Identifying the Regimes and Acoustics of Cryogenic Boiling heat Transfer for Accelerator Applications

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This project aims to advance the development of high-gradient linear accelerators using cryogenically cooled copper technology. These accelerators, essential for future scientific discoveries, rely on efficient cooling systems, such as liquid nitrogen, to enhance performance and reduce costs. However, as the cooling fluids undergo phase changes (such as boiling), they can cause temperature fluctuations, noise, and vibrations that may disrupt the accelerator’s performance. To address these challenges, the research will investigate heat transfer, boiling dynamics, and acoustic effects within the cooling system through a combination of detailed simulations, thermoelastic analysis using finite element models, and hands-on benchtop experiments. The insights gained from these advanced studies will inform the development of design guidelines to optimize future accelerators. The collaboration between Florida A&M University (FAMU) and the SLAC National Accelerator Laboratory ensures a seamless connection between research and practical applications. Beyond advancing accelerator technology, the project will offer professional training to FAMU-FSU College of Engineering students, engaging them in cutting-edge R&D and preparing them to become future scientists contributing to collider technologies.

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

Resonant Microwave Plasma Sources to Improve the Efficiency of Compact Plasma-Based Accelerators

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Laser-plasma accelerators (LPAs) are emerging as a revolutionary technology for particle acceleration, offering electric fields orders of magnitude stronger than those in traditional radiofrequency (RF) accelerators. This advancement holds great promise for creating compact and efficient accelerators with applications in medicine, security, materials science, and potentially a next-generation energy-frontier particle collider. In an LPA setup, an intense laser pulse passing through plasma generates a strong wave that accelerates particles to high speeds, with the plasma creating the electric fields and guiding the laser pulse for sustained acceleration over long distances.

To advance LPA technology, it is essential to develop highly efficient and controllable plasma sources. Microwave resonant structures are ideally suited for this, concentrating electromagnetic energy to achieve high-density plasma with minimal input power. By using a high-quality microwave resonator, we can create stable, long-lasting plasma that meets the stringent requirements of particle acceleration. These “cold plasma” sources operate with low temperatures for heavy particles, high ionization, and stability, ensuring consistent performance without overheating.

This project aims to investigate the principles behind resonant microwave plasmas (RMP) to develop efficient cold plasma sources specifically tailored to compact LPAs. Combining theoretical analysis, modeling, and experimental investigation, we seek to identify the factors that influence the stability and performance of these plasma sources. Cold plasmas already benefit society in areas such as plasma medicine, water treatment, food preservation, material processing, electric propulsion, and environmental protection. By advancing our understanding of RMP technology, we aim to develop a new generation of plasma accelerators that are smaller, more energy-efficient, and equipped for applications in scientific research and practical uses across various fields.

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

Harnessing Nonnegative Matrix Factorization for Advanced Computational Materials Modeling

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We will develop novel scientific machine learning (SciML) algorithms that enhance data reduction, increase interpretability, and bolster performance through advanced mathematical and computational methods. The new SciML algorithms aim to address the inherent and complex challenges of obtaining structure-property information in large-scale – often high-dimensional – and scientific data. Our approach leverages techniques such as deep learning (DL)-assisted non-negative matrix factorization (NMF) and diffusion models (DMs), focusing on developing reliable, efficient, scalable, and interpretable algorithms with validations in inverse material design. These efforts are structured around four synergistic technical objectives, which are central to advancing the DOE mission of improving energy efficiency, environmental sustainability, and scientific discovery.

In Aim 1, we will develop physics-aware NMF models enhanced with structure-aware regularization, informed by time-frequency domain features and physical laws, to foster parsimony, interpretability, and identifiability. These new NMF models seamlessly incorporate domain knowledge, such as crystal symmetries, grounded in rigorous theoretical principles, thus ensuring that the derived representations are both scientifically coherent and practically significant.

In Aim 2 will focus on exploiting NMF-based algorithms developed in Aim 1 to develop scalable machine learning (ML) models to enhance the potential for predicting material properties and guiding synthesis. Our approach aims to improve ML scalability and accuracy by incorporating NMF and structure-aware regularization into deep learning techniques. Additionally, we will utilize NMF for unsupervised feature extraction from complex materials data, enhancing model training and interpretability. We will also develop randomized deep NMF algorithms for efficient data representation and integrate novel DMs to address data scarcity issues. To quantify uncertainty, we will develop scalable Bayesian inference methods to estimate NMF posterior distributions.

In Aim 3, we will integrate NMF and DMs to overcome the current challenges of efficiently processing and interpreting large datasets in high-throughput and inverse materials design. Our NMF models, augmented with DMs for addressing data scarcity, will be applied to high-throughput density functional theory (DFT) datasets to uncover hidden patterns and correlations, facilitating the clustering of similar materials and identifying novel materials in inverse design. This integration promises significant advancements in material discovery and design efficiency. We propose to develop an open-source, distributed computing platform that integrates Aims 1-3 in Aim 4. We will provide Docker images compatible with Windows, Linux, and Mac to ensure easy deployment on various platforms, including GPU servers and cloud environments. Our team's extensive experience in developing and disseminating physics software and ML frameworks, such as BrainGB, TrustLLM, BiomedGPT, ElasTool, and SMATool, PropertyExtractor will guide this effort.

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

High-dimensional characterization of forest mesophication effects on reactive nitrogen emissions by soil microorganisms

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In forests of the eastern United States, wildfire suppression policies have significantly changed the tree structure, soil composition, and moisture levels, a process known as "mesophication". “Mesic” forest soils have increased moisture content and nutrient availability. These mesophication-associated changes are expected to have a major impact on soil nitrogen (N) cycling by microorganisms. Microorganisms involved in N-cycling in forest soils are major sources of nitrogen oxides (NO_x= NO + NO_2) and nitrous acid (HONO) to the atmosphere. These gases are both air pollutants and greenhouse gas precursors. However, we do not know the specific microbial populations and genetic systems responsible for these emissions, making it challenging to predict their contributions to global atmospheric change. Additionally, the specific populations of microorganisms that produce these gases likely vary across ecosystems. Thus, forest ecosystems at different stages of mesophication provide a unique opportunity to study how different environmental factors like soil moisture and nutrient content influence microbial production of NO_x/HONO. This research team will use a novel approach to investigate the microbial origins of these emissions across forests of varying mesophication stages.

This new research is driven by several hypotheses: (1) Soil moisture and N are the primary drivers of microbial emissions of NO_x/HONO in forest ecosystems. Both variables will increase alongside the degree of forest mesophication. (2) In mesic (*i.e.,* moist) forest soils, higher N levels from more easily decomposed leaf litter and increased water runoff from trees contribute to greater NO_x/HONO emissions. (3) The high moisture levels in these soil conditions create small oxygen-deprived zones where anaerobic microorganisms become the main source of NO_x/HONO emissions. (4) Emissions from these microbial processes have a significant impact on regional air quality and atmospheric chemistry across the eastern United States.

Key outcomes of the research include a detailed analysis of soil microbial communities across forests experiencing different levels of fire suppression and resulting mesophication. The study will describe how changes in these microbial populations are connected to the release of NO_x/HONO. Researchers will also determine how specific soil microbial processes, such as denitrification and nitrification, contribute to the production of these gases. Additionally, the team will create a computer model that incorporates isotope data to simulate how nitrogen cycles through the environment and estimate the natural emissions of NO_x/HONO from forest soils at various stages of mesophication. Using these results, they will run simulations to understand how changes in fire management and microbial populations affect atmospheric chemistry and, ultimately, the climate. These findings will be important for both climate modeling and forest management, especially as forests in the eastern U.S. become increasingly dominated by mesic, fire-suppressed conditions.

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

Improving the physical realism of snow processes in E3SM

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Water stored as snow is an essential freshwater resource over extended regions of the world, feeding surface and groundwater systems, sustaining agriculture, energy production, and natural ecosystems. The presence of snow also impacts the land surface temperature and its reflectivity, leading to warming feedbacks between the land and the atmosphere. For these reasons, adequately capturing snow processes is an essential step required to advance the representation of land surfaces in the current generation of Earth System Models such as the Energy Exascale Earth System Model (E3SM).

Improving global snow predictions in these models is important for understanding multiple physical processes, ranging from surface and subsurface hydrology, to the warming rates in the arctic and in mountainous regions, to the interactions between land and atmosphere. Important practical applications of an improved representation of snow include planning resilient agriculture and energy production in a changing climate. To date, E3SM is still affected by biases in snow-dominated regions, and especially in mountainous regions such as the Tibetan Plateau and the Western United States.

Two main challenges in representing snow in E3SM are the relatively coarse resolution of land model simulations, and the simplified physics used to represent snow processes in the model. Objective of this project is to improve the representation of snowpack dynamics in the E3SM land model (ELM) by resolving key physical processes which are still absent: the effects of snow aging on the evolution of snow grain shape, and the variability of snow cover over mountainous terrain. The snow grain shape, linked to its specific surface area, affects how heat penetrates through the snowpack and thus contributes to determining its surface reflectivity to solar radiation (that is, its albedo).

The snow cover is a key quantity which also contributes to the land surface albedo, and is challenging to predict over complex terrain due to its spatial variability. Here we plan to improve the representation of snow cover over mountains in ELM by adopting a data-driven approach based on high-resolution terrain datasets. Together, these model improvements will be comprehensively evaluated by comparing model simulations with in-situ and remote sensing data. This analysis will evaluate how the model reproduces changes in snow cover, snow albedo, and snowmelt rates. We will then employ the updated version of ELM developed as part of this project to investigate the strength of surface albedo feedback, to quantify how the uncertainty in snow model parameters translates to uncertainty in snowpack predictions, and to assess the changing risk of snow drought for the continental United States

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

Exploring the Kinetics and Reaction Dynamics of Peroxy Radical Unimolecular Decay

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The objectives of this research are to implement innovative experimental and theoretical techniques to study the unimolecular decay of peroxy radicals. Furthermore, the research aligns with the Funding for Accelerated, Inclusive Research (FAIR) funding opportunity announcement goals by establishing a partnership between Argonne National Laboratory and Coastal Carolina University, a primarily undergraduate and emerging research institution. Peroxy radicals are reactive organic intermediates ubiquitous in the chemistry of oxygenated environments. The fate of peroxy radicals is highly dependent on the functionalization of the peroxy radical and the conditions of the local environment, such as temperature, pressure, and co-reactant concentrations. Hydrogen atom migration reactions are critical in the unimolecular decay of peroxy radicals: they impact the propensity for the recycling of hydroxyl radicals (an important oxidant), and play a central role in autoxidation, which leads to molecular weight growth and particle formation. Biomolecular reactions of peroxy radicals can compete with unimolecular decay, affecting tropospheric ozone concentrations and the formation of low-volatility molecules. The competition between peroxy radical reactivity between unimolecular decay and bimolecular reaction is sensitive to the rate of the hydrogen atom migration reactions, which highly depends on the functionalization of the peroxy radical. Recent theoretical investigations have shown that the H-atom migration rates of peroxy radicals with different functional groups can vary by as much as fifteen orders of magnitude. Such a vast range in unimolecular decay rates has potentially important implications for the relative importance of critical pathways in Earth's lower atmosphere and low-temperature combustion, such as autoxidation, particle formation, and autoignition. However, the predicted unimolecular decay rates of functionalized peroxy radical are largely uncharacterized due to experimental challenges. Understanding the unimolecular decay of functionalized peroxy radicals demands a holistic approach that uses multiple experimental and theoretical methods. Therefore, their chemistry will be investigated directly in separate complementary experiments at Coastal Carolina University using a new appartus to study the unimolecular decay of peroxy radicals under jet-cooled and collision-free conditions, and at Argonne National Laboratory under thermal conditions, in which the reactivity of peroxy radicals will be studied at a specific temperature and pressure. In both experiments, the peroxy radicals will be generated and stabilized under conditions that minimize unwanted side chemistry and allow direct observation of their unimolecular decay in fundamental pump-probe laser experiments. Peroxy radicals with carbonyl and carboxylic acid functionalization will be specifically targeted due to low energy barriers for their hydrogen atom migration reactions. The results from the experiments will be compared with state-of-the-art theoretical calculations of the predicted unimolecular decay reaction dynamics and kinetics using methods developed at Argonne National Laboratory. The combination of results from this multidisciplinary approach will provide a complete picture of the unimolecular decay of peroxy radicals and transform our understanding of their chemistry in oxygenated environments, such as the Earth's atmosphere and low-temperature combustion.

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

Understanding Degradation Mechanisms and Rates in Acidic Metal Oxide Oxygen Evolution Electrocatalysts

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Green hydrogen, produced from splitting water with renewable electricity, is the most critical, not fully demonstrated technology necessary to enable a clean, sustainable energy system aligned with the DOE mission. Proton-exchange membrane (PEM) electrolysis is the favored pathway currently for green hydrogen but has significant fundamental scientific challenges in terms of the oxygen evolution reaction (OER) catalyst used due to the complexity of materials and reactions involved. Our limited understanding of catalyst degradation, which involves surface reconstruction and metal dissolution under the highly oxidizing potentials and corrosive environments encountered during oxygen evolution under acidic conditions, remains a bottleneck to the development of improved catalysts.

The project objectives are to develop new research capabilities at Texas State University, in partnership with the National Renewable Energy Laboratory, and to understand how surface reconstruction affects metal dissolution rates and degradation mechanisms in metal oxide OER electrocatalysts. The research scope involves the evaluation of how metal substituents, crystal structure, and defects affect surface reconstruction and degradation. Through this collaborative effort, the project will help advance understanding of surface structure-activity-degradation relationships and inform the development of highly active, durable OER electrocatalysts for lower cost, highly durable PEM electrolyzers while expanding knowledge and infrastructure that can applied to numerous electrocatalytic reactions. The project will also expand research capabilities at Texas State University, one of the largest Hispanic Serving Institutions in the U.S., with a large population of students from underrepresented groups and first-generation college students.

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

4D-STEM Nano-Characterization Infrastructure to Enhance Materials Research for Underrepresented Minorities

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This research project aims to significantly enhance the nano-characterization infrastructure at Florida A&M University (FAMU) by adding 4D Scanning Transmission Electron Microscopy (STEM) capability to study advanced high-temperature superconductors and nanostructured high-performance composites and structural materials with advanced data analysis. 4D STEM, a technological breakthrough that uses a pixelated electron detector to capture a convergent beam electron diffraction pattern at each scan location, will open up a new level of quantitative characterization at FAMU, the largest public Historically Black College & University (HBCU). The mapping of atomic/nano-scale information by 4D STEM will resolve the nano-characterization needs to understand energy materials, including strain and stoichiometry variations at the nano and macro scales and the processing-microstructure-property relationships. By acquiring a new direct electron detector for 4D STEM and building the collaboration network with Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL), this research project will provide FAMU students with access to a nationally competitive nanocharacterization capability and facilitate the engagement of underrepresented talent in the microscopy community. A major challenge of 4D STEM lies in handling the massive 4D datasets generated, which can reach terabyte scales for high-resolution experiments. This research project will create a pipeline of 4D STEM data analysis for underrepresented minority (URM) students. Advanced computing resources using modern graphics processing units enable hybrid algorithms that combine multislice and Bloch wave methods for improved accuracy and speed of the data analysis. The rich 4D-STEM data set enables orders of magnitude more efficient recording of complex nanostructural information and opens up new horizons in making new discoveries from “big data” using, for example, machine learning. These research efforts are strengthened by collaboration with ORNL. This research project will provide invaluable training opportunities for URM students and postdocs in nanoscience and nanotechnology research.

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

Probing Coherence Dynamics in Model Systems to Understand Energy Transfer in Photosynthesis

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The multi-step process of photosynthesis begins with the absorption of light followed by transfer of electronic excitation energy to a reaction center, effecting the charge separation necessary to drive the biochemical reactions that feed most life on earth. The entire photosynthetic process in most organisms has about a 1% energetic efficiency. By contrast, the quantum efficiency—which is the ratio of photons absorbed to charge-separated states produced—of the electronic energy-transfer process in photosynthesis can be nearly 100%. This fact is surprising because the structure of a photosynthetic protein is not a perfect lattice like that of single-crystal silicon used in photovoltaic panels. Hence, an improved understanding of energy-transfer mechanisms in photosynthesis is both of fundamental research interest and may offer new design principles for improving solar-energy conversion technologies. One question is the effect of so-called quantum coherences on the overall energy-transfer process. A quantum coherence is the superposition of multiple energetic states, which can be conceptualized as wavepackets of energy that move with time. The question of coherence has persisted for decades, remaining unanswered in part because natural photosynthetic complexes have limited synthetic tunability. The objective of this research is to overcome the issue of limited synthetic tunability of natural photosynthetic complexes by using DNA-templated molecular aggregates as model systems. These tailored molecular aggregates have vast synthetic tunability, and this project will incorporate bilins and chlorins as chromophores. Some bilins and chlorins are natural photosynthetic pigments, but also have synthetic tunability in the laboratory using well-understood chemical reactions. The studies of DNA-templated aggregates will use time-resolved spectroscopic measurements, paired with quantum-chemical computations, to evaluate two key questions: (1) Do the coherences persist longer as the electronic coupling comes into resonance with a vibrational mode? and (2) Does the frequency of the coherence downshift to very long frequencies, as predicted by theoretical model, as the electronic coupling comes into resonance with a vibrational mode? Answers to these questions will improve the interpretation of the coherences that appear in measurements of natural photosynthetic light-harvesting proteins and thereby produce new knowledge into photosynthetic structure-function relationships, which can be used to build new bio-inspired energy-conversion technologies having improved efficiencies or characteristics.

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

Mechanistic Understanding of Electro-Chemo-Mechanical Interplay for Selective and Intercalative Extraction of Uranyl Ions using Disordered Metal Oxides

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Extracting uranium from uranium-bearing mining wastewater remedies the ecosystem and helps address uranium security for the nation's needs. Current uranium separation processes, which are primarily based on adsorption, have limited separation capacity, poor selectivity against competing ions such as sodium and magnesium, and high processing costs. In contrast, electrochemical intercalation chemistry, which allows high capacity and reversibility of cation separations using battery electrodes via a faradaic process, is an energy-efficient recovery technology. While electrochemical separations are energy-efficient, extraction capacity and selectivity limit the electrochemical separation of uranium ions from wastewater. To address these limitations, project objectives focus on understanding and controlling interactions between layered metal oxide battery electrodes and uranium-bearing wastewater to achieve high-capacity and selective separation of uranyl ions. Specifically, a series of electrochemical, chemical, and mechanical processes that involve uranium ion intercalation, uranium oxide deposition, and mechanical deformation of metal oxide host materials are used to investigate how disordered metal oxide layered materials interact with uranium ions. Complementary methods, including wet-chemistry synthesis, electrochemical experiments, in situ strain/stress measurements, in situ synchrotron X-ray total scattering analysis, and electron microscopy are used to gain fundamental insights into molecular and material drivers in separation processes and reproducibility. The iterative Electro-Chemo-Mechanical process feedback loop enables a comprehensive understanding of high-capacity, selective, and stable uranium recovery using intercalative battery electrodes. The knowledge gained could impact how uranium is recovered, thus benefiting the broad chemical science community and advancing an eco-friendly critical material recovery approach.

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

Leveraging Radical Dynamics to Generate Nuclear Spin Hyperpolarization

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This project seeks to advance Nuclear Magnetic Resonance (NMR) spectroscopy by developing innovative methods for enhancing nuclear spin polarization, a critical factor in improving the sensitivity and resolution of NMR-based imaging and analysis techniques. At the core of this research is the exploration of how molecular motion, electron spin resonance, and light can be simultaneously matched and coupled to boost the transfer of spin order from electron to nuclear spins through the Overhauser dynamic nuclear polarization (DNP) mechanism. The project aims to harness these insights to create new free radical polarizing agents that outperform existing ones that utilize instead the so-called cross effect mechanism.

A key focus of the research is the use of Blatter-type radicals as a platform for carefully controlling molecular motions that are predicted to significantly impact the efficiency of spin polarization. By manipulating the molecular structure and dynamics of these radicals, researchers aim to enhance their ability to transfer spin polarization, a process that could dramatically improve the performance of DNP at high magnetic fields. The development of new narrow-line Overhauser DNP polarizing agents, including modified perchlorotriphenylmethyl (PTM) radicals, will be central to achieving these advancements. Prototypical Overhauser polarizing agents will be evaluated in performance using multi-field DNP and compared against high-level spin dynamics calculations in a feedback loop aimed at understanding and improving efficiency. This research will contribute to a deeper understanding of atomic and molecular systems and the fundamental processes that govern their behavior under strong electromagnetic fields. The results of this project have the potential to transform NMR spectroscopy and imaging technologies by enabling more efficient, precise, and chemically stable polarizing agents for a range of applications.

In addition to the scientific goals, this project is committed to building research capacity at the University of Michigan-Dearborn by enhancing personnel expertise, laboratory infrastructure and fostering collaborative relationships with AMES. An integral part of the project is its focus on inclusivity, with initiatives aimed at increasing the participation of women and underrepresented groups in STEM fields. Outreach programs targeting community colleges, K-12 students, and educators will further promote scientific engagement and create pathways for future leaders in the field.

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

Molecular engineering control of photo-induced charge transfer and transport in donor-acceptor frameworks

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Next generation photoconductive materials and photocatalysts are needed to sustainably support current and growing U.S. and global energy demands. This research project explores molecular engineering strategies for realizing new functional materials and discovering novel mechanisms for photo(electro)catalysis, particularly for solar fuels generation. Such materials should exhibit strong visible light absorption and long-lived charge separation with the capacity for charge transport (i.e. photoconductivity) while also affording a high density of accessible catalytic sites — a difficult combination of properties to implement in traditional catalytic systems. Metal organic frameworks (MOFs), as a class of porous solid-state materials composed of metal ions or clusters connected through organic/organometallic linkers, are emerging alternatives for meeting these design targets. MOFs naturally incorporate light-responsive components that provide charge transfer and transport channels while simultaneously offering unique reaction environments with high densities of catalytic sites that are tunable through both framework design and post-synthetic modification. Despite a recent flurry of MOF photocatalyst demonstrations, significant knowledge gaps remain regarding their underlying photophysics and associated catalytic reaction mechanisms that impede rational optimization. This research is therefore geared toward a fundamental understanding of both the photophysical implications of MOF material modifications and how these modifications can strategically promote efficient photo(electro)catalysis. Optical transient absorption (TA) spectroscopy techniques, as a set of laser-based pump-probe methods used to gain information on excited state electronic structure and dynamics, are employed to monitor the photophysics and photoconductivity of these MOF systems as a continuous feedback loop to material design. Characterization of photocatalytic performance involves sustainability-minded benchmark reactions, such as CO_2 reduction. NREL's longstanding expertise in applying these tools to problems involving photoinduced electron transfer and subsequent catalytic processes is intended to closely integrate with efforts at Rutgers-Newark on the materials-driven aspects of the project. Within the framework of the DOE-FAIR program, this mutually beneficial collaborative project involves extensive graduate student training on advanced spectroscopic and analytical tools and therefore is building crucial research capacity at Rutgers-Newark, a non-R1, minority serving (MSI) and emerging research institution (ERI).

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

Chaos, mixing, and energy extraction in active nematics

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The objective of this project is to control the chaos and mixing in active materials, using a combination of experiment, simulation, and theory. Nature already provides many examples of active materials, from flocks of birds to sheets of cells and swarms of bacteria, but active materials are a new paradigm in soft condensed matter physics. In the lab, biomimetic and synthetic active materials have been developed, including self-propelled microparticles and dense phases of biomolecules driven by molecular motors. Although they are non-living, biomimetic active materials share the out-of-equilibrium property of living matter, i.e. they consume energy to maintain their complex structures. Such materials do not fit the framework of conventional thermodynamics, requiring new perspectives and techniques. This project focuses on active nematics, a particularly important class of active materials that consume energy to generate self-sustained flows. These active nematics represent a new class of fluids that exhibit spontaneous, self-driven mixing.

This project is a partnership between two minority serving University of California campuses. UC Merced is an R2 institution in the heart of the central valley of California: a historically underserved region. UC Merced will benefit by partnering with UC Santa Barbara, an R1 institution to build expertise and infrastructure in optical microscopy and micro-fabrication. This collaborative project injects a new perspective into the current understanding of active nematics by uniting concepts from fluid dynamics, chaos theory, and the mathematics of braids. The experimental work requires producing microtubule-based active nematics, using microfluidic techniques to be imaged under a microscope undergoing chaotic motion. The material can be confined in wells of various geometries, dramatically influencing defect dynamics. Various microprinted particles and shapes can also be inserted, both affecting and responding to the fluid flow. Microgears can be placed within the fluid to extract work and potentially perform useful functions.

The research will focus on two specific aims: 1. Tuning the self-mixing dynamics via engineering the boundaries of wells and via inserting motile microparticles. 2. Relating a form of entropy for the active nematics to the amount of work extracted. These aims will be approached in tandem using a synergistic combination of experiment and simulation. Current mathematical models do not account for all aspects of these experiments, and new simulation approaches will be developed and tested. Simulations will also guide experimental plans and be used to interpret experimental results. Compared to the long-established field of equilibrium materials, the field of active matter is still rapidly evolving, dominated by just a few materials. It is hoped that this work will spur interest in new synthetic materials using the principles of active nematics to drive self-mixing flows. Control of these self-mixing flows is the next step to achieve a useful new class of solvents. Such solvents might revolutionize micro-mixing technologies and produce novel biomimetic mixing environments.

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

Developing Novel Electrolytes to Suppress Transition Metal Dissolution Using Multimodal Characterization

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This research aims to develop innovative electrolyte formulations that prevent the dissolution of transition metals from lithium-ion battery cathodes, a key factor in battery performance degradation. By systematically varying electrolyte composition and concentration, the project seeks to understand and control the solvation structures of lithium ions. These solvation structures—how lithium ions are stabilized by surrounding molecules—are critical to how the electrolyte interacts with the cathode surface. Insights into these interactions will inform the rational design of next-generation electrolytes that minimize transition metal loss, enhancing battery stability and longevity. The research will employ a combination of advanced characterization techniques, including X-ray scattering, X-ray fluorescence microscopy, and high-resolution transmission electron microscopy. These tools will be used to investigate the atomic-level changes at the electrolyte-cathode interface, as well as map the distribution of transition metals within the battery. Understanding these dynamics will be crucial for developing electrolytes that effectively inhibit transition metal dissolution during battery operation. The collaboration between Northern Illinois University and Argonne National Laboratory combines expertise in chemistry and materials science with state-of-the-art experimental resources. This partnership will enable a comprehensive investigation of how electrolyte formulations impact battery performance, contributing to the broader goal of advancing energy storage technologies. By addressing one of the critical challenges in lithium-ion batteries, this research will help improve the performance and lifespan of energy storage systems used in electric vehicles and renewable energy applications. The outcomes will have significant implications for the development of more sustainable and efficient batteries, aligning with national priorities to reduce carbon emissions and promote energy independence. Additionally, our scientific training and outcome will be integrated into educational programs to promote STEM education and raise public awareness about energy storage.

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

Development of Novel Li-Based Halide Dual Mode Scintillators for Neutron-Gamma Radiation Detection and Imaging

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This research focuses on a systematic study to investigate and grow novel lithium-based inorganic ternary halide scintillators, with higher detection efficiency for many applications, such as high-energy physics, medical imaging, geophysical exploration, and homeland security. The research specifically looks at lithium (Li) containing scintillation materials capable of dual mode gamma-neutron detectors. These Li-based ternary scintillators are highly sensitive to both gamma-rays and neutrons, with high light yields for both gamma-ray and neutron interactions. Initial results show that they are also capable of efficient discrimination between these different radiation types. The versatility of the proposed Li-containing scintillators is expected to be favorable in many detector applications that can benefit the nuclear industry, for example, for gamma-neutron discrimination as well as high resolution gamma or neutron detectors and imaging. Anticipated public benefits include the development and production of new dual mode gamma-neutron detectors with these favorable properties. This research also seeks to improve detector materials incorporated in radiation detectors or spectrometers that can be utilized in many applications, such as the ones utilized for nuclear nondestructive assay methods, as well as material control and accountancy for nuclear reactor safeguards and nonproliferation efforts. The main task of this research is the growth study of dual-mode scintillators and high-resolution gamma-ray scintillation detectors, as well as the investigation into their material properties. To characterize these scintillation crystal samples, Fisk University (Fisk) conducts measurements of basic scintillation properties such as light yield, decay time, and gamma-ray non-proportionality behavior, as well as other physical and optical properties. In this research Fisk collaborates with Oak Ridge National Laboratory (ORNL) to further characterize the properties of these novel Li-based halide dual-mode scintillators. After the initial gamma-ray characterization, powdered and/or small bulk samples from Fisk are sent to ORNL for crystal structure analyses. Information obtained from these analyses are used to improve the growth systems at Fisk and to further understand the preferrable growth condition for each composition. During this research Fisk sends appropriately processed and encapsulated samples for neutron and/or dual-mode detector characterization at the CG-1A neutron detection test station in ORNL. With this FAIR-funded research-based collaboration, Fisk faculty and students benefit from the state-of-the-art equipment and expertise at ORNL. Advancements in practical and theoretical knowledge are expected at both institutions. Fisk students will have the opportunity to be mentored directly by Fisk and ORNL research personnel at each respective institution as well as gain rigorous research experience that can be adapted in their future academic and/or professional career and development at national laboratories or at other institutions.

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

Collaboration to Introduce Neutron Diffraction to Enhance Research Education by increasing Lab Access (CINDERELA)

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Alabama State University (ASU) and Oak Ridge National Laboratory (ORNL) will collaborate to increase the research capabilities of ASU's chemistry degree program focusing on solid-state inorganic chemistry research. One aim is to engage underrepresented minority undergraduate students in scientific research while providing research opportunities outside of the classroom. This effort also serves as a recruiting tool to increase the viability of ASU's chemistry degree program as well as providing qualified candidates for graduate work to our nation. The partnership with ORNL will provide access to state of the art research tools and professional networking opportunities to enrich the educational experience and have a profound impact in preparing students to advance science. The ASU-ORNL collaboration will investigate the following objective: What is the accuracy of bond valence sum (BVS) to predict the crystallographic locations of trivalent rare-earth (RE^{3+}) substitutions hosted within layered fluoride-based anti-Perovskites by synthesizing the same, determining their crystal structure and measuring the corresponding photoluminescence of these phosphors. An emphasis will be placed on the synthesis, advanced characterization and computer modeling of RE^{3+} substituted and non-RE containing oxyfluoride phosphor materials. These layered oxyfluoride host structures have three distinct positions that can accommodate cationic substitutions to tailor the emission spectrum and create a desired lighting phosphor. Density functional theory (DFT) will guide synthesis and provide predictive modeling in RE^{3+} substituted samples to determine the stability of the structure based on the BVS. The photoluminescence (PL) emission of the resulting phosphors will correlate to the structure stability of DFT modelling. Study of crystallographic structure of air annealed and reduced oxyfluoride samples will help identify the mechanism of the increased PL emission and stability. X-ray diffraction will be used as an essential technique to monitor and identify phases within the synthetic process. Neutron and synchrotron diffraction techniques will further clarify atomic positions within the crystal structure. Refined bond distances and angles from Rietveld analysis will provide experimental bond valence sums and global instability indices for synthetic products from ASU, which will, then be compared with computationally modeled bond valence values from collaborators at ORNL. A joint publication of research results in peer-reviewed journals by undergraduate students in chemistry is expected. CINDERELA funding will effectively allow for chemistry-focused research training for underrepresented African-American undergraduate students, which make up 98% of the enrollment in the chemistry degree program at ASU. Additionally, we will focus on developing the "whole" student by providing a nurturing and challenging educational and professional environment that is scholarship focused. Finally, engaging students and encouraging participation in more advanced research efforts at the undergrad level will positively influence our teaching efforts and shift the culture of our departments.

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

Probing Electronic Instabilities and Magnetic Correlations in Kagome Metals using Advanced Magnetic Resonance Techniques

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Kagome metals have emerged as a fascinating platform for studying complex quantum behaviors. These materials, characterized by a lattice of corner-sharing triangles, exhibit unique electronic properties that can lead to phenomena such as charge density waves, superconductivity, and exotic magnetic orders. Recent discoveries have revealed a rich landscape of behaviors, prompting further investigation into their fundamental properties and potential applications. This research project will elucidate key questions about electronic instabilities and magnetic correlations in kagome metals. The collaboration between California State University, East Bay—a non-R1 minority-serving institution—and Oak Ridge National Laboratory exemplifies the Funding for Accelerated, Inclusive Research (FAIR) program's mission to build research capacity at institutions historically underrepresented in the DOE Office of Science portfolio. The project focuses on three primary objectives using advanced magnetic resonance techniques. First, it will explore the mechanisms behind charge density wave formation, investigating the collective electronic states that emerge from the interplay between the crystal lattice and electron-electron interactions. Second, the research will study how physical strain affects the electronic properties of these systems. Third, the team will examine the magnetic properties of rare-earth-based kagome metals, using chemistry to control the emergence of various magnetic structures. By leveraging nuclear magnetic resonance and electron magnetic resonance, this work generates crucial insight into the electronic and magnetic properties of complex quantum materials, fundamentally improving our understanding of quantum phenomena in strongly correlated electron systems. This knowledge naturally extends towards the development of key quantum technologies, such as more efficient electronic devices, quantum sensors, and quantum computers. Simultaneously, this FAIR project enhances the research infrastructure and expertise at California State University, East Bay, fostering a mutually beneficial relationship with the DOE complex, and Oak Ridge National Laboratory in particular. The collaboration provides unique opportunities for talented students from underrepresented groups to engage in cutting-edge materials research. By involving these students in advanced techniques and analysis, this project will cultivate the next generation of scientists, equipping them with the tools to tackle complex problems in materials science and engineering.

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

Investigation and Prediction of Structural Ordering in Monocrystalline Nitrides Through Classical and Generative Machine Learning and Tunable Energetics

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Disorder in crystalline materials, ranging in both length and dimensionality, can significantly alter the materials and application performance. Processing-disorder-performance relationships are well-studied at some length scales but others, such as zero dimensional (0D) antisite disorder, are less emphasized and less understood. Achieving atomically precise materials through 0D disorder at manufacturing scale would enable unprecedented functionality across a range of applications and would have high technological, economic, environmental, and societal impact. However, to achieve this level of control, a comprehensive understanding of the complex relationship between the synthesis environment and resulting structural ordering is needed. This research will develop world-class plasma-assisted molecular beam epitaxy (PAMBE) capabilities and create classical and generative machine learning (ML) models for predictive PAMBE synthesis. These new capabilities will enable the study, understanding, and control of 0D disorder in energy relevant single crystalline nitrides, specifically cation-anion disorder in NbN and TaN, and mixed-cation disorder in the anti-perovskite Mn_3GaN and the perovskites $NbTaN_3$, and $ThTaN_3$.

Disorder-controlled synthesis of these nitrides requires overcoming the high formation energy associated with the low order structures of these materials. This research will develop and test new corona discharge effusion and plasma sources that will provide a pathway to overcome this energy deficiency issue. These sources will enable the quantitative study of the evolution of 0D disorder during synthesis through in situ measurements the Bragg-Williams order parameter using reflection high-energy electron diffraction. This will be used to probe the effects of the energy of incoming atoms, and various other synthesis conditions, on the formation of 0D disorder in real-time. Simultaneously, machine learning (ML) will be leveraged to correlate the many high-dimensional, non-linear PAMBE growth parameters. This work will create robust training datasets to train both classical and generative ML models to provide predictive capabilities for PAMBE synthesis of monocrystalline nitride thin films.

The identified processing-structure relationships and predictive tools developed in this project will provide a broad understanding of materials synthesis that can be adapted to other deposition and materials systems.

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

Discovering a controlled mechanism to pattern antisite defect qubits in CVD-grown monolayer Transition Metal Dichalcogenides

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As the need for secure communication grows in a globally connected world, quantum computing offers a promising pathway to groundbreaking security technologies through quantum bits or qubits. A qubit, unlike a traditional computer bit, can exist in multiple states simultaneously, enabling exceptional computational power for complex tasks such as encrypted communication and advanced simulations. To achieve qubits on an atomic scale, precise material engineering is essential. This project aims to develop and control specific atomic-scale defects in two-dimensional (2D) transition metal dichalcogenides (TMDs), creating an innovative foundation for qubit-based systems. Leveraging proton irradiation, the research will systematically generate and control defects like antisites in materials such as tungsten disulfide (WS_2) and tungsten diselenide (WSe_2), critical for scalable and stable qubit operation. Through an integrated approach that combines computational modeling and experimental characterization, this project seeks to decode the physics behind defects and establish methods to manipulate these defects without introducing strain or foreign elements, paving the way for qubits that operate at room temperature and are robust enough for practical applications. Aligned with the mission of the Funding for Accelerated, Inclusive Research (FAIR) program, this project also strengthens research capacity at our institution and a partner Minority-Serving Institution, fosters collaboration with experienced partners, and advances equitable engagement in critical areas of foundational science.

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

Harnessing Recycled Aluminum for Enhanced Alloy Performance: Primary Intermetallic Phase Control through Rapid Solidification

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Recycling aluminum (Al) significantly reduces carbon emissions and cost, as it saves up to 95% of the energy required to produce new Al from raw minerals. Despite these environmental and economic benefits, the use of recycled Al in structural applications is limited, primarily due to high levels of iron (Fe) impurities. Excess Fe in Al alloys lead to the formation of large, brittle Fe-Rich Intermetallic Compounds (FeRICs) during casting, severely impairing mechanical properties (fatigue resistance, ductility, and toughness, etc.). While the addition of alloying elements and increasing cooling rates can mitigate the negative effects of excess Fe, the complex interplay between these modifications on FeRIC formation remains poorly understood. This research aims to develop a comprehensive understanding and predictive capability for controlling FeRIC formation in recycled Al alloys. By combining real-time high-temperature characterization techniques, and advanced materials modeling, the project will investigate the mechanisms governing the formation of FeRICs at the microscopic level.

The project will establish a research capability for alloy development at Missouri University of Science and Technology by integrating advanced *in situ* characterization techniques and state-of-the-art materials modeling. Understanding the impact of processing conditions on the FeRIC formation mechanism will lay the foundation for the discovery and design of new and improved Al alloys, while broadly impacting the community through the establishment of experimentally validated solidification models. Ultimately, these findings will help inform the design of high-performance recycled Al alloys, enhancing their usability in high-pressure die casting, welding, additive manufacturing, and other rapid industrial solidification processes, potentially increasing energy conservation and reducing carbon emissions.

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

Vortex Light-driven Structured Quantum Matter

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Light-driven materials offer unique opportunities to create and control new out-of-equilibrium states with novel electronic properties, like the Floquet topological insulator. However, most research has focused on uniform light exposure, leaving space-time-dependent phenomena largely unexplored. This study will use structured light, such as vortex beams, to explore new phenomena that emerge from the combined space- and time-modulations. By intertwining the unique properties of structured light with engineered quantum matter, we aim to uncover new phases of matter. A key focus is overcoming challenges like dissipation and thermalization while optimizing both material modulation and light parameters to reveal these novel states. This research will provide theoretical insights into the conditions required to observe these phenomena, highlighting the benefits and limitations of space- and time-modulated systems. This study will pursue three primary objectives: (1) Emergent Photon-dressed States in Vortex Light Beam Driven Dirac-like Materials, (2) Light-matter Interactions in Space and Time Modulated Systems, and (3) Observables, Dissipation and Interactions in Irradiated Open Systems.

This work will combine numerical and analytical approaches, including effective low-energy and tight-binding models for material descriptions. Time dependence will be addressed by Floquet theory, with effective two-band Floquet Hamiltonians for weak light-matter coupling and non-perturbative inclusion of all relevant Floquet bands for strong coupling. We will handle the resulting space-dependent Hamiltonian by identifying light polarization conditions that preserve conservation laws and employing techniques such as Bessel decomposition, finite differences, and recursive methods for systems with boundary conditions. The Keldysh- Floquet formalism will be adapted for space-time-dependent systems in contact with reservoirs to accurately account for thermalization in physical observables. For numerical calculations, this study will develop efficient graphics processing unit (GPU)-based methods to implement these techniques.

This work will advance space-time-modulated systems, impacting Floquet systems, strain engineering, and thermalization in open systems. The findings of this research will guide experimentalists in exploring complex systems and identifying novel states, thus enhancing both theory and practical applications. Additionally, the project will substantially impact training undergraduate students at Kennesaw State University (KSU), offering valuable research opportunities and internships through collaboration with Ohio University. This initiative will enhance KSU's research capacity while providing meaningful experiences for undergraduate and graduate students and postdoctoral researchers.

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

Title Exciton self-trapping in low-dimensional organic metal halide hybrid materials from GW/Bethe-Salpeter calculations and machine-learning-based force fields

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Organic metal halide hybrid perovskites (OMHHs) are of great interest for solar cells and light-emitting diodes (LEDs). These tunable materials show excellent light absorption in thin films, high carrier mobility, easy charge separation for current extraction, and good defect tolerance. A serious problem, however, is the typical rapid degradation under light, heat, and moisture. While initial research interest was on bulk 3D perovskites, recent research has moved toward low-dimensional materials in which the inorganic component forms sheets, wires, or isolated nanocrystals, because they have reduced degradation. They also show an intriguing phenomenon of strong exciton self-trapping, in which the electron and hole produced after absorption of light deform the surrounding atomic structure and become localized. This phenomenon, which does not occur in traditional hard inorganic semiconductors like silicon, leads to emission of white light which can be used for LED devices. A detailed understanding of exciton self-trapping is key for the emerging area of soft semiconductor science, but it remains so far elusive. There have been few theoretical tools to investigate the early-time behavior after absorption of light. However, recent work on excited-state forces in the GW/Bethe-Salpeter equation (GW/BSE) approach allows a single efficient calculation to give the direction that each atom will move after absorption of light and opens the prospect of accurate calculations of these phenomena. This project comprises three research thrusts:

1. GW/BSE calculations of self-trapped excitons,
2. Parametrization of machine-learning-based force fields for excited states, and
3. Study of exciton structure and transport on longer length scales via force fields.

Results will be compared to experimental data from collaborators. Recent work at UC Merced has provided a practical software implementation for excited-state forces and demonstrated the accuracy of the method. The GW/BSE method will provide accurate electron-hole interactions, and the calculations will be used to parametrize novel force fields that describe the excitation energy. Molecular dynamics with force fields will be used to study longer length and time scales. This work will be enabled by expertise at LBNL's Molecular Foundry on OMHHs and machine-learning force fields and will build on previous collaborations. The project will contribute to the fundamental understanding of excitations in soft semiconductor materials, advance the methodology of excited-state structural dynamics and machine-learning force fields, and inform the design of materials for LEDs. Implementation of new methods will be provided in the widely used open-source code BerkeleyGW (which is DOE-supported) and presented in tutorials for broad availability to the community. The project will build research capacity for further work in this area and enable proposals for future BES funding. Graduate student collaboration with LBNL and summer research at the Molecular Foundry will build the research culture of UC Merced, an institution only 19 years old and still developing.

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

Building the Infrastructure for Physical Property Measurements Toward the Design of Organic-Inorganic Hybrid Materials with Geometric Frustration

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In solid-state materials, chemical bonding varies from strong intermolecular forces in extended solids, such as ionic or polar covalence, to weaker interactions in molecular solids such as Van der Waals or hydrogen bonding. This project develops synthetic strategies and guiding principles for the discovery of organic-inorganic hybrid materials in single compounds comprised of both extended- and molecular-solid chemical bonding motifs. These guiding principles will affect the design of structures with geometric magnetic frustrations, which would broadly affect magnetic properties of crystalline condensed matter. In alignment with the FAIR-FOA to build research infrastructure at diverse institutions, the project acquires the VersaLab instrument to train students on measuring physical properties in teaching labs and through research projects at California State University San Bernardino (CSUSB), a federally designated Hispanic-Serving & Emerging-Research Institution. By employing solid-state synthesis techniques in combination with fundamental principles from both organic chemistry and inorganic extended solids, intermetallic halides will be systematically modified to embed organo-ammonium electron-donating groups (EDGs) with various steric effects. The project involves: (1) establishing general principles for incorporating molecular organic EDGs into inorganic extended solids, (2) structurally characterizing products to uncover the fundamental effects of targeted hybrid organic-inorganic chemical compositions, (3) optimizing single-phase products for physical property characterizations, (4) rationalizing structural formations via computational investigations of chemical bonding and electronic structure theory, and (5) establishing structure-physical property relationships via direct transport and magnetic property measurements. Students will train preliminarily at CSUSB on the VersaLab magnetometer and more in-depth with other advanced structure and physical property characterization equipment (e.g., electron paramagnetic resonance, solid-state nuclear magnetic resonance, cryogenic Evercool system) at Pacific Northwest National Laboratory (PNNL). The collaboration with PNNL aligns with the FAIR-FOA to further expand the capabilities of CSUSB in training students by exposing them to the scientific workforce and diverse instrumentation of a DOE national lab. The overall outcomes of this research will be new predictive relationships between atomic sizes and steric hindrance effects, and a broader application of electronegativity effects, including electron-donation by molecular organic fragments, on the structural formation of crystalline condensed matter. This greater understanding advances the science of synthesis and materials discovery by offering new building blocks to target organic-inorganic hybrids and improve control over materials design and magnetic properties.

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

Exploring the effect of thermal energy by the plasmonic photothermal catalyst in hydrogen generation

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Scientists are developing a method to efficiently produce hydrogen fuel from water using special photocatalyst materials that harness sunlight. Recently, they have added tiny metal nanoparticles to these materials to enhance efficiency. However, researchers disagree on how these metal nanoparticles aid the process. Some argue it results from significantly increased heating in confined spaces, while others believe it is due to very energetic carriers. This debate persists because characterizing the effect of local heating is challenging. This project aims to resolve this mystery by developing advanced imaging techniques to simultaneously measure thermal energy and gas (hydrogen and oxygen) production on a very small scale (billionths of a meter) with a controlled plasmonic nanoparticle array. By studying how tiny metal particles generate and share heat, this project will solve a key mystery: do these materials produce more hydrogen because they get hot, or because they create special high-energy particles? Understanding this will help us make better materials for turning sunlight into clean hydrogen fuel. A gold-titanium material system will be used for water splitting in a photoelectrochemical cell, and the nanoparticle array will be created using electron-beam lithography. A simultaneous temperature and gas detection technique will be developed using highly sensitive surface plasmon resonance (SPR) imaging. The imaging technique's sensitivity will be enhanced through microscope and metamaterial design. This technique will be complemented with ultrafast spectroscopy, gas chromatography-mass spectrometry (GC-MS) or a gas analyzer, and computer simulation. The gas detection generated by SPR will be compared with GC-MS to establish an experimental relationship between simultaneous temperature and gas detection in SPR imaging. Ultra-fast measurements and computer simulations, incorporating advanced physics and chemistry models, will be employed to observe how rapidly these materials generate gas. The measurements will monitor the process from extremely brief moments to longer durations. This will enhance our understanding of heat transfer through the material, which is essential for improving process efficiency. The research outcome will be significant as it allows simultaneous measurement of temperature and gas generation from nanoparticles, providing a direct relationship between thermal energy and hydrogen generation. It will clarify the primary mechanism in enhanced hydrogen generation. This technique has applications in various fields, including clean energy, medicine, and chemical processes. The project aligns well with DOE Basic Energy Science priorities and will leverage the existing capabilities at Texas A&M University-Corpus Christi (TAMU-CC) and the state-of-the-art facilities at Sandia National Laboratories (SNL), preparing the project team thoroughly for this research. This collaboration holds great potential for new discoveries in how light interacts with materials to produce chemical reactions like hydrogen production. The project will foster a constructive partnership between TAMU-CC and SNL, aiding TAMU-CC, a Hispanic Serving Institution (HSI) in the Coastal Bend region of South Texas, in expanding its research capabilities in fundamental science. Students, a post-graduate researcher, and the lead scientist will benefit from access to cutting-edge equipment and the opportunity to exchange ideas with experts in the field.

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

Fundamental studies of the influence of ligands on the molecular structure of noble metal nanoclusters

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Ultra-small nanoclusters are aggregates of two or more metal atoms bonded in specific geometric structures. These materials are at the forefront of chemical research because of their applications in technologies that increase the energy efficiency and selectivity of large-scale industrial chemical reactions and enable solar energy generation. To put the unique size of these materials in perspective, the period at the end of the previous sentence is around one hundred thousand nanometers in diameter. In comparison, nanoclusters are typically one nanometer or smaller. At this molecular scale, nanoclusters exhibit unique size-dependent properties that do not evolve predictably to the bulk phase. Achieving the scalable synthesis of size-focused clusters with predetermined properties is one of the grand scientific challenges in this field. To address this challenge, this project will build capacity at Grinnell College, an emerging research institution, to enable a predictive understanding of how different organic ligand molecules influence the structure and properties of ultrasmall noble metal nanoclusters. This objective will be achieved through the acquisition of new mass spectrometry capabilities that will be used to recruit and train a diverse group of undergraduate students. Understanding the influence of ligands on cluster synthesis and properties requires closely integrated experimental and computational research, which provides an ideal training environment for undergraduates. Students will learn how to use mass spectrometry to characterize the size, charge, and composition of solution-phase synthesis products. Students will also learn how to deposit nanoclusters onto solid supports using the specialized ion soft-landing technique developed at Pacific Northwest National Laboratory. Soft landing allows the preparation of size-selected clusters on surfaces without the solvents, counterions, and contaminants that often confound characterization and theoretical modeling. After deposition, students will learn how to analyze the supported clusters using vibrational spectroscopy and electrochemical characterization techniques. By comparing the experimental results with computational modeling, students will gain insight into the size-dependent molecular-level structures of clusters. This approach will train students in molecular modeling using quantum chemistry calculations. The fundamental knowledge obtained from this project will address knowledge gaps inhibiting the scalable synthesis of size-selected noble metal nanoclusters with tailored properties for a broad range of energy-related applications and build the research capacity at Grinnell College to train a new generation of scientists in cutting-edge experimental and molecular modeling techniques.

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

Excitons in Flatlands: First-Principles Explorations

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This Department of Energy (DOE) FAIR project aims to strengthen computational materials research and education at California State University Northridge (CSUN) through a partnership with the University of California at Riverside (UCR). As a non-R1 minority serving institution, CSUN is one of the largest comprehensive universities in the US with an annual enrollment of ~38,000 students. In close proximity to CSUN, UCR is an R1 minority serving institution with strong research and education programs in basic energy sciences. This FAIR project focuses on the development of first-principles computational methods based on time-dependent density functional theory (TDDFT) and the application of these methods to explore excitonic properties in two-dimensional (2D) van der Waals materials. The 2D van der Waals materials are emerging quantum materials with significant scientific interests and potential applications. Excitons are elementary excitations (i.e., correlated electron-hole pairs) in semiconductors and play crucial roles in optoelectronic properties of semiconducting materials.

Three objectives will be pursued in this FAIR project:

(1) Develop accurate, efficient, and robust real-time TDDFT methods with optimally tuned, screened and range-separated hybrid exchange-correlation functionals to study excitons in 2D van der Waals materials.
(2) Explore excitonic properties in 2D ferroelectric materials and their heterostructures that are both scientifically important and technologically relevant.
(3) Train next-generation materials scientists with diverse backgrounds and encourage them to pursue careers in science, technology, engineering and mathematics fields.

More specifically, the project supports the development of powerful and versatile first-principles methods that combine real-time TDDFT with non-adiabatic molecular dynamics to track real-time dynamics of excitonic states under ultrafast and/or strong electric fields. These methods will enable scientists to examine the interplay of electron excitation, polarization, and magnetism in 2D van der Waals materials and explore the coupling of charge, lattice, spin, and valley degrees of freedom in response to ultrafast laser fields. A number of important scientific problems will be addressed, including elucidation of excitonic properties in 2D ferroelectrics, and their heterostructures with 2D magnets and prediction of ferroelectric excitonic insulators. The project is ambitious, but if successful, it could lay the foundation for attosecond materials science and for critical technologies (optoelectronics, nonvolatile memories, spintronics, quantum information) relevant to the DOE mission.

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

Understanding and Tuning the Interplay between Electronic Topology and Magnetism in Magnetic Topological Materials

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Magnetic topological semimetals (MTS) are a rapidly emerging class of materials at the forefront of condensed matter physics, offering transformative potential for fields such as spintronics, quantum computing, and catalysis. These materials exhibit a unique interplay between magnetism and electronic topology, leading to exotic transport phenomena like the anomalous and topological Hall effects. However, the fundamental relationship between magnetism and topology in MTS remains elusive. This research seeks to explore that relationship by focusing on two families of rare-earth-based, noncentrosymmetric MTS compounds.

This project will investigate two key mechanisms: (i) topology-mediated magnetism, where electronic topology influences magnetic interactions, and (ii) magnetism-driven topology, where magnetism controls topological states. By applying physical and chemical pressure, the project aims to systematically tune the magnetic and electronic band structures of these materials to better understand their electronic and magnetic responses. This approach will allow researchers to uncover how the interaction between magnetic order and electronic topology can be harnessed and manipulated, providing insights that could lead to the development of tunable materials for advanced technological applications.

This research will not only generate new insights into MTS but also promote accessibility and inclusivity in scientific research. The project will enhance Kennesaw State University's research capabilities and provide hands-on training and impactful opportunities for students in collaboration with Oak Ridge National Laboratory, thus fostering the next generation of scientists in this critical field. By investigating these novel materials, this project will contribute to advancing high-impact technologies and enabling scientific breakthroughs in energy-efficient, next-generation devices.

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

Elucidating Oxophilic Pathways of Enhanced Epoxidation Reactions by Optimization of Ag Assemblies on Bifunctional Copper-based Catalysts

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Selective catalytic oxidation is a key process that impacts numerous reactions steered through active sites and beyond to yield desired chemical products of value. Atomic level design of such sites is key to improved efficiencies and mitigation of waste. For instance, the transformation of ethylene into ethylene oxide and propylene into propylene oxide are super selective reactions which are valued at $77 billion on the global market. It is critical that reactions occurring on this scale have high selectivity to mitigate greenhouse gas emission, like the formation of carbon dioxide (CO_2). Currently, silver (Ag) and copper (Cu) materials are used to catalyze the production of ethylene and propylene oxide. High selectivity can be achieved when a second element is added to the Ag and Cu catalysts. Unfortunately, the addition of a second element to catalysts is expensive and, in some cases, toxic yet may not yield improved reactivity. Recently, the use of AgCu bimetallic materials have gained significant attention due to their selectivity enhancement of these reactions. Many questions still surround the highly selective AgCu bimetallic catalysts, including: what happens to the AgCu material during the reaction of ethylene?; what kind of oxygen species are useful for forming ethylene oxide?; and how does ethylene look as it transforms to ethylene oxide?

To answer these questions, experimental, theoretical, and educational approaches used to investigate the objectives will harness the combined expertise of the PI's Baber, Weaver, and Senanayake forming a unique partnership between an undergraduate research institution (James Madison University, JMU) and national laboratory capabilities (Brookhaven National Laboratory, BNL). To investigate the reactivity of the catalysts, temperature programmed reaction spectroscopy and reactor kinetic testing using gas chromatography-mass spectrometry will be used. Density functional theory (DFT) calculations will be used to investigate the structure and energy of ethylene and the intermediates formed on the way to becoming ethylene oxide on the surface of AgCu catalyst.

This project will leverage advanced *in situ* facilities at BNL, including ambient pressure X-ray photoelectron spectroscopy (AP-XPS) and diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), which JMU undergraduate researchers will utilize. This project will benefit faculty and students from JMU as we build upon existing research capacity as a newly minted R2 institution and give undergraduates hands-on research experience at JMU and BNL.

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

Ultrafast Dynamics of Core-shell Nanoparticle Photocatalysts

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Catalysts play a critical and ubiquitous role in industry, being used to produce liquid fuels, synthesize fertilizers, manufacture plastics, and minimize combustion-engine pollution. They accomplish these tasks by providing alternative paths for reactions that are more efficient. However, many catalysts fail to meet today's industrial demands, often due to limitations in their design or the prohibitive cost of rare or complex materials. This has driven the search for innovative catalyst designs. Among the promising candidates are gold nanoparticles, which have gained attention due to their ability to harness light energy to facilitate chemical reactions. These nanoparticles have the potential to overcome some of the material limitations that hinder traditional catalysts and are relatively simple to synthesize, making them attractive for further research. However, their application is currently confined to a small range of reactions, limiting their broader use. The aim of this research is to broaden the scope of gold nanoparticle catalysts by modifying their chemical properties through the encapsulation of a thin shell of another metal, creating core-shell structures. This modification could enable the nanoparticles to catalyze a wider range of reactions that are activated by light. The research objectives include the design, synthesis, and characterization of these core-shell nanoparticle catalysts; benchmarking the light-induced chemistry facilitated by the nanoparticles; and probing the fundamental chemical processes occurring on their surfaces. Understanding these processes is crucial for designing tunable and efficient light-activated core-shell nanoparticle catalysts. By broadening the range of reactions gold nanoparticles can catalyze, this research holds potential for advancing more sustainable and cost-effective catalytic solutions. The development of versatile, light-responsive catalysts could reduce the need for rare materials, lower energy consumption in industrial processes, and contribute to greener technologies in fields ranging from energy production to environmental remediation. The findings of this research may offer a pathway toward more innovative and scalable applications, paving the way for more sustainable, cost-effective solutions across a range of industries.

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

Exploring the Kinetics and Reaction Dynamics of Peroxy Radical Unimolecular Decay

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The objectives of this research are to implement innovative experimental and theoretical techniques to study the unimolecular decay of peroxy radicals. Furthermore, the research aligns with the Funding for Accelerated, Inclusive Research (FAIR) funding opportunity announcement goals by establishing a partnership between Argonne National Laboratory (ANL) and Coastal Carolina University, a primarily undergraduate and emerging research institution. Peroxy radicals are reactive organic intermediates ubiquitous in the chemistry of oxygenated environments. The fate of peroxy radicals is highly dependent on the functionalization of the peroxy radical and the conditions of the local environment, such as temperature, pressure, and co-reactant concentrations. Hydrogen atom migration reactions are critical in the unimolecular decay of peroxy radicals: they impact the propensity for the recycling of hydroxyl radicals (an important oxidant), and play a central role in autoxidation, which leads to molecular weight growth and particle formation. Biomolecular reactions of peroxy radicals can compete with unimolecular decay, affecting tropospheric ozone concentrations and the formation of low-volatility molecules. The competition between peroxy radical reactivity between unimolecular decay and bimolecular reaction is sensitive to the rate of the hydrogen atom migration reactions, which highly depends on the functionalization of the peroxy radical. Recent theoretical investigations have shown that the H-atom migration rates of peroxy radicals with different functional groups can vary by as much as fifteen orders of magnitude. Such a vast range in unimolecular decay rates has potentially important implications for the relative importance of critical pathways in Earth's lower atmosphere and low-temperature combustion, such as autoxidation, particle formation, and autoignition. However, the predicted unimolecular decay rates of functionalized peroxy radical are largely uncharacterized due to experimental challenges. Understanding the unimolecular decay of functionalized peroxy radicals demands a holistic approach that uses multiple experimental and theoretical methods. Therefore, their chemistry will be investigated directly in separate complementary experiments at Coastal Carolina University using a new apparatus to study the unimolecular decay of peroxy radicals under jet-cooled and collision-free conditions, and at ANL under thermal conditions, in which the reactivity of peroxy radicals will be studied at a specific temperature and pressure. In both experiments, the peroxy radicals will be generated and stabilized under conditions that minimize unwanted side chemistry and allow direct observation of their unimolecular decay in fundamental pump-probe laser experiments. Peroxy radicals with carbonyl and carboxylic acid functionalization will be specifically targeted due to low energy barriers for their hydrogen atom migration reactions. The results from the experiments will be compared with state-of-the-art theoretical calculations of the predicted unimolecular decay reaction dynamics and kinetics using methods developed at ANL. The combination of results from this multidisciplinary approach will provide a complete picture of the unimolecular decay of peroxy radicals and transform our understanding of their chemistry in oxygenated environments, such as the Earth's atmosphere and low-temperature combustion.

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

Development of Cold Spray Additive Manufacturing for Tungsten-Based Plasma-Facing Components

Dr. Grant Crawford[1], Professor
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The objective of the project is to investigate and develop cold spray additive manufacturing of tungsten-based materials for plasma-facing component manufacturing and repair. South Dakota School of Mines and Technology (SDM), along with their partners at the University of New Mexico (UNM), will define the multi-dimensional relationships between cold spray processing conditions, microstructural characteristics, and helium-induced degradation behavior of tungsten-based materials produced by cold spray technology. SDM, a non-R1 emerging research institution, is uniquely positioned to lead this research effort due to the combination of state-of-the-art facilities with extensive expertise in additive manufacturing technology. This research program will not only mark the beginning of fusion energy research at SDM, but will also foster a new collaboration with UNM, a Hispanic Serving Institution (HSI) and an emerging leader in fusion energy research. Furthermore, it will provide education and training opportunities for undergraduate and graduate researchers, representing the next generation of fusion energy scientists. This research will systematically study the cold spray processing of tungsten-based materials and establish the response of their microstructures to fusion-irradiation conditions. Cold spray is a solid-state additive manufacturing technique that produces unique microstructural features and can be used for *in-situ* manufacturing and repair. This work will build upon the cold spray deposition expertise previously developed at SDM by processing refractory materials suitable for use as plasma-facing materials (PFMs) for fusion reactors, which are relatively unstudied in the field of cold spray technology. Additionally, this work will establish connections between SDM and experts in the fusion community by partnering with UNM. The project will enable the design of tungsten-based alloys and composites with inherent resistance to irradiation-induced damage. It is hypothesized that: (i) compared to wrought tungsten, microstructurally-optimized tungsten-based cold spray coatings will exhibit less irradiation-induced nanostructuring and bubble formation, (ii) *in-situ* peening during the cold spray process will develop microstructures that limit the formation of helium bubbles, (iii) cold spray coatings will have less radiation-induced degradation in micromechanical properties (e.g., irradiation hardening) when compared to wrought tungsten, and (iv) plasma-facing components repaired by cold spray will retain their initial PFMs performance. Ultimately, successful completion of this research will advance the fusion community’s manufacturing toolbox by demonstrating the feasibility of using cold spray in fusion-relevant irradiation conditions.

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

Building Capacity for Novel High-Temperature Plasma Research at San Diego State University

Dr. Jose Castillo[1], Professor of Mathematics and Director of the Computational Research Center
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The Computational Science Research Center (CSRC) at San Diego State University (SDSU), a research-intensive Hispanic—and Asian American, Native American Pacific Islander-serving institution, is partnering with General Atomics (GA), the operator of the DIII-D National Fusion User Facility for the U.S. Department of Energy, Office of Science, Fusion Energy Science (FES). The main goal of this project is to build capacity for novel high-energy plasma research at SDSU in close synergy with GA.

This project targets two of the three elements of FES' vision as announced in December 2023: *(1) bridging gaps through creating innovation engines*, and *(2) ensuring sustainable pathways for a diverse and exceptional workforce*. Expanding the intellectual capacity at SDSU into fusion plasma science will be achieved through the transfer of expertise in the DIII-D diagnostic data, plasma simulations, and control techniques. The close collaboration with GA will be instrumental in providing the SDSU team with DIII-D data for prototyping computer models. Our approach puts forward two complementary research objectives: **(A)** developing and deploying mimetic methods and **(B)** simulation and dynamical systems analysis of nonlinear structures in fusion plasma. More specifically, the Mimetic Difference Group at SDSU has been building theoretical and practical tools that allow researchers to rapidly implement mimetic difference schemes to numerically solve mathematical models with high accuracy. In parallel, the Nonlinear Dynamical Systems group at SDSU has extensive experience investigating nonlinear structures in complex time and position-dependent systems, such as vortex filaments and vortex rings, which have been observed in nuclear fusion plasmas and whose dynamics and control are thought to be key in developing more efficient plasma confinement and compression.

The synergy between SDSU and GA promises mutual long-lasting benefits. We foresee a vibrant exchange of ideas in fusion research between the two sites through these shared research efforts, student training at both sites, and joint meetings. In particular, we will establish a seminar series that will integrate horizontally (between the two sites) and vertically (research, graduate and undergraduate, students and postdocs at SDSU) a springboard to develop successful approaches to understand and improve the operation of the DIII-D fusion plasma facility.

The overall success of this program is aligned with the goal of enhancing inclusion in DIII-D related research and broadening its user community. This partnership will introduce new student-scientists from SDSU's diverse population to the field of fusion plasma physics, in anticipation of fusion's future as a clean source of abundant energy.

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

Fast-Neutron Source Localization using a Single-Photon Camera

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Research will support the fabrication a novel fast-neutron imaging camera for localizing and reconstructing the source of D-D energetic neutron emission within a reaction vessel in three dimensions by determining the neutron tracks back to the source. This detection system would be universal for D-D neutron generation in plasmas (or target based) in any form of fast neutron reactor. The most immediate need for this imaging system is motivated by the theory that many of the D-D fast-neutrons originate not in the central plasma, but rather the walls or grid (cathode) within the reactor. Our neutron camera relies on a novel 3D reconstruction algorithm that leverages physics-based machine learning to reconstruct neutron traces from just a handful of scintillation photons in extremely photon starved settings. The use of such a detection system would not only help other groups working with D-D or D-T reactions for the study of neutron scattering and plasma diagnostics, but also more broadly for neutron scattering and neutron radiography with a wide range of applications from medical imaging to border security.

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

Modeling Ion-Irradiated Mechanical Properties of Novel High-Powered Target Materials

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The research project will develop a reliable framework to accelerate the development of novel materials for next-generation accelerator target facilities. A reverse modeling strategy will be used to design an optimum test matrix. This framework will enable modeling and predicting ion-irradiated mechanical properties using reduced test data, thereby accelerating the development of novel High-Entropy Alloys (HEA) materials for beam window applications. Our research project will include nanoindentation testing and material characterization of several HEAs exposed to ion irradiation. Irradiated mechanical property prediction model and property correlation metamodels will be developed considering traditional and machine learning approaches. Extrapolation will be performed using a data superposition approach to predict the HEAs' material responses under higher irradiation conditions and the results will be validated against test data. The combined optimum testing matrix and robust modeling techniques will be used to help downselect suitable HEA compositions that are most resistant to beam-induced radiation and thermal shock damage. The development and selection of novel HEAs will ensure reliable operation and improved lifetime of beam windows in next-generation accelerator target facilities, such as the 2.4 megawatts Long-Baseline Neutrino Facility, that will support advancements in high-energy physics research.

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

Pioneering Millimeter-Wavelength Line Intensity Mapping Surveys for Large-Scale Cosmology

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Over the last several decades, ever-more precise studies of the large-scale distribution of matter in the Universe have led to important shifts in our understanding of fundamental physics. Maps of the Cosmic Microwave Background (CMB) along with spectroscopic galaxy surveys form the basis of the LCDM model of cosmology, wherein the dynamics of the expanding Universe are driven by competing forces of dark matter and dark energy. Despite the remarkable success of this model, the true nature of these forces remains a mystery. Indeed, tensions between large-scale structure and other measurements of cosmic expansion may hint that even our current limited understanding of cosmic expansion may be faulty.

This project explores a novel survey technique known as Line Intensity Mapping (LIM) with the potential to significantly expand upon current large-scale structure observations. Where spectroscopic surveys require directly imaging thousands of individual galaxies, LIM surveys map the unresolved emission from many galaxies at once, reducing the sensitivity and resolution requirements necessary to map large volumes at great distances. LIM experiments at millimeter wavelengths are particularly exciting, as they can leverage the vast observational experience built up by the CMB community at these wavelengths. This potential, to expand the reach of large-scale structure surveys using the heritage of CMB experiments, makes LIM an exciting near-future opportunity for precision cosmology.

Several demonstrator-scale LIM instruments are currently operating or under construction, but these first-generation observatories lack the sensitivity necessary to compete with modern cosmological surveys. In this project, we will create a fast end-to-end simulation pipeline capable of creating mock LIM signals, observing them with mock instruments, and forecasting constraints on cosmic expansion and dark energy. This will enable us to simulate different cosmologies and instrument designs, laying the groundwork for a wide range of future LIM experiments.

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

DOE-FAIR: Cryogenic Charge Amplifiers for Sub-GeV Dark Matter Detectors

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Cryogenic charge amplifiers with resolution approaching single-electron sensitivity are a promising avenue towards direct detection of sub-GeV dark matter. This project continues development of a novel two-stage cryogenic charge amplifier based on commercial CryoHEMTs. The research is spearheaded by California State University East Bay (CSUEB), a minority-serving institution in the San Francisco Bay Area. Undergraduate students are actively involved in the research program, contributing significantly to various aspects of the project's design and execution. Initial testing and development take place at the CSUEB cryogenics facility. Collaboration with SLAC enables access to sub-Kelvin temperature testing at the SLAC Millikelvin Facility.

During the first phase of the project, efforts are concentrated on enhancing the CSUEB cryogenic infrastructure, developing a preliminary warm electronics board, and refining the CryoHEMT noise model, particularly for low-capacitance HEMTs. This includes measuring current noise and noise variations with respect to bias power and temperature for CryoHEMTs suitable as amplifier inputs. The second phase will focus on developing an active amplifier reset mechanism, a refined cryogenic amplifier package, and an improved warm electronics package. Measurements of the standalone charge and energy resolution using a suitable semiconductor target material will also be performed.

The final product is a complete high-resolution charge amplifier system easily adaptable to any insulating cryogenic detector material which produces charge excitations with immediate applications to sub-GeV dark matter direct detection.

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

Preparing for the Exascale of the CMS Experiment

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Through the support of this grant, the PI, Dr. Allison Hall, will build research capacity at USNA to develop solutions to critical computing challenges faced by the Compact Muon Solenoid (CMS) experiment in the Exascale era through collaborations with scientists and computing professionals at Fermi National Accelerator Laboratory (FNAL), including co-investigators Dr. Bo Jayatilaka and Dr. Nick Smith.

The High Luminosity LHC (HL-LHC) upgrade of the LHC will drastically increase the collision rate and will enable CMS to search for even rarer physics processes. This huge influx of data, however, presents considerable computing challenges in how to efficiently store and analyze exabyte-scale datasets. The primary objective of the proposed computing research is making a credible plan for how to transition the current CMS computing model (including both central offline production and user analysis) to one that takes advantage of the benefits of object stores. In particular, the Fermilab Tier 1 computing center is mission critical for the success of the entire experiment and is the largest dedicated CMS computing resource outside of CERN. Currently, CMS uses a tiered data storage approach, with the RAW detector output stored on tape and end-user analysis formats stored on disk. At each data tier, only a subset of the total information is kept. If an analysis needs data from earlier tiers, the entire dataset needs to be staged to disk and reprocessed. This is an issue especially for analyses (such as those the PI has been leading looking for long-lived particle decays) that rely on low-level detector information for optimal results. Fermilab has been exploring a novel solution to this problem using object stores. Object stores, compared to the current file-based organization of CMS data, allow for highly granular data access. The feasibility of this approach has been demonstrated, and the PI and postdoc supported by this grant will work closely with Fermilab to make a road map for implementation at the Fermilab Tier 1, including a proof-of-concept test using cloud computing resources.

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

Building ASU Isotope Research Infrastructure and Expertise to Advance Isotope Production and Basic Research Capabilities

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The overarching goal of the planned project is to enhance research infrastructure and expertise at Alcorn State University (ASU) to advance isotope research capabilities and strengthen the collaborative relationships between ASU and Brookhaven National Laboratory Isotope Research and Production Department (BNL-IP). The project's research objectives are 1) development of purification and separation methods of medically relevant isotopes. 2) Chelation and stability studies of 225Ac 3) developing nano-based methods to enhance delivery of therapeutic 225Ac radionuclide at tumor site and 4) Computational investigation of 225Ac coordination chemistry. The research areas to be enhanced range from isotope separation, purification, radiochemical synthesis, nanotechnology, computation and related science of radiation monitoring and measurements, radionuclide delivery methods, and nuclear and radiochemistry. The grant will fund an upgrade of the PI's Laboratory, acquisition of radioanalytical instruments including a high purity germanium detector (HPGe) detector, dedicated equipment for radioactive work AR-2000 radio-TLC Imaging Scanner, Glove box and a thermomixer, radiation monitoring and measurements devices, chemical supplies, and support for students, postdoctoral fellow and faculty involved in this initiative. Development of radiochemistry expertise will be supported by access of ASU faculty, postdoctoral fellow and students to scientific expertise and advanced instrumentation at BNL-IP facilities to rapidly accelerate isotope research at ASU. The infrastructure built through this project will help to fulfill the university's goal to build research capacity and expand critical instrumentation, enable development of new modules devoted to an in-depth understanding of nuclear and radiochemistry, and computational analysis for integration into existing courses in the Department of Chemistry and Physics curriculum. The project takes advantage of the complementary techniques available at ASU in the Departments of Chemistry & Physics, and the broad expertise available at the BNL-IP facility and Radioisotope Research and Production Laboratory (RRPL), and will involve ASU faculty, undergraduates, as well as BNL Scientist collaborators. The project will include extended research and training visits to BNL by ASU faculty and post-doctoral researcher involved in this initiative, student engagement in research internships at BNL, short training courses on nuclear and radiochemistry (both onsite and distance), experiments and activity measurements at BNL, thus broadening expertise and skills to other isotope production, separation, purification, radiochemical synthetic approaches, techniques and facilities, thereby providing knowledge and expertise in isotope research and production. The collaborative team will hold monthly research-focused group meetings via real-time video teleconferencing for project updates. The students engaged in this program will be involved in basic research which will support their B.S. senior project. The ASU faculty involved in the project will systematically engage high school students in the surrounding schools and undergraduates at ASU to encourage, recruit and broaden participation by providing opportunities for students from underrepresented groups to participate and contribute to the project's research activities. The research outcome will be disseminated through conferences, workshops and publications, with a goal of publishing in peer reviewed journals. This project also responds directly to the critical shortage of highly qualified scientists in the field of nuclear science and radiochemistry, Health Physics, and radionuclide R&D in the U.S. and brings diversity to nuclear and radiochemistry as well as to the national labs.

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

Expanding the *Potential* for Chemical Separations with Carbon Supports

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A key focus of this research is the separation of ^{153}Sm, a beta-emitter used in nuclear medicine. Its production through the neutron-irradiation of ^{152}Sm requires the removal of the long-lived ^{154}Eu impurity from the final product. Achieving complete separation of these adjacent lanthanides often involves the reduction of Eu^{3+} to Eu^{2+} using a chemical reductant prior to the separation step. This challenging separation underscores the need for innovative approaches in extraction chromatography. This research will replace conventional non-conductive resin supports with conductive frameworks that incorporate redox functionality and controlled architectures for enhanced chemical separations. This research will expand the capabilities at the University of Massachusetts Lowell (UML) to transform the field of extraction chromatography by leveraging the morphology and electrical conductivity of carbon materials. The objectives are twofold: (1) to build radiochemical separation research capacity at UML, relevant to the U.S. Department of Energy Isotope R&D and Production (DOE IP) missions through collaboration with the Isotope Science and Engineering Directorate (ISED) at Oak Ridge National Laboratory (ORNL) and investments in analytical equipment; and (2) to develop and apply conductive carbon-based supports with increasingly organized structures to extraction chromatography, adding the functionality of deliberately controlled electrode potentials. By establishing UML, a Minority Serving Institute (MSI), as a leader in radiochemical separations, particularly relevant to the DOE IP mission, this research paves the way for future innovations in isotope research, development, and production. The collaborative efforts with ORNL not only enhance scientific capabilities but also strengthen university-national lab partnerships, fostering a culture of knowledge exchange and collaboration. Additionally, the training and mentorship provided to graduate and undergraduate students will help build a skilled workforce for radiochemistry and related fields. Ultimately, the outcomes of this research have the potential to improve nuclear medicine, environmental stewardship, and national security through more efficient and selective radiochemical separations.

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

Novel Holographic Approaches to the Non-perturbative Dynamics of Proton Spin

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This project is an interdisciplinary research collaboration between SUNY Old Westbury (SUNY OW), a Minority Serving Institution (MSI), and the Nuclear Theory Group (NT) at Brookhaven National Laboratory (BNL), to pioneer techniques based primarily on holographic duality to understand where proton spin comes from. We call this collaboration UPSHoT (Understanding Proton Spin with Holographic Theories).

The UPSHoT collaboration will attack the problem of proton spin by developing novel techniques for strongly interacting systems. The PI O'Bannon and co-Is Estes and Lippert are experts in holographic duality, a technique that translates intractable problems in strongly coupled systems to solvable problems in Einstein's theory of relativity in higher-dimensional spacetimes. The PI is also expert in "defect quantum field theory," which describes strongly interacting objects like protons as "defects" of the quantum vacuum. Co-I Venugopalan recently developed a powerful "worldline" formalism which uncovered the central role of topological objects called sphalerons in proton spin. Physicists conjecture that these sphalerons played an important role in how matter came to dominate over antimatter as the universe evolved.

This project will focus on how topology influences the quark contribution to proton spin. Key objectives include a) develop novel models of protons in holographic duality, defect quantum field theory, the worldline formalism, and combinations thereof, b) produce a comprehensive classification of anomalies in these holographic models and extract universal results, c) use the results to make predictions quantifying the potential of the EIC to discover the existence of sphalerons.
UPSHoT thus aims to jump-start holographic approaches to the mysteries of proton spin, ideally producing far-reaching impacts on EIC physics and beyond!

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

Monte Carlo Simulations for Polarized and In-medium Parton Evolution in the Nuclear Realm

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This goal of this project is to understand the fundamental components of nuclear matter - the quarks and the gluons - is a central question of nuclear physics. This project aims to deepen that understanding by developing, and applying in detailed phenomenological studies, advanced simulation tools that will allow us to investigate the nuclear realm at particle colliders. Through Monte Carlo (MC) simulations, the project will provide insights into how nuclear constituents behave when polarized, and in extreme conditions. This will illuminate how protons and neutrons are formed through the confinement of quarks and gluons, and how their spin is distributed among these constituents.

The project's main objectives are:

1. Simulating electron-proton collisions with the effects of spin: We will develop MC tools to simulate interactions where electrons collide with protons, both having their spins aligned in specific directions. This will be essential in clarifying the inner spin structure of protons.
2. Electron-ion collisions probing nuclear structure: Extending our MC, we will simulate collisions between electrons and a range of nuclei (from light elements like deuterium to heavier ions). This will allow exploration of how quarks and gluons interact with the dense environment of nuclei, providing a new level of understanding on the forces that bind nuclear matter.
3. Modeling jet evolution within a nuclear medium: We will simulate the behavior of jets - streams of particles produced in high-energy collisions - as they traverse through the dense nuclear environment in which they are produced. Studying these interactions will provide insights into a unique state of matter called the quark-gluon plasma, believed to resemble conditions shortly after the Bing Bang.

To achieve these goals, the project leverages HERWIG, a powerful and flexible MC simulation framework. By incorporating new features in HERWIG for handling particle spin and complex nuclear interactions, the simulations will reach a precision level critical for upcoming collider experiments, such as the planned Electron-Ion Collider (EIC) at the Brookhaven National Lab. These simulations will directly support experimental programs, enabling scientists to interpret experimental data, and guiding the next generation of measurements. The findings of this endeavor could offer unprecedented insights into nuclear interactions. The partnership between Kennesaw State University and Georgia State University will foster a collaborative, inclusive research environment, positioning both institutions as leaders in theoretical nuclear physics.

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

Inelastic Neutrino-Nucleus Scattering Research by NCCU at ORNL

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This proposal supports the inelastic neutrino-nucleus scattering (INNS) program being carried out by the North Carolina Central University (NCCU) Neutrino Group at the Spallation Neutron Source (SNS) located at Oak Ridge National Laboratory (ORNL). NCCU is a public, liberal arts, masters' granting, Historically Black University (HBCU). PI Markoff (NCCU), Co-I Barbeau (Duke University) and ORNL partner Co-I Newby are COHERENT collaborators engaged with a suite of detectors measuring neutrino interactions. The COHERENT collaboration recently published measurements of INNS in lead (208Pb) and iodine (127I) that were lower than expected. The initial interest of the collaboration results from this inelastic interaction being a source of background neutrons that can interfere with low-energy recoil measurements of elastic neutrino scattering. This proposal seeks to fund a systematic program of improved measurements in different target configurations to check the initial results and to explore the discrepancy to determine whether the trend of low reaction rates exists in other nuclei.

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