neutrinos in core-collapse supernovae and in similar hot/dense environments, determining the sensitivity of supernova neutrino flavor transformation to the unknown neutrino mixing parameters, and learning how these properties affect Galactic supernova neutrino burst signals, we are presented with a situation where the missing neutrino properties will be imprinted into the signal itself. The goal of this project is accordingly to prepare for the detection of neutrinos from the next Galactic supernova, and to anticipate how these future observations can be used to improve our understanding of neutrinos.

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

Direct Production of 99MTC Using a Small Medical Cyclotron

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Over 80% of nuclear medicine procedures require the use of the radioisotope 99mTc. Compounds that make use of this isotope are used in many studies, from cancer diagnosis to assessment of heart function. Recently, there have been many reports of the "isotope crisis" related to a shortage of 99mTc. Currently, 99mTc is produced via nuclear fission using highly enriched uranium (HEU), which is a concern because of nuclear proliferation risks. In addition to this, the United States is dependent solely on currently unreliable foreign sources of this important medical isotope. Clearly, a need exists to probe alternative domestic production routes of 99mTc. This application describes an investigation toward the non-HEU production of 99mTc with a small medical cyclotron, of which there are many located through the United States. The overarching goal of this project is for Washington University to develop the in house capability to routinely produce 99mTc for nuclear medicine patient procedures and to translate this capability to other nuclear medicine departments. Our facility is uniquely situated to explore the scope of this project as we have the expertise in cyclotron targetry and a very close relationship with the medical community because of our location within the department of radiology at one of the best medical schools in the country. Overall, the project introduces a straightforward domestic solution to the current crisis while also addressing the proliferation issues associated with the current method of production.

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

Transport Studies of Quantum Magnetism: Physics and Methods

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The goal of this project is to uncover and identify new states of matter resulting from the strong correlation in various quantum spin systems. The work will be focused on understanding the properties of the new ground states by studying elementary excitations via thermal and electrical transport properties. It will also involve the development of a new experimental method for thermometry that is tailored for thermal transport measurement and is also expected to have a more general impact on ultra-low-temperature thermometry.

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

Combating the Data Movement Bottleneck

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On next-generation supercomputers, the power cost of moving data is the critical metric for software while limited bandwidth further constrains the amount of data that can be moved. The objective of this project is to alleviate the data-movement bottleneck in extreme-scale computing to accelerate numerical simulation and data analysis. The research will focus on software solutions to reduce the amount of data transferred between memory banks, across distributed compute nodes, and between main memory and secondary storage. This project will take a three-pronged approach based on maximizing data locality by optimally reordering data elements, improving compute locality using parallel stream processing, and integrating high-speed data compression. These complementary techniques will limit the total size of data moved, minimize data accesses, and make effective use of multilevel caches to keep data as close to the processor as possible. This effort will lead to new tools for greatly reducing data movement with commensurate increases in performance and reductions in power consumption on next-generation massively multi-core computer architectures.

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

Bio-Inspired Electro-Photonic Structure for Dye-Sensitized Solar Cells

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The objective of this research project is to redesign and enhance the optical and electronic properties of dye-sensitized solar cells in a comprehensive manner through bio-inspired optical designs for light absorption and concomitant multi-scale reconstructions of the metal-oxide electrode structure for electron transport. The project will seek to utilize a “butterfly-wing” photonic crystal design for the anode of the solar cell to provide simultaneously a needed optical enhancement in the red wavelengths of the spectrum and a shortened, more efficient electron transport pathway for charge collection. The investigator will coordinate an array of experiments (1) to explore the synthesis of novel photonic structures for the solids based on examples taken from nature and (2) to determine their electronic properties. These results will be integrated into a comprehensive three-dimensional mathematical model and will allow the optimum parameters to be defined for the design of a high-efficiency, dye-sensitized solar cell.

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

Multi-System Analysis of Microbial Biofilms

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Microbial biofilms impact many biogeochemical processes including the fate and transport of contaminants in the subsurface. The present research will employ state-of-the-art technologies to determine the chemical composition of biofilms in relation to their highly hydrated native-state structure/architecture. The research will extend the mechanistic understanding of extracellular polymeric substance (EPS)-metal ion interactions using high-resolution cryogenic imaging and analysis techniques at the Environmental Molecular Sciences Laboratory (EMSL) and will develop new spectroscopy methods for obtaining spatially resolved chemical information. Synchrotron X-ray-based analyses will be used to obtain high-sensitivity, element-specific chemical distributions within biofilms that have been imaged using EMSL microscopies and spectroscopies. These integrated technologies will characterize the chemical and physical interactions of hydrated biofilms and catalytic components of EPS as they interact with redox-transformable metal ions and influence biogeochemical reactions. Determining the chemical composition and spatial coordination of biofilm-associated EPS will significantly advance understanding of how molecular-scale biogeochemical reactions can influence subsurface contaminant fate and transport at larger scales.

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

Fundamental Electroweak Interaction Studies Using Trapped Atoms and Ions

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Ion and atom traps at radioactive ion beam facilities have opened up a new vista in precision low- energy nuclear physics experiments. They provide ideal sources for studying the decays of rare isotopes: The trapped samples are extremely cold (< 1 mK) and localized (< 1 mm^2), and the trap forces are weak enough that the daughter particles escape with negligible distortions to their momenta. This project will construct a large-diameter, open Penning trap and couple it to T-REX (Texas A&M University Reaccelerated Exotics), which is the upgraded radioactive ion beam facility at the Cyclotron Institute at Texas A&M University. The flagship experimental program will test our understanding of the fundamental symmetries underlying our current theory of electroweak interactions by measuring the b − n correlation parameters and ft values from isospin T = 2 superallowed ¯-delayed proton decays. Comparison of these precision measurements to theoretical predictions will either confirm the Standard Model to a higher degree or point to new physics and help guide theorists toward developing the New Standard Model. In addition, the versatility of this system will also make it a general purpose decay station where any number of other low-energy experiments will be possible (mass measurements, laser spectroscopy, electron-capture studies, etc.).

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

Weak Interaction Study Using Laser Trapped 6He Atoms

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High-precision measurements of how radioactive nuclei decay have played an essential role in today's understanding of the fundamental laws of nature, which are summed up in what is known as the Standard Model of particle physics. However, modern cosmological observations, such as the presence of Dark Matter and the lack of antimatter in the universe cannot be explained by the Standard Model. Thus, the quest for direct experimental evidence of "New Physics" is an exciting endeavor currently being pursued on many fronts in fundamental research. Here, the decay of 6He, a radioactive isotope of helium, will be studied in exquisite detail to test the "Weak Interaction" component of the Standard Model. Atoms of 6He suspended in vacuum by laser light represent an ideal laboratory in which to detect the decay products and measure their properties with high precision. Combined with the detailed theoretical understanding of this rather simple nucleus, telltale signs of new interactions would reveal themselves as small deviations from the Standard Model predictions. Techniques developed for this experiment will also enable studies of other noble gas isotopes in a quest for additional hints of "New Physics."

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

Quantum Field Theories for Cosmology

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This research spans a wide range of subjects in theoretical cosmology and in field theory. In the first part, effective field theory techniques will be applied to the study of fluids and of cosmological perturbations. Such an approach—now standard in particle physics—is quite unconventional for theoretical cosmology. The research addresses several concrete questions where this formalism will prove valuable, both within and outside the cosmological context, concerning, for instance, the quantum mechanical properties of fluids and of superfluids, the post-inflationary reheating phase of early cosmology, and the effects of large matter inhomogeneities at short scales on the dynamics of cosmological perturbations and of the universe as a whole at much larger scales. In the second part, more fundamental questions and ideas will be investigated for the present universe as well as for the very early one, using quantum field theory as a guide. The questions to be addressed include the following: Is the present cosmic acceleration caused by a new, 'dark' form of energy or are we instead observing a breakdown of Einstein's general relativity at cosmological distances? Is the cosmic acceleration accelerating? Is the Big Bang unavoidable? Related to this, is early inflation the only sensible cure for the shortcomings of the standard Big Bang model and the only possible source for the observed scale-invariant cosmological perturbations?

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

High-Average Power Laser Experiments at the Large Plasma Device

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The goal of this project is to obtain highly detailed measurements of laser-driven collisionless shocks and highly nonlinear plasma waves in a large magnetized plasma (i.e., the Large Plasma Device at the University of California, Los Angeles) using a new, high-average-power slab-laser system (25 J at 4 Hz). Magnetized collisionless shocks are launched by rapidly exploding laser plasmas and a large (≤50 cm) diamagnetic laser-plasma cavity, which acts as a fast moving magnetic piston upon the highly magnetized ambient plasma (17 m x 0.7 m at 1012-1013 cm^{-3}). In comparison with earlier work on pinches, these experiments can be performed with arbitrary shock propagation angles (from quasi-perpendicular to quasi-parallel) and can thus access weakly supercritical shocks in both the dispersive and dissipative regime. The 1 Hz repetition rate of these experiments allows us to create shocks reproducibly for tens of thousands of times, leading to highly detailed measurements of (1) the magnetohydrodynamic (MHD) response of the ambient plasma, (2) the dissipation of the shock, and (3) the effect on the particle velocity distribution. Particle acceleration in the shocks will also be studied using preformed non-thermal particles.

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

Measuring the Importance of Valence to Chemistry of Nanocrystal Surfaces

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Surface structure is central to the properties of colloidal semiconductor nanocrystals. Yet the valence of atoms on nanocrystal surfaces and its influence on the binding and exchange of their ligands remain an essentially unexplored avenue of research. Current descriptions of semiconductor nanocrystal surfaces do not adequately distinguish between dative ligand interactions (L-type binding) and ligands that balance their charge with nonstoichiometric crystals (X-type binding). To address this problem, this project will investigate the relationship between nanocrystal stoichiometry and the exchange of both X- and L-type surface ligands. Nuclear magnetic resonance spectroscopy will be used to measure the thermodynamic binding constants and the mechanisms and kinetics of ligand exchange. The project will develop methods (1) to exchange surfactant ligands allowing the fabrication of thin films composed of nonstoichiometric nanocrystals with an intact metal-ligand surface layer and (2) to controllably deposit films of nanocrystals using layer-by-layer dip coating and electrodeposition where the X-type organic surfactant ligands have been replaced with a halide ligand shell. These techniques will furnish nanocrystal thin films with a small inter-nanocrystal separation and enhanced electronic coupling. Fabrication of field effect transistor devices using these methods will allow the details of atomic surface structure to be correlated with electrical transport characteristics. To date, nanocrystal researchers have heavily relied on an L-type ligand model when describing nanocrystal surfaces. Clarifying the importance of X-type ligands to nanocrystal surface chemistry and its relationship to stoichiometry can have a dramatic influence on nanocrystal research and will lead to powerful methods for precisely tailoring nanocrystal surfaces. In particular, these methods may offer major improvements in nanocrystal-based thin film optoelectronic devices.

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

Developing Novel Techniques for Readout, Calibration and Event Selection in the NOVA Long-Baseline Neutrino Experiment

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The long-baseline neutrino experiment known as NOvA (NuMI or Neutrinos at the Main Injector Off-Axis ve Appearance Experiment) uses a fine-grained, low-Z, fully active detector that offers unprecedented electron neutrino identification capabilities for a detector of its scale. This research involves the development and implementation of novel techniques for channel readout, detector calibration, and event reconstruction that make full use of the strengths of the NOvA detector technology. In particular, custom event reconstruction algorithms that use the rich information available in the substructure of hadronic and electromagnetic showers will be designed. Exploiting this information provides not only substantial improvement in background rejection for the electron neutrino search but also better shower energy resolution (improving the precision on measured oscillation parameters) and a high-energy electromagnetic calibration source (through neutral pion events). Further, a new electronics readout scheme compatible with the existing hardware that can reduce near detector event pile-up and offer powerful timing information to the reconstruction wil be developed and deployed, allowing for cosmic ray muon tagging via track direction determination, among other things. In conjunction with the above, the project involves leading the calibration of the NOvA detectors, including characterizing individual electronics channels, correcting for spatial variations across the detector, and establishing absolute event energy scales.

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

Atomic Layer Deposition of Superconductors, an Innovative Approach to Improve the Performance of High Energy Physic Accelerators

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After 40 years of research and development, niobium superconducting radio frequency (SRF) cavity performance may be reaching fundamental intrinsic materials limits. Presently, the state of the art for Nb cavities involves using reproducible operating field gradients of 35 MV/m, for which the peak equatorial RF field of 140 mT has almost reached the depairing limit set by the thermodynamic critical field of about 200 mT. Based on theoretical models by Alex Gurevich of Florida State University, the research seeks to build cavities with cost effective deposition methods that will reduce significantly the operating and capital accelerator cost. The goals require a close-coupled effort that (1) develops an atomic layer deposition (ALD) synthesis process of high temperature superconductors on coupons or dummy cavities, (2) provides complementary production deposition techniques that can produce high-quality, thick (~µm) Nb films on coupons and cavities, (3) allows for the rapid surface science characterization required to optimize synthetic/deposition methods on coupons, (4) provides the best cavity base material to use, (5) develops methods to scale PEALD (plasma-enhanced atomic layer deposition) to real cavities, (6) provides for fast turn-around vertical cavity tests, and (7) allows for reuse of the base cavities.

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

Real-Time Studies of Nucleation, Growth and Development of Ferromagnetism in Individual Protein-Templated Magnetic Nanocrystal

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The aim of this project is to determine the nature of protein-templated nanoparticle formation. Using advanced electron microscopy techniques, the research intends to uncover the mechanism of particle nucleation and growth, the emergence of crystal structure, and the development of ferromagnetism in individual bio-templated magnetic nanocrystals. Magnetic nanoparticles with narrow size distribution, large magnetic moment, and controlled magnetic anisotropy have important technological applications. Bio-inspired synthetic routes offer room-temperature pathways to a variety of magnetic nanostructures having shapes and sizes not realizable via conventional inorganic chemical techniques. However, despite significant research effort in this area, fundamental understanding is lacking on how the supramolecular assembly of biomolecules dictates nanoparticle formation and functional properties. The work will make possible in-situ nanoparticle synthesis and dynamic studies of the emergence of crystallinity and evolution of magnetic response in individual protein-templated magnetite nanoparticles free of artifacts associated with the conventional sample preparation and characterization.

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

Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level

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This project aims to develop a comprehensive framework that will lead to a fundamental description of both structural properties and reactions of light nuclei in terms of constituent protons and neutrons interacting through nucleon-nucleon and three-nucleon forces. This is a long-sought goal of nuclear theory that is now within reach as new promising techniques and the required computational power to implement them are becoming available. This project will provide the research community with the theoretical and computational tools that will enable (1) an accurate prediction for the fusion reactions that power stars and Earth-based fusion facilities; (2) an improved description of the spectroscopy of exotic nuclei, including light borromean systems; and (3) a fundamental understanding of the three-nucleon force in nuclear reactions and nuclei at the drip line.

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

Physics of Lattice Defects and Defect-Impurity Complexes in Materials Used for Superconducting RF Cavities

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The proposed research seeks to understand the role of lattice defects such as dislocations, vacancies, and vacancy-hydrogen complexes in the performance of superconducting radio frequency (RF) cavities. Based on the results of the preliminary studies, the work aims to fill the gap in knowledge and allow further progress in gradients and quality factors. It is intended to perform systematic studies on samples by utilizing state-of-the-art surface analytical techniques such as electron backscattered diffraction (EBSD), focused ion beam (FIB), transmission electron microscopy (TEM), positron annihilation spectroscopy, and elastic recoil detection (ERD). The effect of lattice defects on RF superconductivity will be directly studied by introducing localized irradiation damage into niobium cavities and characterizing the RF performance with advanced thermometry. The expected outcome is the capability to tailor a superconducting RF cavity surface to sustain the highest surface magnetic fields based on a detailed understanding of near-surface lattice defect structure and its effect on RF performance.

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

Engineering self-assembled bioreactors from protein microcompartments

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The goals of this research are to understand how organisms such as bacteria segregate certain metabolic processes inside of specific structures, or "microcompartments," in the cell and apply this knowledge to develop novel engineered microcompartments for potential use in nanotechnology and metabolic engineering. For example, in some bacteria, self-assembling protein microcompartments called carboxysomes encapsulate the enzymes involved in carbon fixation, enabling the cell to utilize carbon dioxide more effectively than if the enzymes were free in the cell. This research will determine how structures such as carboxysomes assemble and function in bacteria and develop a means for creating novel, synthetic microcompartments for optimizing production of specific energy-rich compounds.

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

A Physicochemical Method for Separating Rare Earths: Addressing an Impending Shortfall

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The objective of this project is to develop new approaches to chemically extract cerium (Ce), praseodymium (Pr), neodymium (Nd) and terbium (Tb) ions from mixtures of rare earth ions. Nitroxyl radicals will be synthesized and evaluated for selective binding of high value rare earths through oxidative intermediate valence effects. This research will develop new fundamental knowledge in f-element chemistry and the potential for new element-specific extractants. The extractants are expected to reduce the costs of strategically important materials made from the elements Ce, Pr, Nd and Tb.

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

Data Locality Enhancement of Dynamic Simulations for Exascale Computing

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Computer simulation is important for scientific research in many disciplines. Many such programs are complex, and transfer a large amount of data in a dynamically changing pattern. Memory performance is key to maximizing computing efficiency in the era of Chip Multiprocessors (CMP) due to the growing disparity between the slowly expanded memory bandwidth and the rapidly increased demands for data by processors. The importance is underlined by the trend toward exascale computing, in which the processors are expected to each contain hundreds or thousands of (heterogeneous) cores. Unfortunately, today’s computer systems lack support for a high degree of memory transfer. This project proposes to improve memory performance of dynamic applications by developing two new techniques that are tailored especially for the emerging features of CMP. The first technique is asynchronous streamlining, which analyzes the memory reference patterns of an application during runtime and regulates both control flows and memory references on the fly. The second technique is neighborhood-aware locality optimization, which concentrates on the non-uniform relations among computing elements. This research will produce a robust tool for scientific users to enhance program locality on multi- and many-core systems that is not possible to achieve with existing tools. Further, it will contribute to the advancement of computational sciences and promote academic research and education in the challenging field of scientific computing.

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

Fundamental Instability Measurements in Magnetically Driven Z-Pinch Liner Implosions

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The magnetic pressure generated by large, pulsed currents can be used to directly compress initially solid metal tubes (liners) to extreme conditions. The Sandia Z facility can generate 100 megabars of magnetic pressure (25 MA at a radius of 1 mm), similar to the radiation-driven ablation pressure on fusion capsules designed for the National Ignition Facility. Achieving extreme conditions in the laboratory for fusion or dynamic materials studies requires the compression of matter and current to small radii. The most important factor limiting the controlled compression of dense matter to small radii using magnetic pressure is the magneto-Rayleigh-Taylor (MRT) instability. In liner implosions the MRT instability arises at the outer plasma-vacuum interface, where the driving magnetic pressure plays a role analogous to a light fluid pushing on a heavy fluid (the plasma liner) as in the classical fluid Rayleigh-Taylor instability. The MRT instabilities in fast z-pinch systems are complex, and we rely heavily on advanced simulation tools to model them. Surprisingly, there are few data that can be used to validate these simulation tools, particularly in the ~100 ns regime where plasma effects and strong shocks can be important. The principal investigator recently led the first well-characterized MRT growth measurements on ~100 ns time scales using initially solid Al liners. This research will enable several additional experimental campaigns on the Sandia Z facility to study both fundamental and applied aspects of the MRT instability. Data collected in these experiments are expected to ultimately improve our physics understanding and help us validate critical simulation tools, thereby benefiting fusion and dynamic materials applications based on magnetic pressure drive.

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

Cosmology with the Lyman-Alpha Forest

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This project will investigate the nature of dark energy, the mysterious component of the universe responsible for its accelerated expansion, using quasars, which are the brightest objects in the universe. Using data from the Baryon Oscillation Spectroscopic Survey (BOSS) experiment, the three-dimensional structures in the early universe will be determined by measuring the shadows that intervening neutral hydrogen in space casts on the spectra of quasars, known as the Lyman-alpha forest. Such data offer a unique probe of the distant universe and will also provide constraints on dark matter, neutrinos and cosmic inflation. A comprehensive framework will be built based on novel and robust techniques to analyze the Lyman-alpha forest spectra, with strong emphasis on understanding the systematic errors arising from astrophysical and instrumental effects. This will result in new constraints on cosmological parameters and pave the way for the future experiments studying the nature of dark energy.

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

New Dimension Reduction Methods for Multi-scale Nonlinear Phenomena

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This project will develop a new dimension-reduction method for complex, multiscale, non-linear problems and design scalable, communication-minimizing algorithms for the implementation of this method on leadership-class computers. Many mathematical models of natural and/or engineered systems are multiscale and nonlinear and have a common feature: Their discrete approximations are systems of ordinary differential equations (ODEs), which can contain an enormous number of unknowns. Direct simulation of these models can be extremely expensive. The dimension reduction methods will provide a rigorous mathematical foundation for approximating large systems of ODEs with models containing a much smaller number of unknowns. By doing this, the new method will address computational challenges posed by large-size ODE models. These outcomes would constitute a breakthrough in multiscale modeling with a strong potential for significant advances in various engineering and science applications.

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

Defining Fe and H Speciation During Olivine Carbonation Under Highly Reducing Conditions

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Rock weathering significantly affects atmospheric and groundwater chemistry, particularly the exchange of carbon dioxide between air, water and rock components. However, it is difficult to unravel chemical reactions between fluids and rocks in the subsurface, including microbially mediated biogeochemical processes. The goal of this project is to examine the connection(s) among the geochemical behavior of iron and the extent of hydrogen, methane or carbonate mineral formation during the aqueous alteration of olivine at near-surface temperatures and pressures. An integrated suite of surface sensitive x-ray scattering and spectroscopic techniques will be used to interrogate the dynamic structure and reactivity of the mineral-water and mineral-microbe interfaces. Stable isotope measurements of hydrogen, water, and methane will also reveal whether similar microbial dynamics might be successfully detected and interpreted in in-situ systems. These investigations will provide first-order insights into geochemical and microbial processes in the shallow earth during the exchange of atmospheric carbon dioxide with the geosphere.

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

Interpreting New Data from the High Energy Frontier

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This research aims to maximize the discovery potential of the Large Hadron Collider (LHC) by using theoretical insights in high energy physics to galvanize the search for new physics. The LHC will push the frontiers of fundamental physics through high energy particle collisions. However, gleaning evidence for new physics from the overwhelming standard model background is a challenging task, and innovative methods in data analysis and interpretation are needed to convert raw experimental measurements into evidence for new physics. In this research, three aspects of LHC physics in which theoretical insights can play a crucial role will be addressed. First, to propose new LHC searches, novel LHC signals for new physics scenarios involving supersymmetry and dark matter will be identified. Second, to increase experimental sensitivities in existing LHC searches, the PI will propose new data analysis techniques to better measure and identify jets produced in high energy collisions. Third, to make signal extraction more robust, the PI will improve Standard Model background predictions. Through this research on new physics searches at the high energy frontier, this project will help achieve the ultimate goal of the LHC: to discover what new phenomena lie beyond the standard model.

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

Microbial Communities in Biological Carbon Sequestration

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Wetland ecosystems are known to cycle and potentially store massive amounts of carbon on an annual basis. Carbon dioxide captured from the atmosphere by plants moves below the water or soil surface through the action of roots or the death of biomass, where it is subject to the processing by complex communities of microorganisms. This can result in the degradation of organic carbon back to carbon dioxide or methane or to more stable forms that may be stored for long periods of time. Relatively little is known about the organisms performing these processes or what conditions influence the storage or release of carbon. The current research will use cutting-edge genomic techniques to examine microbial community structure and functional properties in a restored wetland habitat in San Francisco bay, with an emphasis on characterizing processes that result in increased biosequestration of organic carbon over time. The study will leverage resources at the Department of Energy Joint Genome Institute to link activities of dominant environmental microbes to major carbon cycle processes to enhance our understanding of critical biogeochemical cycles and ecosystem sustainability.

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

Innovative Techniques for Improved Diagnosis and Control of Edge Localized Modes in 3-D Toroidal Plasmas

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The next step toward a magnetic fusion reactor is the large international experiment currently being built in France called ITER. A major challenge for ITER and future fusion reactors is controlling the intense flux of heat deposited on the confinement chamber wall by high-energy, long-pulse plasmas. Furthermore, local concentrations of heat flux can seriously damage the wall surface. Thus, interactions of the plasma with the material wall must be monitored and controlled in three dimensions (3-D). Of special concern are sudden large impulses of heat resulting from plasma instabilities such as the Edge Localized Mode (ELM). These impulses create peaked values of heat flux that are many times the steady-state wall flux levels and thus can augment the erosion of wall surface. This research aims to build tools to improve the understanding of ELM excitation, mitigation, and suppression mechanisms toward the design of more effective control methods. The design principles and mathematical tools developed and validated in this work can, in principle, help diagnose a wide range of 3-D edge physics phenomena closely related to those examined here. The implementation of two diagnostics for measurement of these 3-D edge perturbations will be pursued: The first diagnostic aims to measure the plasma edge magnetic field structure during the mitigation and/or suppression of ELMs by applying external 3-D fields know as resonant magnetic perturbations. The other diagnostic will be used for precise tracking of high-speed, cryogenic pellets used for triggering ELMs. Both of these diagnostics rely on the processing of 2-D data to determine 3-D plasma characteristics. Therefore, a unifying analysis method to extract this 3-D information will be developed using common mathematical techniques. The new information given by this analysis can aid in the fundamental understanding of ELMs by providing novel, high-fidelity 3-D information during ELM control experiments in present-day experiments.

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

Miracles in Scattering Amplitudes: from QCD to Gravity

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The present research in the area of theoretical high energy physics will be centered around both theory and phenomenology of scattering amplitudes in quantum field theories and gravity. Recently, remarkable advances have been made in this area, with a broad spectrum of results ranging from new precision predictions in Quantum Chromodynamics (QCD) that will be very important for understanding Large Hadron Collider (LHC) data to the miraculous structures in N=4 Yang-Mills and N=8 supergravity. This research involves deepening our understanding of gauge and gravity theories by exploring hidden structures of scattering amplitudes (ranging from integrability to twistors to the theory of motives) and using these rich structures as much as possible to aid practical calculations relevant to collider physics. These hidden structures not only help researchers calculate and make predictions for experimentally relevant processes but also lead to deeper understanding of fundamental properties of field and gravity theories. The research will contain three major areas, (1) QCD and Collider Physics; (2) N=4 Yang-Mills and AdS/CFT (Anti DeSitter Space/Conformal Field Theory); and (3) Quantum Gravity. The funds will be used to train graduate students and postdocs.

This research was selected for funding by the Office of High Energy Physics (HEP) and the DOE Experimental Program to Stimulate Competitive Research (DOE EPSCoR).

Physics and Control of Locked Modes in the DIII-D Tokamak

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The objectives of this project are (1) to control instabilities in tokamak plasmas by means of externally applied magnetic field perturbations and microwave-generated electric currents and (2) to improve our understanding of the instability dynamics both by analyzing the unstable magnetic fluctuations that they generate and by comparing the experimental results with computer model predictions. Tokamaks are devices that confine toroidal (doughnut-shaped) fusion plasmas by means of an equilibrium magnetic field configuration. Coherent helical modifications to the equilibrium magnetic field called locked modes can form in high-performance tokamak plasmas, degrading confinement and resulting, in some cases, in an abrupt termination of the plasma. Such an event, called a disruption, can be detrimental to the tokamak device. This experimental study will deepen theoretical understanding of these locked-mode-related instabilities, improve the precision and scope of our predictions, and test and validate specific techniques for avoidance and control. Magnetic field perturbation measurements, advanced analysis, and comparison between experiment and computer models will be employed to study the dynamics and growth of locked-mode-related instabilities. To be evaluated is the ability to control locked modes by a combination of (a) externally applied magnetic field perturbations to modify their location and (b) a microwave-generated current to modify their size. Of particular utility to the international ITER tokamak under construction in France is the development of a capability, made possible by the sensitivity of these locked-mode-related instabilities to desired and undesired magnetic field perturbations and imperfections, to diagnose and correct imperfections (“error fields”) inherently present upon the construction of a perfectly designed tokamak equilibrium magnetic field.

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

RF Breakdown Dependence on Electric and Magnetic Fields and Pulsed Heating

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The objective of this project is to understand breakdown of high gradient phenomena in an accelerator structure. Electric field, magnetic field and pulsed heating are thought to affect breakdown based on innumerous experiments. However, it is not clear how the combination of the fields and heating is governing breakdown since they are coupled in an accelerator cavity. This research aims at delineating these different effects by designing a special radio-frequency (RF) cavity that permits the coupling of two different RF modes and the use of a laser for selected pulsed heating. A good understanding of these effects is important for designing structures capable of supporting high accelerating gradients, beyond current state of the art, for devices such as klystrons and magnetrons used for generating reliable RF power for driving accelerators. Better understanding of the associated physics and generation of breakdown can lead to significant cost saving for future high gradient accelerator applications such as linear colliders; compact linear accelerators for light sources, medicine, and industry; satellite communication systems; and fusion reactors.

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

Electron Temperature Fluctuation Measurements and Transport Model Validation at Alcator C-Mod

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The objective of this project is to merge experiment and theory by using advanced turbulence simulations to aid in the design of a new turbulence diagnostic system that will be used to test the fundamental physics of turbulent transport in tokamak plasmas. The research project will develop a novel correlation electron cyclotron emission (CECE) diagnostic system for measuring turbulence in the core plasma of the Alcator C-Mod tokamak at the Massachusetts Institute of Technology (MIT). Gyrokinetic theory describes how small-scale turbulent fluctuations are responsible for the observed transport of particles, heat, and momentum in tokamak plasmas. The new and unique data obtained with the CECE diagnostic system will be used in detailed validation studies to probe the limits of gyrokinetic theory and to assess the accuracy of models for turbulent-driven transport in tokamaks. This diagnostic approach will measure electron temperature fluctuations, which provide direct information about the underlying physics of heat transport. When combined with advanced models and simulations, these data can be used to indirectly probe the turbulent transport of particles, momentum, and energy as well. This research project aims to transform the traditional approach to testing advanced gyrokinetic turbulence simulations by introducing an innovative method for merging diagnostic development with code validation. This includes using for the first time quantitative predictions of turbulence characteristics to guide the design of a new fluctuation diagnostic system.

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

Quantum Mechanical Simulations of Complex Nanostructures for Photovoltaic Applications

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This research project involves theoretical studies of complex semiconducting nanomaterials and their interfaces with other materials for next-generation photovoltaic cells. The central challenge in materials simulation is to address complexities in real materials rather than considering the properties of idealized materials or structures. For photovoltaic devices, it is of paramount importance to be able to accurately predict excited-state properties of complex nanostructures that are the result of optical absorption. However, current quantum mechanical simulation methods are either computationally too demanding or not sufficiently accurate. The primary objectives of this project are (1) developing a new theoretical approach for electronic excitation calculations that is both accurate and applicable to large and complex systems and (2) applying the new methodology to investigate complex nanostructures that have great potential of opening new routes toward designing a material's transport, electronic, and optical properties for photovoltaic and other optoelectronic applications.

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

Functional Domain Walls as Active Elements for Energy Technology

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This project aims to understand and exploit novel physics and functionalities of domain walls in transition metal oxides for their use as active elements to direct matter and energy. Heterophase and homophase domain walls are mobile, nanoscale elements existing in a wide range of materials; they can host remarkable, emergent functionalities that are absent in the bulk. This may lead to a variety of new energy technologies that are superior to existing ones. This research seeks to understand the fundamental mechanism governing diffusion and recombination of point defects facilitated by domain walls, demonstrate ultra-sensitive transduction of external disturbances on domain wall motion, explore and exploit effects of domain walls in electrothermal transport for nanoscale thermal management, and finally probe the physical behavior of correlated electrons confined within domain walls as a quasi-two-dimensional electron liquid.

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

Enhancement of the Trigger Capaiblity for New Physics at the Large Hadron Collider

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The Large Hadron Collider (LHC) is designed to address some of the most fundamental questions of physics by producing rare events of new physics in the tremendous background. To increase the sensitivity to new physics, the availability of more sophisticated event characteristics at early trigger stages will be crucial to ensure high background rejection with high signal efficiency. The track information of the event is reconstructed typically with reiterative software on CPUs (central processing units) and is very time consuming in the LHC environment. The research will involve the designing and building of a hardware system with massively parallel processing that will reconstruct global tracks with near-offline resolution. Subsequently, sophisticated algorithms will combine the precisely reconstructed tracks with other trigger information to perform early background rejection and signature identification. This will substantially improve the potential for new physics discoveries.

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

Utilizing Molecular Self-Assembly to Tailor Electrical Properties of Si Nanomembranes

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The objective of this project is to use silicon (Si) nanomembrane, a well controlled two-dimensional single crystalline semiconductor, as a prototype system to explore the mechanistic basis of electronic interactions at the hetero-interface and to develop strategies to tailor the nanomembrane's transport properties by surface functionalization and self-assembly. Understanding and control of hetero-interfaces between organic and inorganic materials is crucially important for the development of organic electronics, molecular electronics, molecular/biological sensors, and energy converting devices. However, an atomic- and molecular- level understanding of charge transfer behaviors at the interface and how they influence the properties of inorganic materials remains elusive. This work exploits the precision of molecular assembly on Si nanomembranes and combines the scanning probe microscopy characterization of local interfacial electronic structures with the electrical transport measurements of nanomembranes to elucidate the interfacial phenomena. The fundamental insights provided by this research may lead to the rational design of nanomaterials with controlled properties via regulation of surfaces and interfaces.

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

Real Time TEM Imaging of Materials Transformations in Liquid and Gas Environments

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The objective of this project is to study the physical and chemical processes in materials with high spatial resolution using in situ liquid or gas environmental transmission electron microscopy (TEM). Understanding how materials grow and function at the nanometer or atomic scale in their working environments is essential to developing efficient and inexpensive energy conversion and storage materials and devices. With real-time imaging in liquids or gases, this project will develop environmental cell TEM and result in better understandings of growth and chemical reactions of nanocrystals and mass transport induced structural changes in electrochemical processes important for energy applications.

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