Enhanced Radiated Power via Engineered Eigenbasis Collapse

Dr. Tsampikos Kottos[1], Lauren B. Dachs Professor
Dr. Zin Lin[2], Assistant Professor
Dr. Patrick Sebbah[3], Professor (unfunded)
Dr. Ilya Vitebskiy[4], Principal Research Physicist (unfunded)
1: Wesleyan University, Middletown, CT 06457
2: Virginia Tech Research Center, Arlington, VA 22203
3: Bar-Ilan University (Israel)
4: Airforce Research Lab, Dayton, OH 45433

This fundamental theoretical and experimental research proposal is driven by the Department of Energy's needs for the development of high-power radiofrequency, microwave, and laser sources for innovative medical, industrial, and basic research particle accelerator technology. The proposed collaboration between an emerging research institution (Wesleyan), an R1 minority-serving institution (Virginia Tech), an international institution (Bar-Ilan), and a federal lab (AFRL) will leverage the complementary expertise and scientific culture of these groups and will assist in building experimental radiofrequency/microwave research capabilities that the Wesleyan group strives to develop during the past years.

The proposed research shall explore new photonic avenues and formulate fundamental principles that will allow for transcending the existing limits set by the traditional Purcell physics on the power-emissivity of electromagnetic sources. This will be achieved by enforcing new interaction rules dictated by special electromagnetic field degeneracies, which determine the coupling between an emission source and its engineered environment. The effort shall promote novel fundamental concepts and engineering strategies for developing high-power lasers, masers, and radiofrequency sources under extreme light-matter interaction conditions induced by these electromagnetic field degeneracies. To create these special degeneracies, we shall exploit spatial, temporal, and phase degrees of freedom available in radiofrequency and microwave electromagnetics combined with high-dimensional optimization involving inverse design computational methods. Examples of proof-of-concept demonstrations include degeneracy-based high-performance up/down frequency converters, high-average power pulse generators, directional amplifiers, and compact high-power beam combiners. It is expected that the outcomes of the current study will be relevant for a variety of physics and engineering frameworks, ranging from optical, microwave, and acoustic waves to matter and quantum waves.

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

Intra-Beam Scattering and Beam Cooling for Circular Modes

Dr. Béla Erdélyi[1], Professor
Dr. Brahim Mustapha[2], Accelerator Physicist
1: Department of Physics, Northern Illinois University, DeKalb, IL 60115
2: Physics Division, Argonne National Laboratory, Lemont, IL 60439

High energy colliders and storage rings require high collision luminosity and beam brightness for future scientific discoveries and applications. Flat beams could enable this need, because one of the transverse beam sizes is very small, which enhances the luminosity and brightness. However, at low energy, flat beams cannot sustain high beam currents due to space charge effects, which cause significant tune shifts and unstable motion. In order to resolve this dilemma, flat beams can be propagated as circular mode beams through the lattice while maintaining intrinsic flatness through coupling, then converted to flat beams at high energy.

We investigate the effects of IBS on circular mode optics using particle tracking simulations. The results of these simulations will be used to verify and eventually improve the IBS analytical formulae for the case of coupled beam optics. To this end, we are developing accurate and efficient large-scale computational beam dynamics tools for phenomena where collisional processes play a significant role. The prime example is electron cooling of heavy ions, one of the most challenging nonlinear beam dynamics applications of interest to high energy and nuclear physics. Our computational framework is currently the only tool available that can address it based on first principles. Therefore, a holistic approach to circular beam modes for improving future colliders needs a better understanding of IBS on its own, in relation to space charge, and its contribution to electron cooling. We are in a unique position to be able to address all these topics.

The research's broader impact is in the education of the next generation of accelerator scientists, which has been identified as critical in the long-term health of many scientific endeavors at accelerator facilities. Moreover, the coding infrastructure that will be developed will serve as a free resource for other current and future accelerator-based facilities.

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

Entanglement Estimation for Quantum Computing: Theory, Algorithms, and NISQ-level Verification

Dr. Lu Wei[1], Assistant Professor
Dr. James Osborn[2]
1: Texas Tech University, Lubbock, TX 79409
2: Argonne National Laboratory, Lemont, IL 60439

Entanglement is the workhorse enabling quantum algorithms that offer substantial computational speedups over their classical counterparts. However, a quantitative understanding of how the amount and type of available entanglement relates to the performance of quantum algorithms remains elusive. In this project, we employ the ingredients of generic states and entanglement estimation to uncover the deep connection between entanglement and algorithm performance. This is achieved by systematically studying the behavior of certain algorithms across major generic states ensembles as measured by different entanglement estimators. As an integral part of the project, some of the project results will be evaluated, verified, and benchmarked by making use of IBM Quantum Simulators and Argonne Leadership Computing Facility (ALCF) resources in collaboration with the co-PI at Argonne National Laboratory (ANL). The synergy of the PI's effort on entanglement estimation and the co-PI's current focus on quantum algorithms is necessary to advance the understanding on the role of entanglement in quantum algorithm analysis. In entanglement estimation, we consider entropy-based estimation, where the exact moments of the entanglement entropies over different models of generic (random) states will be derived. Based on the results, we will investigate entanglement phase transitions between separable and entangled states and identify the corresponding critical system parameters. We also consider metric-based estimation, where the key entanglement metrics of fidelity and volumes in quantum computing will be studied. The ultimate goal is to develop a rigorous but non-asymptotic entanglement estimation theory based on recent progress in understanding the statistical behavior of finite-size quantum systems. In applications to quantum algorithms, the project progress on entanglement estimation will be utilized to establish the framework connecting the performance of quantum algorithms to the degree of entanglement of quantum states. As case studies, we will focus on quantum simulation algorithms in the context of quantum approximate optimization algorithms and quantum circuit cutting methods in the context of state tomography, an area the co-PI is actively contributing to. In results evaluation, some of the project findings will be evaluated using IBM Quantum hardware platforms and simulators. The simulators will be utilized for studying quantum algorithms under realistic noise models. Performance of the considered quantum algorithms will be simulated by measuring different entanglement indicators in the presence of practical imperfections modeled as noise. ALCF resources at ANL, including leadership-class supercomputers, will also be leveraged to benchmark algorithm performance.

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

Developing temperature-jump X-ray crystallography to study dynamic biosynthetic enzymes at synchrotrons and XFELs

Dr. Michael Thompson[1], Assistant Professor, University of California, Merced
Dr. Aina Cohen[2], SLAC National Accelerator Laboratory
1: University of California, Merced, 5200 N Lake Road, Merced CA 95342
2: SLAC National Accelerator laboratory, 2575 Sand Hill Rd., Menlo Park CA 94025

Molecular motions underlie many important biochemical functions, such as enzyme catalysis, but these motions are challenging to study because they involve distances of less than a nanometer, and timescales ranging from picoseconds to milliseconds. Modern X-ray light sources, including synchrotrons and X-ray free electron lasers (XFELs) built and maintained by the DOE, offer new opportunities to study molecular motion with atomic resolution imaging. These instruments produce ultrafast, high-brilliance X-ray pulses that act as a "molecular high-speed camera," enabling the observation of molecular motions in real time using a technique known as time-resolved crystallography. A major caveat to these experiments is that the measured samples contain billions of individual molecules, and in order to study the motions of interest, the molecules must be synchronized, which is not a trivial task. A variety of rapid perturbations have been explored for this purpose. To make time-resolved crystallography a general tool that can be applied to study the dynamics of any protein of interest, we are exploiting the inextricable link between temperature and molecular motion. Specifically, we are developing the use of infrared laser-induced temperature-jump (T-jump), wherein the molecules of interest are rapidly heated with a nanosecond pulsed infrared laser to stimulate and synchronize their motions for time-resolved imaging. In this proposal, we describe a collaborative effort to pilot the use of new hardware and software for imaging protein motions across DOE structural biology facilities at SLAC National Laboratory. Because temperature is a universal means by which to perturb protein motions, we expect the methods we develop will be broadly applicable to the study of many different biochemical systems, and the tools we develop will be made available to the large user base of these facilities. To demonstrate the power of these new time-resolved molecular imaging methods that utilize T-jump, we will study lipoxygenase enzymes that are found in plants and animals, which catalyze important biosynthetic reactions that also have broad industrial applications. The catalytic function of lipoxygenase enzymes is hypothesized to be linked to a specific set of molecular motions within the enzyme. We will test this hypothesis by using T-jump to map molecular motions in several lipoxygenase variants with different catalytic properties. This comparative analysis will lend insight into which of the observed motions are functional in catalysis. Experiments performed at both synchrotron (SSRL) and XFEL (LCLS) facilities will allow us to observe molecular motions across broad timescales ranging from nanoseconds to milliseconds. Our work will help shed light on the fundamental relationship between molecular motions and catalytic function in enzymes. This knowledge will inform the future engineering of artificial enzymes with designer catalytic properties that can act as environmentally-friendly chemical reagents for industry.

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

Evaluating water, sediment, and nutrient transport rates and accumulation patterns in alluvial ridge basins between the abandoned river channels (Resacas) of the Rio Grande Delta

Dr. Tian Dong[1], Assistant Professor, University of Texas Rio Grande Valley, Edinburg, Texas
Dr. Jonathan Schwenk[2], Los Alamos National Laboratory, Los Alamos, NM
1: University of Texas Rio Grande Valley, 1201 W University Dr, Edinburg, TX 78539
2: Los Alamos National Laboratory, P.O. Box 1663, MS P288, Bikini Atoll Road, Los Alamos, NM 87545

River deltas are vital ecosystems and social centers in coastal regions. However, deltas face climate change threats and human activities today, leading to land loss. River deltas distribute sediment and build land near the coast by abruptly shifting course through channel avulsion. Within a delta, much of the area is occupied by alluvial ridge (AR) basins, depressions formed by relict channels from past avulsions. How materials, like sediment and organic carbon, accumulate in AR basins remains less understood. Moreover, climate change and natural disasters disproportionately affect under-served communities, especially those of the Rio Grande Delta (RGD) in south Texas. The RGD region contains seven major relict channels of the Rio Grande, known locally as *Resacas*. Despite experiencing frequent flooding, the patterns of water and sediment transport in the AR basins of the RGD remain unclear. This project aims to study the processes of mass accumulation in deltaic AR basins by combining field observations, remote sensing data, and numerical modeling. The research will determine the connectivity of the channel network and the direction of water flow within the AR basins. The topography of the channel network will be analyzed via flow routing using digital elevation models. Instruments will be deployed to measure water and sediment transport rates in three AR basins, representing a range of natural and human conditions. Sediment core samples will be collected for radiocarbon age dating to determine sediment and nutrient accumulation rates over long periods. The field data will be combined with numerical models to simulate material transport and accumulation patterns under different scenarios, providing insights into the impact of climate change on the RGD and its communities. This project will be the first comprehensive study of mass accumulation rates and patterns in the RGD, the second-largest river delta in North America. Furthermore, it aims to provide valuable data to the under-served community, enabling them to understand delta inundation patterns for better policymaking and engineering practices. The results of this research will also help to validate the transport rate and direction of the E3SM-Land model.

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

Understanding the Role of Duckweed Transcription Factor in Triacylglycerol Metabolism and Abiotic Stress Tolerance in Plants

Mrs. Bagyalakshmi Muthan[1], Research Associate, West Virginia State University
Dr. Changcheng Xu[2], Brookhaven National Laboratory
1: West Virginia State University, 201 Campbell Conference Center, Institute, WV 25112
2: Brookhaven National Laboratory, 50 Bell Ave, Upton NY 11973

In nature, plant oils represent one of the most energy-rich sources of renewable hydrocarbons. They are stored as triacylglycerols (TAGs) or oils, which can be used as alternative feedstocks for biodiesel production. As an alternative feedstock, plant-based oils have several advantages over other fuels, including high energy content, no need for fermentation, compatibility with existing fuel technologies, and being environmentally friendly. Life cycle analyses have shown that the production and use of jet fuel from oilseeds can results in lower greenhouse gas emissions as compared to petroleum-derived fuels. However, supplies of these energy-rich oilseeds compounds are limited due to low crop yield and limited available arable land   This project aims to use a combination of genomic, molecular biological, and biochemical analyses to explore transcription factor regulatory networks that regulate TAG/oils production in plants, and how they can be manipulated to increase the carbon conversion to oils in oilseed plants. Specifically, transcriptional regulators that have been found to increase oil content when over-expressed in *Arabidopsis* will be targeted to better understand the mechanism by which seed oil storage is enhanced. The central hypothesis of this project is that a transcription factor described in duckweed is also required to regulate TAG metabolism in Brassicaceae oilseed crops such as *Camelina*, Canola, and Pennycress. Three objectives will be pursued, which are to 1) determine requisite duckweed transcription factor functions in oil storage metabolism; 2) to alter oil content and agronomic performance in *Camelina*; and to 3) define an overall metabolic engineering strategy to leverage duckweed transcription factors for increasing TAG yield. Knowledge gained from this research will unlock new and creative avenues to use genetic engineering to enhance the TAG in oilseed crops, which will help fulfill the world's growing fuel needs.

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

Advancing Atomistic Understanding of Electronic Energy Transfer

Dr. Liang Shi[1], Associate Professor
Dr. Christine Isborn[1], Dr. Henrik Larsson[1], Dr. Britta Johnson [2]
1: University of California, Merced, CA 95343
2: Pacific Northwest National Laboratory, Richland, WA 99354

Electronic energy transfer (EET), a process of fundamental importance in both natural and artificial light-harvesting systems, is heavily influenced by the multifaceted interactions between electronic and nuclear degrees of freedom in condensed phases. The interplay of these factors involving multiple energy and time scales is complex, thus the experimental spectra used to probe EET are often difficult to interpret. This project aims to elucidate the effects controlling the dynamics of EET by advancing atomistic scale understanding through simulations that span from simple models that can be solved exactly to condensed phase atomistic dynamics.

This project will use atomistic simulations to provide deeper insights into the environmental correlations between chromophores, the fluctuating excitonic couplings in complex environments, and the state mixing between bright and dark states. Large-scale electronic structure methods will be validated against correlated wavefunction methods, and molecular dynamics simulations will be performed with force fields derived from electronic structure calculations. Key advancements in our approach over standard techniques will be the incorporation of the couplings between electronic excitation and nuclear motions derived from atomistic simulations. The effect of these couplings on EET dynamics will be examined by various dynamical simulation methods, ranging from classical simulations, to semi-classical molecular dynamics simulations, to quasi-exact state-of-the-art quantum dynamics methods.

The methods Id In this project will provide the simulation community with reliable protocols for modeling EET with atomistic detail, with the gained physical insights leading to the further improvement of EET efficiency in artificial light-harvesting systems. The collaboration between the University of California Merced (UCM) and Pacific Northwest National Laboratory is not only essential to the proposed research, but is also beneficial to the training of diverse student populations at UCM, a Hispanic-serving institution with a large number of first-generation college students.

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

Atomic Level Structure-activity Relationship of Small Molecule Activation on Single Atom Catalysts Supported on 2D Boron-based Materials

Dr. Fang Xu,[1] Assistant Professor
Dr. Darío J. Stacchiola[2]
1: University of Texas at San Antonio, TX 78249
2: Brookhaven National Laboratory, Upton, NY 11973

Borophene is an emerging 2D catalytic material for energy and environmental applications. The hollow hexagon structure on borophene is predicted to provide strong metal-support interactions allowing to stabilize single-atom catalysts (SACs) and small clusters, which have been proven to enhance catalytic performance in numerous reactions. This proposed research project aims to experimentally study small molecule activation (H_2, CO_2, and C_2H_4) over SACs and small clusters supported on boron-based 2D materials. Advanced microscopy and spectroscopy, including cutting-edge ambient pressure techniques, at the University of Texas at San Antonio (UTSA, PI) and Brookhaven National Laboratory (BNL, Partner) will be used to study the boron growth, visualize the atomic structure of the surface, quantify surface composition across pressure regimes, and measure reaction kinetics. The combined results will reveal structure-activity relationships over SACs and small clusters supported on novel 2D boron-based materials. The proposed research project also presents a distinctive and valuable opportunity to introduce students from the San Antonio area to cutting-edge equipment and a national laboratory setting. Two graduate students from UT San Antonio each year will be sponsored by this project and complete a half-year rotation at CFN, BNL. Thus, a significant portion of the funding will be used to train and educate underrepresented minority students in the field of materials and chemical sciences. This represents an important step toward creating a cohort of minority role-model scientists and developing the future workforce in the field of science and engineering.

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

Atomic to mesoscale models of phase transitions for energy materials

Dr. Nicole Adelstein, Associate Professor
Dr. Liwen (Sabrina) Wan[2], Dr. Tae Wook Heo[2], Dr. Marissa Wood[2]
1: San Francisco State University, San Francisco, CA 94132
2: Lawrence Livermore National Laboratory, Livermore, CA 94551

Objective: Numerous energy production and storage technologies rely on materials with many metastable phases (polymorphic); often one phase is more effective than others for a given application. These polymorphic phases can coexist and undergo phase transformations during synthesis or device operation since their energies are relatively similar, unlike for example graphite and diamond. Transition metal (TM) oxides with nickel, manganese, and cobalt are promising polymorphic materials for catalysts, battery electrodes, and supercapacitors. However, their long-term performance and efficiency are impacted by phase transitions between their competing polymorphic phases. Extensive work has been done to address the thermodynamic differences between the polymorphic phases. In application, kinetics is also a primary driving force for any undesired phase transformations, which is far less understood. Our simulations are designed to determine the kinetics of phase transitions and phase nucleation and growth, focusing on MnO_2, since significant simulations of its thermodynamics have already been performed.

Methods: Multiscale simulations that employ three cutting-edge computational techniques will bridge the quantum, atomic, and mesoscales to provide an innovative and comprehensive model of polymorphic MnO_2. Quantum and atomic scale simulations will determine phase transition pathways, transition states, and energy barriers. A phase-field method will provide microstructure-level mesoscale simulations to determine phase evolution. Machine learning force fields (MLFF) will be developed to perform meta-dynamics simulations that will determine nucleation and growth parameters. The MLFF will also be used to simulate interfacial energies and elastic properties for the mesoscale model. MnO_2 synthesis and characterization using X-ray diffraction and SEM by Lawrence Livermore National Laboratory (LLNL) will inform the microstructural models and can provide experimental validation of the simulations.

Impact and Outcomes: The proposed research will advance the fundamental capabilities to model the kinetics of phase transformations at the atomic and mesoscale, which will have significant impact in many energy fields. In particular, the atomic-scale energy barrier calculations and machine learning force fields (MLFF) meta-dynamics simulations of nucleation and growth will provide insights into the phase transformations of the technologically important MnO_2. Additionally, simulations of the kinetics of TM oxides will enable engineering of the microstructure to optimize battery cathodes and O_2 evolution catalysts. Our simulations will be one of the few studies that tackles solid-solid nucleation and growth of complex TM oxides or the mesoscale phase evolution of polymorphic materials. The MLFF development will use the most rigorous methods for training and testing the potentials so that they can be trusted to accurately simulate the complex phase transitions between polymorphic TM oxides.

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

Controlling Densification-Induced Structural Transformations in Metal-Organic Frameworks for Size Selective Separations

Dr. Sameh K. Elsaidi, Assistant Professor
Dr. Wenqian Xu
1: Illinois Institute of Technology, Chicago, IL 60616
2: Argonne National Laboratory, Lemont, IL 60439

The primary method employed for the densification of metal-organic frameworks (MOFs) is pelletization, which involves the application of pressure with or without a binder to convert MOF powders into practical and usable forms. However, it is imperative to thoroughly investigate the structural changes, alterations in porosity, and resulting gas adsorption properties following the densification process, in order to fully comprehend the performance of densified MOF materials in practical applications. This research project proposes a universal approach for the densification of MOFs, with the goals of improving particle adhesion and minimizing intergranular voids. By leveraging the high densification of MOF nanocrystals, the approach can induce controlled shearing, squeezing, or rearrangement of the crystal lattice, leading to modifications in pore structure, shape, and size, ultimately influencing the separation properties of the densified material. Successful implementation of this concept would yield insights into the factors driving structural changes during densification, establish detailed relationships between structural transformations and separation performance, elucidate mechanisms governing these behaviors, facilitate the modulation of structural composition and architecture for optimizing separation properties, and provide guidelines for designing and understanding structural flexibility in MOFs.

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

Data-driven learning of dissipation from microscopy of chemically active materials

Dr. J. R. Green,[1] Professor of Chemistry and Physics
Dr. J. P. Patterson
1: University of Massachusetts, Boston, MA 02125
2: University of California, Irvine, CA 92697

Materials chemistry has taken the first steps to identify chemical networks that drive the transient formation of materials. These dissipative materials stand out in their potential to function dynamically, forming patterns and generating work. In supramolecular hydrogels, there is an opportunity to optimize this functionality by designing the chemical kinetics at the molecular scale to control the fiber number, lengths, and lifetimes assembled at the mesoscale. While these materials are expected to have applications from energy materials to tissue engineering, there is not yet a pathway to their practical implementation. A key roadblock is that there is little more than a binary answer to the question of whether a given assembly process is, in fact, dissipative, preventing both design strategies and the optimization of function. Machine learning can guide experiments and accelerate design processes with data-driven models, but is not yet able to optimize energy efficiency or timed formation of structure. The proposed project will address these challenges by establishing the necessary framework for learning dissipation directly from experimental data, using theory and computation to guide further experimentation and material design.

Energy dissipated by nonequilibrium materials can have a strong influence on their structure, function, and efficiency. In the field of self-assembly, dissipation is typically considered a negative byproduct of structure formation. This project will test the hypothesis that it is instead an untapped thermodynamic resource that can be used to catalyze the formation of structure. The strategy will be to measure dissipation in active supramolecular materials monitored with multiscale in-situ microscopy through four specific aims: (i) quantify the structural dynamics of chemically active nanomaterials from in-situ electron microscopy, (ii) develop data-driven methods to measure the dissipation associated with material assembly, (iii) train and GPU accelerate these methods on physically-relevant reaction-diffusion models, and (iv) validate our AI models of the dynamics against experimental data. Together, these aims will culminate in a closed feedback loop between theory and experiment, generating AI-ready datasets that clarify the role of dissipation in the assembly of responsive and self-healing nanomaterials.

Overall, the project aims to arm materials design with (i) experimental and simulation datasets, together with data-driven theory for the dissipation of chemically-active materials, (ii) principled explanations that will accelerate their timely and efficient use in practical applications, and (iii) predictive, dynamical models of dissipative materials. Success in these aims will equip the materials community with a codebase, algorithms, and benchmark datasets that are a pathway to design materials in nonequilibrium regimes where structures have unique optical, mechanical, or photonic properties. The large datasets will be AI-tested and AI-ready, with an industry collaboration ensuring the open-source codebase is capable of massive parallelization across GPUs

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

Designing Photoresponsive Nanosponges for Efficient and Reversible Capture and Release of Carbon Dioxide

Dr. Yangyang Liu,[1] Associate Professor
Dr. Long Qi[2]
1: California State University, Los Angeles, CA 90032
2: Ames National Laboratory, Ames, IA 50011

The overarching goal of this project is to develop photoresponsive porous materials that can efficiently capture carbon dioxide (CO_2) from the air and can be easily regenerated utilizing visible light/sunlight. The designed core-shell metal-organic frameworks (MOFs) are expected to undergo multiple reversible CO_2 capture and release cycles without sacrificing their overall CO_2 adsorption capacity. The specific objectives are 1) designing shell MOFs by incorporating visible light-responsive functional groups through linker functionalization, 2) synthesizing and characterizing photoresponsive MOFs with optimal core-shell combinations, and 3) studying the CO_2 capture and release properties of the photoresponsive core-shell materials using visible light as the trigger for material regeneration.

This project hypothesizes that efficient and reversible CO_2 capture and release cycles can be realized using porous materials integrating visible light-responsive shells and CO_2-binding cores. These core-shell MOFs with photoresponsive "gates" are designed to achieve controlled CO_2 capture and release utilizing visible light/sunlight, minimizing the energy required for materials regeneration. The partnership with Ames National Laboratory will facilitate the investigations of the solid-state photoswitching and CO_2 adsorption mechanisms in the core-shell MOFs, guiding the rational design of better-performing materials. This project is expected to discover new materials with high CO_2 capacity, excellent CO_2 selectivity over N_2 and other gases, and outstanding hydrolytic stability. These materials can maintain their structures and CO_2 adsorption capacity after multiple CO_2 capture/release cycles with minimal energy requirement for materials regeneration.

The proposed research provides a new direct air capture concept by integrating photoresponsive functionalities in MOFs for energy-efficient CO_2 sorption and release. These materials could, in theory, regenerate utilizing sunlight, an energy source that is naturally occurring but not parasitic to the power plant. The work is proposed to elucidate the fundamental design principles and atomistic mechanisms for efficient and robust photoresponsive porous materials to achieve on-demand and regulated interactions with CO_2. The proposed research activities and internship opportunities are expected to increase the number of underrepresented students and junior researchers engaged in energy and decarbonization research. The mutually beneficial relationships between California State University, Los Angeles and Ames National Laboratory will have a significant, long-term impact on energy-focused fundamental research and the development of a diverse workforce at both institutes.

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

Development of Containerless HTXRD Technique for In-Situ Materials Characterization in Extreme Environments

D. Lipke,[1] Associate Professor
Dr. C. Benmore,[2] Dr. R. Weber,[3]
1: Missouri University of Science and Technology, Rolla, MO 65409
2: Argonne National Laboratory, Lemont, IL 60439
3: Materials Development Inc., Evanston, IL 60202

This project will advance the state-of-the-art in high temperature materials research by establishing a hyperbaric aerodynamic levitation facility for in-situ containerless melting studies using high-energy X-ray scattering techniques available at the Advanced Photon Source beam sector 6-ID-D. Levitators are ideal tools for studying solidification phenomena of importance to any material that undergoes liquid-solid phase transitions during its natural history or industrial processing. Understanding the emergence of non-equilibrium states in crystals and glasses via dynamic arrest from supercooled liquids is experimentally challenging, and levitators play a key role in developing fundamental knowledge of this technologically important phenomena that cuts across multiple areas of importance for the energy, economic and national security of the United States, including steel and glassmaking industries, additive manufacturing, high purity crystal growth, and high temperature materials research for nuclear, defense, energy generation and transportation applications.

The levitator will operate at specimen temperatures above 2500°C and at pressures up to 15 MPa in oxidizing, reducing, and inert atmospheres. These conditions will be obtained by use of a custom sample environment comprising a pressure vessel, a nozzle to levitate specimens upon a pressurized fluid jet, a diamond window for laser admittance to heat the specimen, and optical and X-ray windows for sample observation. The levitator will provide important new experimental capabilities for materials researchers by expanding the operational pressure regime by more than an order of magnitude as compared to current generation levitators. Benefits of this new capability will include reduced sample volatilization rates, better retention of specimen chemical composition, and access to extended redox regimes especially for the stabilization of high oxidation states in transition metal compounds. Planned experiments enabled by the capabilities of the new levitator include first-of-its-kind observations of the fragile-to-strong transition in silica (important to verify theoretical understandings of melt dynamics and glass formation), the effects of ferric ion abundance on network coordination in iron silicates (important for understanding slag interactions in steelmaking), and of ion speciation during solidification of metal-insulator transition lanthanum nickelate perovskites (important for understanding mechanisms of crystal growth of defect-sensitive quantum materials).

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

Electrochemical nitrate reduction to ammonia on single-atom alloy catalysts

Dr. Shyam Kattel,[1] Assistant Professor
Dr. Xiaofeng Feng
1: Florida A&M University (FAMU), Tallahassee, FL 32307
2: University of Central Florida (UCF) Orlando, FL 32816

Sustainable production of fuels/chemicals using renewable energy is essential to reduce the energy dependence on fossil fuels and to mitigate the negative environmental impacts of greenhouse gas emissions. Ambient electrochemical processes that convert wastes/pollutants to valuable chemicals using the electricity generated from renewable sources are ideal in this regard. Ammonia, one of the widely used chemicals in agriculture and industries, is currently produced via the energy- and carbon-intensive Haber-Bosch process, while the increasing use of nitrogen fertilizers has caused nitrate contamination of water resources. It is thus appealing to develop renewably powered ammonia production technologies at ambient conditions from abundant nitrogen feedstock such as nitrate. Therefore, the electrochemical reduction of nitrate to ammonia presents an attractive approach for a low-carbon and convergent ammonia manufacturing technology that concurrently remediates nitrate-polluted water systems.

The development of such technology relies on a fundamental understanding of the nitrate reduction reaction. This project combines theoretical and experimental approaches to obtain an atomic-level understanding of the catalytic mechanisms of the electrochemical nitrate reduction to ammonia and to develop earth-abundant, low-cost, and selective single-atom alloy catalysts for efficient nitrate conversion to ammonia. The goal of this proposed research is to gain a mechanistic understanding of this proposed reaction and to formulate materials design principles for predicting active, selective, and stable single-atom alloy catalysts.

This FAIR project aims to build research infrastructure and expertise at FAMU to study electrochemical reactions at the electrified solid–liquid interfaces. It will strengthen the catalysis science research at FAMU and UCF, provide cutting-edge research experience to underrepresented minority undergraduate students, graduate students, and postdoctoral scholars and create a pipeline to train the next generation of minority scientists and engineers. This collaborative theoretical and experimental effort is anticipated to have a tremendous impact on the education and research training of underrepresented minority students at both FAMU and UCF in the cross-disciplinary field of heterogeneous catalysis, which requires approaches that can integrate state-of-the-art computational and experimental methods.

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

Emergent phases, transport, and nonequilibrium dynamics of interacting Majorana fermions

Dr. Armin Rahmani,[1] Associate Professor
Dr. Jianxin Zhu[2]
1: Western Washington University, Bellingham, WA 98225
2: Los Alamos National Laboratory, Los Alamos, NM 87544

This research focuses on interactions between many Majorana fermions, particles with fascinating properties that can emerge in whirlpool-like electronic structures called vortices in special materials known as topological superconductors. They can be thought of as mathematical counterparts to electrons but with no electric charge. The project's goals are first to construct realistic models of interacting Majorana fermions relevant to quantum materials and then explore distinct phases of quantum matter that emerge in models with different arrangements of vortices as a function of physical parameters such as the distance between vortices and electronic voltages applied to the system. The research will also focus on how these distinct phases transition from one to another. The project will examine how interacting Majorana fermions respond when the system is driven out of equilibrium by suddenly changing or periodically driving various physical parameters. Another critical component of this research is identifying signatures of Majorana fermions coupled to metallic or superconducting materials, which are electronically probed. Finally, the project utilizes quantum computing devices for studying interacting Majorana fermions, providing physical realizations for table-top analogs of supersymmetry and black hole physics that arise from interacting Majorana fermions.

The research approach involves mathematically combining pairs of Majorana fermions into more familiar particles called regular fermions. Established methods used to study correlated electrons are then applied to analyze the interacting Majorana models. In conjunction with analytical techniques, the project relies on two powerful numerical methods: the density-matrix renormalization group (DMRG) and numerical variational approaches. Time-dependent DMRG will be used to study the dynamical properties of interacting Majorana fermions. The project uses a combination of boundary conformal field theory and DMRG for investigating one-dimensional wires connected to Majorana-based structures. Finally, the project leverages the quantum computing device as a novel experimental platform.

This project will provide valuable training and internship opportunities for a postdoctoral researcher and an undergraduate student through direct collaboration between academia and National Laboratories, providing access to state-of-the-art computational facilities and contributing to the research capabilities and resources.

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

Emerging Properties through Controlled Phase Transformations for High Energy Sodium Ion Batteries

Dr. Hui (Claire) Xiong,[1] Professor
Dr. Wanli Yang[2]
1: Boise State University, Boise, Idaho 83725
2: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

The development of high-energy low-cost batteries remains a formidable challenge and the bottleneck for today's sustainable energy applications. The performance issues are believed to be associated with the high-voltage operation of the batteries. This proposal aims to ***elucidate the emerging properties through controlled phase transformations in layered sodium transition metal oxide (LSTMO) cathode materials for high-energy low-cost Na-ion batteries (SIBs).*** The ***research objectives*** are to (1) synthesize P-type Mn-rich LSTMO cathodes with controlled phase transformations during cycling through low-temperature heat treatment and Li substitution; (2) quantify cationic and oxygen redox reactions through state-of-the-art synchrotron-based soft X-ray spectroscopy; (3) track transition metal (TM) interlayer ordering, migration, and Na^+/vacancy ordering through neutron scattering and advanced analytical electron microscopy; and (4) clarify the fundamental mechanism of oxygen redox and develop design strategy for high energy cathode materials. The proposed work involves design, synthesis, and processing of LSTMOs along with advanced structural and chemical characterizations to unlock the mechanisms associated with TM and oxygen redox processes. The collaboration will work to reveal the fundamental association between the controlled phase transformations and electrochemical redox reactions to achieve optimized materials for high energy SIBs.

We will test ***the hypothesis that phase transformations in high energy high stability LSTMOs can be controlled by modulation of interlayer cation ordering and low-temperature processing***. We plan to combine phase modulations in material synthesis and processing with state-of-the-art multimodal spectroscopic and microscopic characterizations to tackle the fundamental mechanism of both the cationic redox and anionic redox activities in LSTMOs at high voltages. Additionally, we will identify the specific structural location and environment of TMs and light elements (Na, Li) for understanding TM migration and Na/vacancy ordering through neutron diffraction, *operando* synchrotron X-ray diffraction , and *in-situ* heating transmission electron microscopy . The fundamental mechanism revealed through these multimodal characterizations will then be carefully analyzed for further material optimizations towards high-performance SIBs. The ***scientific outcomes*** will be a mechanistic understanding of how materials synthesis and processing affect redox behaviors in LSTMOs, and how phase transformation tailor electrochemical properties of oxide materials, followed by practical material optimizations for high-energy SIBs.

The knowledge obtained through this work will provide foundational understanding and development for solid-state energy materials chemistry, synthesis, and processing science — supporting DOE missions in energy security while also promoting global competitiveness in energy storage technology development and manufacturing to boost the national economy and open new synthesis and processing pathways for new solid-state materials. Practically, we anticipate that the outcome of this research will be an unprecedented improvement in battery science and technology for electric grid applications.

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

Empowering research and engineering of biological CO2 uptake mechanisms by integrating molecular structure, genomic diversity, bioinformatics, and metabolomics

Dr. Rob Burnap,[1] Professor
Dr. Mostafa S. Elshahed,[1] Dr. Wouter Hoff,[1] Dr. Noha H. Youssef,[1] Dr. Jianping Yu[2]
1: Oklahoma State University, Stillwater, OK 74078
2: National Renewable Energy Laboratory, Golden, CO 80401

Photosynthesis forms the energetic basis for the Earth's biosphere, food production, and is responsible for the abundance of oxygen in the atmosphere. It also is the major mechanism to mitigate rising CO_2 levels in the atmosphere and provide biofuel and biomimetic solutions for sustainable energy production. This project investigates the cyclic electron flow (CEF) in oxygenic photosynthetic organisms. CEF is critical for overall photosynthetic efficiency and the robustness of the photosynthetic mechanism in changing environments. The overall goals are to understand CEF and its integration with metabolism including organisms engineered for bioproduct synthesis. Our scientific partners at the National Renewable Energy Laboratory (NREL) have developed highly useful cyanobacterial strains that include award-winning ethylene-producing strains that have been engineered to divert the photosynthetic reactions to produce this energy-rich product, which provides an experimental paradigm for understanding the coupling of the light reaction, including CEF, with biosynthetic metabolism. Moreover, their expertise in metabolomics will both serve the research goals, but also provide a segue for Oklahoma State University (OSU) researchers to expand their extensive capabilities in metabolic reconstruction from large genomic and metagenomic datasets. The focus will be on the electron transport complexes that have been shown to balance photosynthetic outputs, drive inorganic carbon uptake, and influence overall metabolic fluxes in the process. There are two broad outreach efforts for the project: Outreach geared for Oklahoma high school teachers, thereby reaching a broad audience of high school students. Expertise in bioinformatics and computational analysis will be used to develop exercises using broadly applicable computer skills involving bioinformatics. The curriculum development will involve teachers incorporating this knowledge into lesson plans that meet state teaching rubrics. Outreach also involves partnerships with a vibrant Native Americans in science program at OSU, the Louis Stokes STEM Pathways and Research Alliance (LSAMP) and leverages several local scholarship programs such as the Wentz, Beckman, and Niblack programs at OSU. Overall, the project is a unique integration of high level scientific research into a critical research topic that lends itself to partnering with innovative educational outreach programs.

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

First Principles Multiphase Modeling of Mesoscale Gas Transport in Porous Reactive Systems

Dr. M. Barisik,[1] Assistant Professor
Dr. R. Ranjan,[1] Dr. R. Sankaran,[2] Dr. S. Irle,[2]
1: University of Tennessee at Chattanooga, TN 37403
2: Oak Ridge National Laboratory, Oak Ridge, TN 37830

Mesoscale transport, interphase dynamics, rarefaction, and surface chemical reactions in a non-equilibrium multiphase gas environment is observed in many energy and material synthesis applications such as ablative thermal protection system for spacecraft, catalytic vacuum microreactors, chemical vapor deposition/infiltration processes for advanced materials, etc. Therefore, an improved fundamental understanding and accurate and efficient modeling of such processes in such multiphase heterogeneous porous reactive systems are key to the development of novel applications with improved properties and performance. The presence of a wide range of length- and time scales in such processes, which spans about six orders of magnitude, makes it challenging to employ a first principles computational modeling strategy, thus requiring alternate techniques. The proposed research will address this challenge by first examining the fundamental physics at the molecular and mesoscopic scales, and then establishing a novel and transformative multi-scale modeling framework, which will accurately include the subscale physics due to homogenization and upscaling to enable investigation of mesoscale and macroscale transport processes in porous reactive systems. The key focus of the proposed research will be on (a) the development of surrogate kinetic models for meso- and macro-scale studies by using molecular scale studies, (b) an enhanced computational model for mesoscale multiphase transport and surface reactions by utilizing algorithms such as dynamic load balancing, floating molecules list, and parcel number density control within the framework of direct simulation Monte Carlo (DSMC) technique, (c) computationally efficient sensitivity assessment of the process at mesoscales by using a non-intrusive probabilistic framework of the uncertainty quantification tool, (d) assessment of macroscale continuum model for state evolution in porous reactive systems, and (e) demonstration of the performance of homogenization and upscaling models for macro-scale studies by comparing with the ongoing experimental studies of the chemical vapor infiltration process. The proposed research will employ scale-specific modeling techniques such as density functional theory (DFT), kinetic Monte Carlo (kMC), and molecular dynamics (MD) for molecular scale studies; an enhanced DSMC, subscale-explicit/aware DSMC for mesoscale studies; and subscale-aware continuum models for macroscale studies. Apart from providing a validated multi-scale modeling framework, the proposed research will lead to an improved understanding of the role of finite-rate chemistry models accounting for surface complexations and interactions between by-products; the non-equilibrium heat and mass transport, and gas/surface momentum/energy coupling at mesoscales; and an accurate characterization of the subscale processes at meso and macro-scales.

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

Inhibition of Impurity Adsorption and Nucleation at Mineral-Water Interfaces via Chelator Adsorption

Dr. Jacquelyn Bracco,[1] Assistant Professor
Dr. Sang Soo Lee[2]
1: Queens College, City University of New York, Flushing NY 11367
2: Argonne National Laboratory, Lemont, IL 60439

Organic chelators are commonly used in energy/water productions and industries to inhibit nucleation and growth of scaling minerals that cause detrimental consequences such as clogging and failure of oil and gas pipelines or reduction of reverse osmosis membrane capacities in desalination plants and municipal water systems. Each of these systems has its own complex solution conditions, which can lead to diversities in the structure and chemistry of mixed-phase mineral scaling. However, the impact of chelators on the formation and removal of individual scaling materials is not well understood at the mechanistic level. To address this knowledge gap, we will resolve the mechanisms by which chelates bind to mineral surface, analyze the impact of chelators on ion adsorption, and quantify the effect of chelators on nucleation and growth. The overarching goal of this project is to develop a fundamental understanding of the molecular scale mechanisms by which organic chelating agents modify surface structure, ion adsorption, and nucleation of common scaling minerals at geologically and environmentally relevant conditions. We will use high-resolution microscopic approaches to study minerals' evolving morphologies during dissolution, nucleation, and growth and synchrotron-based x-ray scattering measurements to probe ion adsorption and reaction layer formation at the mineral surfaces. These studies are enabled through the partnership of Queens College (QC where Bracco is the leading PI) with Argonne National Laboratory (ANL where Lee is the partner PI) under the support of the FAIR initiative, which aims to build research capacity, infrastructure, and expertise at institutions historically underrepresented in the Office of Science portfolio. A key component of this collaboration is to provide new research opportunities and national laboratory experience to undergraduate and graduate students at QC, a Hispanic Serving Institution (HSI) and Asian American and Native American Pacific Islander-Serving Institution (AANAPISI). These students will receive training in novel x-ray scattering and microscopy techniques at ANL through summer internships and visits throughout the semester. QC will also host outreach seminars by ANL staff that will be open to students at local community colleges. Overall, the fundamental understanding obtained from our study will have a broad impact on various disciplines of science including geoscience, separation, catalysis, and interfacial molecular sciences, directly addressing Department of Energy (DOE)'s missions, including topics in Basic Research Needs for Energy and Water. Our efforts will also be consistent with the DOE's Chemical Sciences Geosciences, & Biosciences (CSGB) synergistic research themes, in regard to developing a new understanding of Chemistry and Complex Interfaces, Reaction Pathways in Diverse Environments, and Chemistry in Aqueous Environments.

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

Intrinsically Porous Polyoxometalate-Based Frameworks for Critical Metal Recovery

Dr. Z. Peng, University of Missouri-Kansas City
Dr. P. Thallapally,[2] Dr. M. Momenitaheri[1]
1: University of Missouri-Kansas City, MO 64110
2: Pacific Northwest National Laboratory, Richland, WA 99354

As the world transitions to renewable energy technologies, demands on critical metals are expected to surge, exacerbating the already dire critical metal shortage issue and threatening the US economy and national defense. With dwindling terrestrial ore mining and increasing environmental concerns, aqueous saline sources are increasingly being recognized as one of the major sources of critical metals. One critical technical challenge is how to selectively extract the desired critical metals, often in very low concentrations, from the saline sources and then effectively release them afterward for recovery.

This project hypothesizes that intrinsically porous polyoxometalate (POM) molecular clusters and POM-derived porous frameworks (POMFs) with precisely controlled pore sizes and chemical environments are potentially effective, selective, and electrically switchable adsorbents for critical metal ions from saline sources. This hypothesis is rooted in POMs' unmatched structural and compositional tunability, ease of synthesis, and high thermal stability. More importantly, POMs are robust redox active materials that can undergo repeated reduction-oxidation cycles. The redox process does not alter the overall structure but can result in changes in the size and chemical environment of the pores, which in turn affects the binding affinity and selectivity toward different metal ions. Such a property may allow electrochemical switching of the adsorption and desorption of critical metal ions, addressing the challenging paradox of sorption-based recovery where a sorbent must have favored adsorption isotherm during capture but unfavored isotherm during release. To test this hypothesis and to accelerate materials discovery, a closed-loop approach that encompasses data science adaptation, computationally aided materials design, materials synthesis, and performance evaluation is adopted. The technical approach of the project includes 1) *building comprehensive mega-databases of POMFs* and expanding our calculation programs to predict their properties. These databases and calculation programs can be the launch pad to initiate machine learning programs to design not only adsorbents for critical metal recovery but also POM-based materials for other applications such as catalysis and energy storage. (2) *Materials design through modeling and simulation*. To understand, predict and develop porous POMs with the right pore size and to establish structure-property relationships, we will perform high-throughput electronic structure calculations combined with molecular dynamic simulations to survey and predict selective metal adsorption capabilities of doughnut-shaped POMS (*ds*-POMs) with varied compositions.
(3) *Synthesis of predicted promising ds-POMs with varied chemical compositions and controlled pore sizes.* (4) *Preparation of POM-derived porous frameworks (POMFs)* using the most promising *ds*-POMs as building blocks. (5) *Performance evaluation of ds-POMs and POMFs as selective critical metal adsorbents* with or without electrochemical reduction. At the conclusion of the project, the hypothesis that POMs with precisely tuned pores and porous structures are electrochemically switchable critical metal ion-capturing materials from aqueous saline sources will be thoroughly tested.

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

Light Mediated Synthesis of Single Atom and Single Atom Alloy Catalysts

Dr. Sanchari Chowdhury,[1] Associate Professor
Dr. Pabitra Choudhury,[1] Dr. Prashant Padmanabhan[2]
1: New Mexico Institute of Mining and Technology, Socorro, NM 87801
2: Los Alamos National Laboratory, Los Alamos, NM 87545

Single-atom and single atom alloy catalysts are promising systems to enhance different catalytic reactions including CO_2 reduction, water splitting and solar energy conversion. The goal of this proposal is to develop a mild light mediated plasmon enhanced deposition method to synthesize stable transition metal based single atom and single atom alloy catalysts deposited on metallic nanostructures hosts. Single atoms alloy catalysts consist of the catalytically active metals such Pt, Ni, Pd, Rh which are atomically distributed on less reactive noble metal hosts such Ag, Au and Cu which can support strong plasmonic properties. Besides traditional metals, refractory plasmonic transition metal nitride nanostructures are emerging as a promising support for single atom catalysts. We will focus on the deposition of transition metal catalysts such as Pt and Ni on noble plasmonic metals host such as gold nanoparticles to synthesize single atom alloy catalysts. We will also study deposition of the single atom catalysts on titanium nitride which exhibits long term stability, strong plasmon resonance under solar light and a promising catalytic support. Plasmonic nanomaterials can efficiently absorb and concentrate light at the nanoscale to generate intense electromagnetic fields. The photoexcited electrons can undergo nonradiative decay, generating highly energetic electrons which can reduce metal precursors adsorbed on the surface to deposit metal atoms on the surface. We hypothesize that the reduction rate of metal precursors can be easily manipulated by varying light intensities and wavelengths to efficiently deposit single atoms on the surface of plasmonic metallic structures in a controlled manner. Importantly, deposition of catalysts on plasmonic supports allow us to develop photo active single atom catalysts as the support can absorb light and transfer the energy or photo-excited charge carriers to catalysts to drive reactions. Over the past decade, single-atom and single atom alloy catalysts have attracted extensive attention due to their high atom efficiency, strong metal support interactions and excellent catalytic performance. However, the challenges for the wide scale applications of single atom and single atom alloy catalysts are the complexity of the synthesis processes (multiple steps, expensive processes, energy extensive etc.) for stable high loading catalysts or precise control over the alloying. The proposed plasmon enhanced synthesis of single atom and single atom alloy catalysts can overcome these challenges due to the several advantages over current methods. We will combine experimental and theoretical study to understand how the plasmonic properties of the supports, catalyst support interactions and the reaction conditions can be tuned to synthesize single atom catalysts with high loading which are and stable in a harsh condition. The outcome of this study will guide the synthesis of single atom catalysts on wide range of catalytic support materials including many metals and few transition metal nitrides and carbides, chalcogenide, and oxide nanostructures, which exhibit plasmonic properties.

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

Macroscopic quantum states in antiferromagnets: Bose-Einstein condensation of anti-ferro-magnons

Dr. Dmytro Bozhko, Associate Professor
Dr. Zbigniew Celinski,[1] Dr. Valentine Novosad[2]
1: University of Colorado Colorado Springs, CO 80918
2: Argonne National Laboratory, Lemont, IL 60439

Bosons are particles of integer spin that support the formation of the fundamental macroscopic quantum state – Bose-Einstein condensate (BEC). Since its experimental discovery in 1995, BEC became a hot topic in physics. BECs have been experimentally observed in a variety of different systems, including real particles such as ultra-cold gases as well as quasiparticles like exciton-polaritons and photons. Quanta of collective spin excitations (magnons) in ferrimagnets, quantum magnets, and liquid helium ^{3}He were also found to form BEC under special conditions. The BEC phenomenon has already found its first applications for quantum computing noise reduction. Recently, antiferromagnetic (AFM) materials have attracted remarkable interest from the scientific community due to their unique properties – high operating frequencies combined with significantly suppressed stray fields.

This proposal aims to realize for the first time the BEC of magnons in AFMs (anti-ferro-magnons) and study its properties in a wide frequency range from GHz to THz in a broad range of temperatures from ambient to the quantum limit. The range of materials for investigations includes fluorides, oxides, and synthetic AFMs. The main scientific objectives of this 3-year proposal are: (1) Realization of AFM BEC through rapid cooling using a broad range of micro-structured AFMs; (2) Realization of microwave-pumped anti-ferro-magnetic BEC employing AFMs that exhibit resonances in tens of GHz; (3) Realization of magnon BEC in synthetic AFMs such as Fe/Cu/Fe and Fe/Cr/Fe through both parametric microwave pumping and rapid cooling techniques; (4) Observation and study of macroscopic quantum phenomena in AFMs: anti-ferro-magnonic BEC supercurrents, Bogoliubov waves, magnon Josephson effect, and second sound. Besides the four listed above scientific aims, the important objective of this proposal is to build significant research and educational capacity at the University of Colorado Colorado Springs to explore the quantum properties of magnetic systems that will allow to enhance quantum workforce development in DOE.

The proposed aims will be realized using a combination of state-of-the-art fabrication and measurement techniques. The samples will be grown using molecular beam epitaxy and nanostructured using electron beam lithography and reactive ion etching. The AFM BEC will be detected using time-, space-, and wavevector-resolved Brillouin light scattering and microscopy, and microwave spectroscopy. To perform these measurements in a wide range of temperatures, the team will build a cryostat capable of reaching temperatures of 3 K together with optical and microwave access. Measurements of AFM dynamics in the single-quanta limit will be performed at Argonne National Laboratory in the dilution ^{3}He-^{4}He fridge.

The expected outcomes of the proposal will help us to understand the fundamental aspects of AFM physics as well as make progress in applied material science. We plan the experimental demonstration of anti-ferro-magnonic BEC achieved in a fundamentally different way from earlier experiments as well as to provide important insights into the properties of AFMs at low and ultra-low temperatures.

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

Manipulate Spin Selectivity via Chiral Molecules in Solar Energy Conversion

Dr. Jing Gu,[1] Associate Professor
Dr. Yong Yan,[1] Dr. Matthew Beard,[2]
1: San Diego State University, San Diego, CA 92182
2: National Renewable Energy Laboratory, Golden, CO 80401

The clean energy infrastructure of the future will depend on efficient, low-cost, and long-lasting systems for the conversion and storage of solar energy. While many approaches have been taken to reach new heights in solar energy conversion, the kinetic challenge of oxygen evolution reaction (OER) remains the primary limitation for the water splitting reaction, hindering the advancement of the field. To increase the efficiency of OER, this research will develop a novel approach that suppresses the production of the competing byproduct, hydrogen peroxide (H_2O_2), and reduces the overpotential by systematically controlling the spin of electrons. To control the electron spin at room temperature and without external magnetic fields in the photoelectrochemical (PEC) process, it will employ chiral materials that take advantage of chiral-induced spin selectivity (CISS) at the semiconductor-catalyst interfaces to enable a direct correlation of spin selectivity with the efficiency of solar energy conversion. The research will also develop novel ultrafast spin-dependent spectroscopic studies to answer fundamental questions about how chirality impacts light harvesting, spin-selective charge separation/transport, and respective catalytic kinetics.

The long-term goal of this project is to deepen our fundamental understanding of how to induce and exploit the coupling of photoexcitation, charge injection, charge separation, and transfer to create new mechanisms that direct light-matter interaction for more efficient solar energy conversion. Specifically, two types of chiral semiconductor-catalyst interfaces will be deliberately designed. In the first interface, hybrid metal oxide/chiral molecules, synthesized using atomic layer deposition and molecular layer deposition, will be sandwiched between the semiconductor and catalyst. In this interface, it is hypothesized that the hybrid chiral layer will perform as a pseudo “p-n” junction, facilitating spin-selective charge separation and transport, thus, improving the selectivity and overpotential of OER. In the second interface, molecular photosensitizers will be adsorbed on the nanocrystalline TiO_2-modified FTO glass. Similar to Lego bricks, the chiral layer will be positioned at different locations to direct the spin-polarized carriers for efficient solar energy conversion. In addition, the research will employ spin-dependent ultra-fast pump-probe spectroscopy to elucidate the key carrier dynamics that shed light on CISS-induced light harvesting, charge separation, and transport kinetics. Lastly, the PEC performance of the photoelectrodes will be correlated with their spin-selective carrier dynamics.

The performance of a photoelectrode depends on the efficiency of light harvesting, charge separation, transport, and chemical conversions. The key steps involve dynamic electron excitation, injection, separation, and transfer. The electron spin is reported to affect the PEC process, yet the fundamental understanding of spin’s correlation with key PEC steps remains elusive. The enhanced understanding of key spin-controlled mechanisms that influence the performance of the semiconductor-catalyst interfaces provided by this study will be critical to the further development of solar energy conversion infrastructure, spin-selective electronic devices, sensors, and catalysis.

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

Optoelectronic Properties of Artificially Tailored Quantum Materials

Dr. Komalavalli Thirunavukkuarasu,[1] Associate Professor
Dr. Wei Pan[2]
1: Florida A&M University, Tallahassee, FL 32307
2: Sandia National Laboratory, Albuquerque, NM 87123

This project aims to advance the field of artificially tailored quantum materials (ATQMs) for quantum information science (QIS) applications by exploring ATQMs composed entirely of compound semiconductors. Such compound-semiconductor-based ATQMs will enable the tunability of three fundamental parameters associated with quantum materials: electron-electron interactions, spin-orbit coupling, and band topology. Such tunability, in turn, will enable both unraveling mysteries associated with quantum-materials phenomena already observed but poorly understood as well as the discovery of new quantum-materials phenomena not yet observed. Eliciting and understanding both kinds of phenomena are the goals of the project's objectives: (1) investigate novel optical and electronic properties in semiconductor moiré superlattices (MSLs); (2) explore moiré excitons and excitonic insulators in semiconductor MSLs; (3) achieve flat bands with strong e-e correlations and emergent novel electron physics in semiconductor MSLs. To accomplish these objectives, the following technical tools and capabilities will be used: advanced materials synthesis, nano-scale device fabrication, and quantum-transport and magneto-optical-spectroscopic experimental studies of ATQMs.

An immediate impact of this proposal's switch to compound semiconductors for quantum materials research will be in enabling a new scientific window into quantum-materials phenomena. The ability to fabricate semiconductor MSLs with desired tunable quantum states offers the possibility of new device concepts and new ideas in advanced optoelectronics and data processing. Semiconductor-based MSL devices could be platforms to explore new types of electronic switches, transistors with superior properties, and even new ways to store information based on exotic quantum mechanical states. Thus, a longer-term impact is more impactful: by making semiconductor heterostructures a powerful new QIS materials platform, future QIS applications can build on, and be compatible with, the sophistication and maturity of state-of-the-art semiconductor synthesis and processing.

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

Photocatalyzed Degradation and Chemical Recycling of Polymers Using Visible Light Photo-oxidation Catalysts

Dr. S. E. Brown-Xu,[1] Associate Professor
Dr. L. X. Che[2]
1: Northeastern Illinois University, Chicago, IL 60625
2: Argonne National Laboratory, Lemont, IL 60439

The 2019 Basic Energy Sciences Roundtable on "Chemical Upcycling of Polymers" identified the growing need to develop a circular plastic economy in which waste plastics are chemically recycled into value-added chemical products, feedstocks, or fuels. In particular, the development of new energy-efficient catalysts and control over mechanistic pathways to promote selective chemical reactions is required to achieve this goal. This research will investigate photochemical polymer transformations using earth-abundant photo-oxidation catalysts (BiCuOS, $BiFeO_3$, and MnO_2) that are active with visible light irradiation. In situ X-ray absorption spectroscopy and FT-IR experiments will reveal the effects of the electronic and structural properties of the photocatalysts in the active state and determine the role of reactive intermediates in the photocatalytic mechanism. Time-resolved studies, both UV-vis and X-ray transient absorption spectroscopy, will identify structure-mechanism-function relationships that exist between the photophysical properties of the catalysts and the efficiency of photo-induced hole transfer to the polymer chain. The proposed studies will capitalize on the PI's expertise in correlating excited state and charge transfer dynamics with photoinduced structural changes in order to predict and control photochemical reaction trajectories. The project aligns with the DOE mission of advancing fundamental scientific understanding of photochemical and photoinitiated charge transfer pathways with the aims of reutilizing plastic waste and reducing the consumption of fossil fuels for energy and chemical production.

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

Probing CO_2 Dissolution and Mineralization in Deep Saline Aquifers with Experiment and Simulation

Dr. Aaditya Khanal,[1] Assistant Professor
Dr. Mojdeh Delshad,[2] Ryosuke Okuno[2]
1: University of Texas at Tyler, TX 75799
2: University of Texas at Austin, TX 78712

Underground sequestration of CO_2 released from significant point sources, such as power plants and heavy industries, is a possible technology for reducing greenhouse gas emissions into the atmosphere. However, large-scale implementation of geological CO_2 sequestration requires a clear understanding of the underlying physics behind numerous complex processes currently inadequately understood. This project aims to examine dissolution and mineralization trapping mechanisms, which are critical to ensure the long-term storage of CO_2 in subsurface formations, such as deep saline aquifers, using experimental, numerical, and data-driven approaches. In addition, this project will also evaluate the impact of various geological and geochemical uncertainties present in subsurface formations on the trapping mechanisms. Finally, the effect of injected CO_2 on the flow properties of the aquifer, such as porosity and permeability, will be investigated to improve the storage security of the sequestered CO_2. The experimental data, simulation results, and data-driven models expected from this project will be instrumental in improving the current technologies involved in sequestering CO_2 in deep saline aquifers. Furthermore, this project will yield transferable insights to improve current and future CO_2 geo-sequestration projects, which are critical to meet our climate goals without a sudden disruption to the existing energy infrastructure. The project outcomes will address the global environmental challenges and advance national energy security and prosperity through transformative science. This project will build research capacity and infrastructure at The University of Texas at Tyler (UT Tyler), an emerging research institution, through a mutually beneficial collaboration with The University of Texas at Austin (UT Austin), an R1 minority-serving institution. Through this collaboration between institutions, students from diverse backgrounds in local high schools, community colleges, and other educational institutions will be able to engage in fundamental research, providing them with valuable exposure to education and career pathways in energy and environmental engineering. The investigators will also promote equitable and inclusive research by recruiting students from underrepresented groups in STEM fields through short hands-on projects, presentations, and directed recruiting events. Finally, the outcomes of this project will broaden public knowledge about the various aspects of energy generation, carbon emissions, and technologies that can mitigate the impact of the emissions.

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

Quantum Properties and Physics of Defects in 2D Transition Metal Dichalcogenides

Dr. Birol Ozturk[1], Associate Professor
Dr. Can Ataca[2]
1: Morgan State University, Baltimore, MD 21251
2: University of Maryland Baltimore County, Baltimore, MD 21251

Quantum sensing is a paradigm shifting approach for the detection of extremely small changes in temperature, magnetic and electric fields. Defects in wide bandgap semiconductors are promising qubit platforms that can operate at room temperature as opposed to other leading quantum systems requiring cryogenic temperatures such as superconducting circuits. Two-dimensional (2D) Transition Metal Dichalcogenides (TMDs), specifically TmX2 compounds (Tm = W, Mo, X = S, Se, Te), are wide bandgap semiconductors which have gained considerable attention in recent years. These materials possess remarkable properties and offer exciting possibilities for various applications. However, the defects present in 2D TMDs have received less focus despite the extensive research on these materials. Therefore, this project aims to investigate and address the defects in 2D TMDs. By doing so, we can advance our understanding of these materials and their potential for ultrasensitive quantum sensing. The project will focus on characterizing various unknown parameters of the defects, such as zero phonon line emission energies, zero field splitting frequencies, Debye-Waller factors, and coherence times.

Objectives of this project are: 1) Develop methods for controlled formation of defects at targeted sites on two dimensional (2D) Transition Metal Dichalcogenide (TMD) samples, 2) Establish gate voltage controlled defect emission methods, 3) Identify quantum properties of defects in 2D TMDs, 4) Demonstrate quantum sensing of magnetic fields with defects in 2D TMDs, 5) Develop a comprehensive understanding of the nature of quantum emitters in 2D TMDs and their relation to defects, 6) Recruit and train minority students on quantum science and 2D TMDs for the next generation STEM workforce.

To achieve the objectives of the project, we will form intentional defects in samples of 2D TMDs using techniques such as Atomic Force Microscopy (AFM) indentation, electron beam irradiation, and annealing. These intentional defects will allow us to study their quantum properties. We will employ techniques such as Raman spectroscopy, confocal photoluminescence spectroscopy, continuous wave, and pulsed optically detected magnetic resonance (ODMR) methods to analyze the quantum characteristics of these defects. Additionally, computational simulations will be conducted to further investigate the quantum properties of the defects in these materials. These simulations will help us better understand the underlying mechanisms and provide theoretical predictions that can guide our experimental efforts. To enhance the efficiency of our research outcomes, machine learning algorithms will be utilized, which will play a crucial role in data collection, analysis, and computational simulations.

The outcomes of this project will pave the way for the development of highly sensitive detectors that can be applied across a diverse range of fields including brain signal monitoring, GPS-free navigation, Quantum Light Detection and Ranging (LIDAR), and quantum telecommunication.

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

Rational Design of Concentrated Electrolytes for Beyond-Li-ion Batteries with Machine Learning and Quantum Calculations

Dr. Mirza Galib,[1] Assistant Professor
Dr. Bryan M. Wong
1: Howard University, Washington, DC 20059
2: University of California Riverside, CA 92521

Li-ion batteries have made transformative technological advances in portable electronic devices and electric vehicles. However, a limited supply of Li in the Earth's crust has motivated the scientific community to explore other metal cations(e.g. Na, K, Ca, Mg, and Al) as alternatives to Li-ion batteries. Designing suitable electrolytes is a challenging task which currently impedes the commercialization of the beyond-Li-ion batteries. In this project, we will use quantum calculations and machine learning to rationally design new ionic liquid electrolytes for the beyond-Li-ion batteries. More specifically, we will develop a computational framework to rationally screen the best performing ionic liquids from a target chemical space including i) alkyl and ether-based phosphonium cations with two commonly used anions ($TFSI^-$ and FSI^-), ii) three commonly used organic solvents (acetonitrile, dimethyl sulfoxide, and methanol), and iii) five metal anodes (Na, K, Ca, Mg, and Al). Phosphonium protic ionic liquids are prospective electrolytes as they have a low cost and possess better physiochemical properties. We will first develop machine learning models from *ab inito* data that can simulate long time dynamics for any metal anode-electrolyte-organic solvent combination for the above-mentioned chemical space. Leveraging the low computational cost of the machine-learned force field, we will carry out several nanosecond-long molecular dynamic simulations with state-of-the-art enhanced sampling techniques (e.g., umbrella sampling and metadynamics) to investigate: (1) electrolyte decomposition reactions, (2) migration and adsorption of decomposition products at the electrode surface, (3) ns-long dynamics of the solid electrolyte interphase (SEI), and (4) energy barriers and kinetics of ion transfer and desolvation in the SEI. We will build a comprehensive data set from our computations to characterize the elementary steps involved in the formation of SEI, which will then be used to develop structure-property relationships to rationally select the best-performing ionic liquids from that target chemical space. We will also employ time-dependent DFT methods to calculate spectral signatures that can be directly compared to X-ray absorption experiments. Overall, this project will systematically explore the vast chemical space of ionic liquids and develop a rational design strategy to select next-generation ionic liquid electrolytes for beyond-Li-ion batteries by combining quantum mechanics, statistical mechanics, and machine learning. In addition, the framework developed in this work would be easily extendable to larger chemical spaces with additional cation/anion combinations, other anodes based on carbon/alloys, and the cathode-electrolyte interphase.

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

Solution-based Synthesis of Structurally Well-defined Carbon Nanobuds and Their Energy Applications

Dr. Yunxiang Gao,[1] Assistant Professor
1: Prairie View A&M University, Prairie View, TX 77446

Carbon nanobuds (CNBs), composed of fullerene buds covalently bonded to other carbon nanostructures such as carbon nanotubes or graphene directly via their carbon lattice, show potential for exceptional performance in various energy applications due to their tunable surface chemistry, as suggested by numerous theoretical simulations. However, experimental synthesis of well-defined CNBs remains a challenge due to limited successful reports of CVD-based synthesis, along with difficulties controlling bud density and species.

Theoretically, using well-defined fullerenes and other carbon nano-substrates as two soluble reactants in wet chemistry synthesis might offer better control over nanobud structure. However, this approach faces significant hurdles, such as the lower reactivity of the less-curved graphene's carbon lattice, and the self-polymerization of the highly curved, more reactive fullerenes in reactive priority.

Our project aims to develop an innovative, fully solution-based synthesis strategy for high-quality CNBs, which allows us to control fullerene-bud species and bud density, while ensuring high production yield and minimal side products. We plan to improve the reactivity of nano-carbon substrates through metal-free hetero-doping, and to prevent fullerene self-polymerization by covalently attaching individual fullerenes to solvated sacrificial micro-/nano-templates. Optimization of CNB synthesis will involve investigating variables such as the size of the solvated sacrificial templates, fullerene-bud coating density on these templates, and the use of alternatively doped carbon nano-allotropes as substrates. To evaluate the structural and morphological properties of the synthesized CNBs, we will utilize comprehensive characterization techniques including Scanning Electron Microscopy (SEM), Brunauer–Emmett–Teller (BET) method, X-ray Photoelectron Spectroscopy (XPS), Raman-AFM (Atomic Force Microscopy), Transmission Electron Microscopy (TEM), Thermogravimetric Analysis (TGA), Fourier-transform Infrared Spectroscopy (FT-IR), and UV-visible Spectroscopy.

The synthesized CNBs will be characterized and evaluated for their catalytic activity in Oxygen Reduction Reactions (ORR) for fuel cell applications, and as catalyst supports for single-atom transition metal catalysts in Electrocatalytic CO_2 Reduction Reactions (eCO_2RR). We will conduct theoretical simulations using molecular dynamics and Quantum Mechanics/Molecular Mechanics (QM/MM) approaches to study the reactivity of various doped carbon allotrope species towards the carbon lattice of fullerene, and to understand the CNB-supported CO_2 reduction process.

Successful synthesis of CNBs in solution with precise structural control may yield exceptional electrocatalytic performance, thereby contributing to the development of more sustainable energy applications.

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

Structural influences in electrochemical dehydrogenation of liquid organic hydrogen carriers

Dr. Elizabeth J. Biddinger,[1] Associate Professor
Dr. Oliver Gutierrez-Tinoco,[2] Dr. Juan Lopez-Ruiz[2]
1: City College of New York, New York, NY 10031
2: Pacific Northwest National Laboratory, Richland, WA 99354

The need for storage and transport of energy increases as more renewable electricity comes online. Molecular hydrogen (H_2) has been proposed as a clean means to store energy in chemical bonds, but storing and transporting it is challenging because of its flammability and gaseous state. Alternatively, the energy associated with hydrogen in chemical bonds can be stored in liquid organic hydrogen carriers (LOHCs) avoiding handling compressed or cryogenic H_2. Hydrogen storage in LOHCs requires "loading" by hydrogenating an organic molecule and then "releasing" the hydrogen by dehydrogenation. This strategy leverages the carbon backbone of organic molecules to exchange hydrogen, reversibly, without emitting CO_2. Electrochemical cycling of LOHCs could intensify the reaction scheme, bypass the step of H_2 generation, enable benign operating and storage conditions, and be directly powered by the renewable energy grid without the need for combustion-derived heat.

Faculty and students at The City College of New York (CCNY) will work with scientists at Pacific Northwest National Laboratory (PNNL) to understand the reaction mechanisms that govern the storage and release of energy in the form of electric potential or H_2 utilizing organic molecules. The central theme of the proposal is the conversion of LOHCs using electrochemical systems at mild conditions with strong emphasis on enabling the reversible hydrogen removal from the reduced form of the organic carriers. The aim will be at understanding and controlling the electrochemical environment, and molecular structure, that enables hydrogen transfer while suppressing undesired side reactions. The hypothesis is that the applied potential will enable dehydrogenation (otherwise feasible only at high temperatures), while the accurate tunning of the interactions at electrode/electrolyte interfaces will selectively accelerate the kinetics of the electron and hydrogen transfers. Through the collaboration, CCNY aims at developing the capabilities needed for advanced *in situ* characterization of electrochemical reactions and determination of dehydrogenation kinetics under continuous flow reaction systems. Investigations will include the electrode/electrolyte interface properties and how they influence electrochemical dehydrogenation (ECD), development of kinetics and mechanisms for ECD, and influence of molecular structure on ECD reactivity and selectivity. The reaction of benzyl alcohol to benzaldehyde will serve as the model ECD reaction. Learnings will be expanded to other alcohol to aldehyde reaction systems.

To support the scientific investigations, the team will 1) develop at CCNY flow electrochemical reactors for enhanced kinetic analyses and flow *in situ* FTIR cells for dynamic analyses of adsorbates, 2) use *in situ* NMR techniques at PNNL to identify products and reaction intermediates, and 3) educate CCNY PhD students via a 10-week computational electrochemistry workshop as well as 3-4 months/year internship at PNNL to learn new techniques and transfer knowledge. The expected outcome of the work is to identify what environment and structure, or electrochemical properties, enable dehydrogenation.

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

Super-resolution 3D Atomic Force Microscopy of Electrochemical Interfaces

Dr. Tao Ye,[1] Associate Professor
Dr. Ashlie Martini,[1] Dr. David Prendergast[2]
1: University of California, Merced, CA 95343
2: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

The electrochemical processes of batteries, supercapacitors, and fuel cells predominantly take place at the interface between the electrode (electron conductor) and the electrolyte (ion conductor). The efficiency of these processes depends on the microscopic structure of the solvent molecules and ions that reside just a few nanometers from the electrode. Many important questions concerning the microscopic structure of the electrode-electrolyte interface remain unanswered, including how the solvent molecules and ions are arranged into layers, how the arrangement is influenced by the electrode surface, and how this arrangement changes in response to an applied potential. A team from UC Merced and Lawrence Berkeley National Laboratory will develop super-resolution electrochemical 3D atomic force microscopy (EC-3D-AFM) capable of mapping the 3D arrangement of solvent molecules and ions under electrochemical control. Using EC-3D-AFM, they will image the interface between an electrolyte and an atomically flat electrode at different electrochemical potentials. In addition, they will develop a computationally efficient machine learning method to accurately assign subnanometer features within a 3D force map to the time averaged density and orientation of solvent molecules and ions within the electrochemical interface. The combined experimental and simulation investigation will help the team to understand how the time averaged 3D spatial distribution of solvent molecules changes in response to the electrode potential. Data from experiments will be used to calibrate the atomistic simulations so that the simulations can reliably predict the potential-dependent orientations of water molecules, hydrogen bonding patterns, as well as the dynamics of water and ions within electrochemical interfaces. Such an unprecedented level of structural information may enable researchers to test and refine theoretical models for interfacial capacitance as well as electron transfer at electrode-electrolyte interfaces. Advances toward a molecular level understanding of these important interfaces will ultimately aid the development of materials for electrochemical energy storage and conversion.

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

Understanding phycoerythrin biogenesis: Structural and biochemical studies of bilin lyase-isomerase MpeV

Dr. W. Schluchter,[1] Professor and Chair, Eurofins Professor of Molecular Biology
Dr. X. Yang[2]
1: University of New Orleans, New Orleans, LA 70148
2: University of Illinois at Chicago, IL 60607

Photosynthetic cyanobacteria play critical roles in the global carbon cycle and biomass production. These organisms harvest light energy using huge antenna complexes composed of phycobiliproteins carrying a large array of bilin pigments. Bilin attachment, a critical step in the biogenesis of these phycobiliproteins, is catalyzed by a family of enzymes called **bilin lyases**. These enzymes are responsible for the extensive pigment diversity, thus the wide adaptability of cyanobacteria to various light and nutrient environments. Despite the importance of this enzyme family, the molecular mechanisms underlying the bilin attachment process remain elusive at both the structural and mechanistic levels. In this project, the PI will collaborate with the Co-PI to investigate a group of novel bilin lyases in the MpeV family that have the unique capability of attaching a bilin chromophore via double ligation at Cys50 and Cys61 on the β-subunits of phycoerythrin. We will take an integrated approach of bioinformatics, mutagenesis, biochemistry, homology modeling, and structural biology to identify the molecular determinants underlying the lyase-isomerase functions and to establish the structural basis for the double ligation reaction, an intriguing and unique feature of the MpeV family. Specifically, we will pursue crystallographic studies on the bilin lyase MpeV and its homologs, both in their apo- forms and in complex with substrates. The proposed studies will provide mechanistic insights into this important enzyme group critical for phycoerythrin biogenesis. Findings will also lead to tool enzymes for fluorescent protein production and an engineering framework for developing bio-inspired components that convert solar energy into chemical fuels.

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

Understanding the Mechanisms of Robust Coatings for Extreme Temperature Composites

Dr. Hema Ramsurn,[1] Associate Professor
Dr. Michael W. Keller,[1] Sanwu Wang,[1] Dr. Matthew R. Ryder[2]
1: University of Tulsa, Tulsa, OK 74104
2: Oak Ridge National Laboratory, Oak Ridge, TN 37830

The overarching goal of this proposal is to understand the microstructural evolution and the formation and oxidation mechanisms of anti-oxidative coatings for composites intended for extreme environments. By filling the critical knowledge gap of how processing parameters influence coating robustness, we believe we can significantly enhance the performance of these materials. The proposed work focuses on carbon/carbon (C/C) composites, which consist of carbon fiber reinforcement embedded in a graphite matrix. These advanced materials have low density, high strength-to-stiffness ratio, high thermal and electrical conductivity, and are resistant to ablation, particle erosion, and thermal shock. These lightweight structures are thus ideal for high-temperature structural applications like hypersonic aerospace vehicles, nose cones and wing leading edges of space shuttle orbiters, rocket nozzles, heat shields, aircraft disc brakes, and nuclear fusion reactors. However, one of the current limitations is that C/C composites oxidize at temperatures above 500 °C and thus are limited to inert atmospheres. Although there have been several studies to design reliable oxidation-resistant coating systems that can perform up to 1700 °C, the difference in thermal expansion between the C/C composites and the coating cause cracks to form, compromising the protective efficiency. In this study, we want to leverage the novel densification process of C/C composites developed at the University of Tulsa (TU) with anti-oxidative coatings to develop new materials for extreme environments. Modeling the solid-solid interface will probe the adhesion between the carbon surface of the composite and the protective coating, while the solid/gas interface will be studied to understand how the surface corrodes in an extreme environment. The adherence of anti-oxidative coatings to our novel carbon composites can lay the foundation for the next generation of high-temperature structural materials.

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

Understanding the role of chemical pressure on thermal expansion tunability in earth-abundant materials

Dr. J. A. Cooley,[1] Assistant Professor
Dr. K. H. Stone[1]
1: California State University Fullerton, CA 92831
2: SLAC National Accelerator Laboratory, Menlo Park, CA 94025

Thermal expansion, the way materials change shape when you heat or cool them, is an advantageous property to understand and control. Many objects that people rely on every day (*e.g*. building materials, energy transportation and storage materials, aerospace parts, *etc*.) can wear out or fail more easily if their thermal expansion is not matched well, thus less robust materials create more waste and compromise safety. While many materials exhibit positive thermal expansion and expand as they are heated some exhibit negative thermal expansion and shrink with increasing temperature. These two opposing types of expansion can be coupled in materials such that there is control over the thermal expansion of the final material. This project will study how to control these thermal expansion properties so that new types of materials can be engineered.

This project is a collaborative effort which will be conducted at a primarily undergraduate institution (PUI) which is also a Hispanic Serving Institution (HSI). Undergraduate and Master's students will be involved to attempt to understand how to tune the thermal expansion of certain combinations of earth-abundant elements that shrink instead of expanding upon heating. Part of this effort will involve development temperature-dependent diffraction measurement capabilities at a DOE National Laboratory to the benefit of not only this project, but also the broader user community. Students recruited to work on this effort will conduct experiments in-house at the university and at national laboratories, and disseminate findings to the public through local, national, and international conference presentations. Furthermore, local outreach will allow students to work to increase the amount of citizen science, public scientific literacy, and overall public interest in materials chemistry.

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

Conceptual and engineering design and construction of a Hampton University located stellarator

Dr. C. Lowe,[1] Research Professor
Dr. N. Pablant[2]
1: Hampton University, Hampton, Virginia 23668
2: Princeton Plasma Physics Laboratory, Princeton, NJ 08543

This grant supports the design and construction of a stellarator experiment, STAR_Lite, at Hampton University, an Historically Black College/University (HBCU) in partnership with the Princeton Plasma Physics Laboratory (PPPL). The experiment will be important to the world stellarator program through innovative design and by addressing key physics issues related to stellarator optimization and stability in which a university-scale experiment can make important contributions: design optimization, non-resonant divertor operation, fast plasma response to external magnetic perturbations, and the effect of plasma currents on plasma stability. The STAR_Lite program will be organized around long-term national and international collaborations with world-leading plasma scientists to enhance Hampton's contributions to the advancement of fusion plasma science. The STAR_Lite program will enable the creation of a new experimental physics group at Hampton University and have a strong focus on undergraduate and graduate education thereby bringing a new and diverse set of expertise into the fusion workforce. Diversification of the US fusion workforce will be a natural result of engaging underrepresented students, scientists, and engineers in research of worldwide importance in collaboration with internationally known researchers.

The Stellarator for Research and Training (STAR_Lite) will have a plasma radius between 0.3m and 0.5m and will be optimized for particle trajectory, core confinement, non-resonant divertor robustness and MHD stability. Although STAR_Lite is in its early conceptual design phase, it is envisaged that the primary coils will have an open geometry, likely helical, in order to study the issues and benefits of an open-access design for experimental flexibility and for power-plant maintenance. At the end of this 3-year program, we expect to have designed and constructed a complete stellarator device, have mapped the magnetic flux surfaces and be prepared for a first plasma operational phase.

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

Localized electrons, ionization potentials, and non-thermal states in warm dense matter from the thermal projection-based initial maximum overlap method

Dr. Aurora Pribram-Jones,[1] Assistant Professor
Dr. Frank Graziani[2]
1: University of California, Merced, CA 95343
2: Lawrence Livermore National Laboratory, Livermore, CA 94551

This project will expand an established partnership between UC Merced and the High Energy Density Sciences (HEDS) Center at Lawrence Livermore National Laboratory (LLNL). We will enhance the partnership between a Hispanic-serving institution and a world-class research laboratory, strengthening ongoing efforts to advance frontier science through inclusive excellence and developing a diverse and expert technical workforce for fusion energy sciences. By applying a new computational approach, the thermal projection-based initial maximum overlap method (PIMOM), we will investigate the electronic properties and phase transitions of target materials along the fusion ignition pathway. The project offers a high-impact opportunity for the fusion energy sciences community by improving simulation capabilities for core excitations in fusion-relevant materials and providing a new set of models for investigating key fusion physics principles. These goals represent fundamental scientific insights important for fusion applications at partner institution LLNL and beyond, as well as practical advances in computational capabilities within the field. Additionally, this project would enhance the burgeoning HEDS research program at UC Merced and further facilitate potential national laboratory career paths for UC Merced undergraduate, graduate, and postdoctoral researchers.

This project will be carried out in close collaboration with Graziani and colleagues at the HEDS Center at LLNL, who will ensure connections to current experimental and computational practice in HEDS. These efforts would provide an entirely new computational capability to researchers at both UC Merced and LLNL and would facilitate inclusion of quantum chemical expertise into the ongoing collaboration of LLNL HEDS researchers with the Pribram-Jones Group. Quarterly, in-person meetings will be facilitated by the close proximity of UC Merced and LLNL. These interactions will be further solidified by student summer positions on-site at LLNL and participation in ongoing joint professional development activities, which are critical to fostering inclusive and accessible career pathways for UC Merced's exceptional research students.

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

Scale up of Normalizing Flows for Likelihood-free Inference with Fusion Simulations

Dr. Marcus Alfred,[1] Associate Professor
Dr. Michael Churchill[2]
1: Howard University, Washington, DC 20059
2: Princeton Plasma Physics Laboratory, Princeton, NJ 08543

The physics objective of the proposed research is to continue work to scale up likelihood-free inference (also known as simulation-based inference, SBI) with normalizing flows to quantify anomalous transport coefficients in fusion devices. This merges machine learning and Bayesian principles to give deeper and more thorough analysis of experimental data and comparison to simulation. The infrastructure objective this project seeks to build research capacity, infrastructure, and expertise at Howard University through a mutually beneficial relationship between Howard University (HU) and the Princeton Plasma Physics Laboratory (PPPL). By researching how to use Artificial Intelligence and Machine Learning techniques to discover improved and faster ways of matching computer simulations with experiments involving magnetically confined plasmas, HU and PPPL will use the funding for an initial investment in sustainable research personnel to dramatically expand HU's research capacity in Fusion Energy Sciences while strengthening growing ties with PPPL. This effort may have a direct impact on the development of the science and technology needed to develop fusion as an energy source. Fusion represents a step to advance the energy security of the United States and may ultimately play an enormous role in ensuring America's security and prosperity by addressing its energy challenges.

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

Estimating the Ultimate Sensitivity of Dwarf Galaxies to the Indirect Detection of Dark Matter

Dr. Christopher Kelso,[1] Professor
Dr. Daniel Hooper[2]
1: University of North Florida, Jacksonville, FL 32224
2: Fermilab National Accelerator Laboratory, Batavia, IL 60510

For decades, astronomers and physicists have understood that there exists a new type of matter, unlike that which we see around us. This "dark matter" does not seem to interact appreciably with light and thus far has only been detected through its gravitational interactions. The nature of this dark matter remains one of the most intriguing, unsolved problems in modern physics. A variety of experiments around the world and in space have attempted to observe dark matter and its interactions for many years. One experimental strategy is referred to as "indirect detection," whereby observers use telescopes to search through space for regions with an unexpectedly high number of particles that might be caused by dark matter particles annihilating with each other (or decaying) throughout the cosmos. One such telescope is the NASA and DOE sponsored Fermi Gamma-Ray Space Telescope that orbits the earth about every 90 minutes and scans the entire sky for high energy photons called gamma-rays.

This project has the potential to have a direct impact on the viewpoint held by the scientific community regarding the effect of the upcoming, DOE funded Legacy Survey of Space and Time (LSST) telescope on the indirect search for dark matter. Many scientists within the community have the strong expectation that LSST will discover many "dwarf galaxies" that are much smaller than our own Milky Way galaxy but are orbiting the Milky Way as they are trapped by its gravitational pull. These new dwarf galaxies are anticipated to lead to a significant increase in the Fermi telescope's ability to discover or constrain the properties of dark matter. This work will provide quantitative estimates for exactly how significant that increase is likely to be, thus making those expectations much more robust. In addition, we will provide a first estimate of the ultimate sensitivity that will be accessible for the indirect detection of dark matter using dwarf galaxies as targets. This aspect of the work is inspired by a well-studied, similar statistical limit created at the point in the future when neutrinos will provide an irreducible background referred to as the "neutrino floor/fog" for experiments that search for a direct interaction between a dark matter particle and the detector (direct detection experiments).

This work will also make a key contribution to the investigation of an excess of gamma-rays coming from the galactic center, first identified in 2009 that might be due to the annihilation of dark matter. Since that time, several groups of researchers have confirmed the presence of the excess, including the Fermi Collaboration itself. This galactic center excess remains one of the most intensely researched subjects in dark matter indirect detection as well as gamma-ray physics in general. The work of this proposal intends to provide a definitive answer as to whether the ultimate sensitivity of the Milky Way dwarf galaxies will be sufficient to confirm or refute the dark matter interpretation of the galactic center excess.

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

Accelerating Dark Energy Science from Emission-Line Galaxy surveys and participation of women and underrepresented minority groups in Midwest

Dr. Shun Saito,[1] Assistant Professor
Dr. Andrew Hearin[2]
1: Missouri University of Science and Technology, Rolla, MO 65409
2: Argonne National Laboratory, Lemont, IL 60439

Revealing and understanding the nature of Cosmic Acceleration or Dark Energy is one of the most fundamental questions in physics. In this project, the team proposes to develop a simulation-based forward modeling approach to unlock the full potential of Dark Energy science from Emission-Line Galaxy (ELG) surveys such as the Dark Energy Spectroscopic Instrument (DESI). The scientific goal of this project is to develop a theoretical framework and analysis pipeline to model ELGs using existing N-body simulations and to infer Dark Energy parameters by making full use of scales probed by galaxy surveys while marginalizing over theoretical uncertainties in galaxy formation and evolution physics. As a byproduct, the proposed work will provide unique high-fidelity synthetic catalogs of ELGs, which will be useful in a wide range of communities.

The collaboration is based at a cosmology group recently established at Missouri S&T, an emerging research institution, and is largely benefited from the state-of-the-art high performance computing facility at the Argonne Laboratory Computing Research Center. Meanwhile, the project is designed to promote the participation of women and underrepresented minority groups in astrophysics research in rural areas of Missouri, where such opportunities were nascent. Leveraging the newly developed Women in Physics group and a physics bridge program that PI develops at S&T, the proposed project will provide the team members in underrepresented categories with excellent training opportunities and unique mentorship from various international collaborations.

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

Demonstration of Home-Grown Crystals for Future SuperCDMS Experiment (DHGC-FSE)

Dr. Dongming Mei, Professor
Dr. Francisco Ponce[2]
1: University of South Dakota, Vermillion, SD 57069
2: Pacific Northwest National Laboratory, Richland, WA 99354

Project Objectives: The proposed project aims to advance Cosmic Frontiers experiments in High Energy Physics by developing low-threshold, cryogenic germanium (Ge) detectors to explore the properties of dark matter (DM) and neutrinos. These detectors will be made using home-grown crystals from the University of South Dakota (USD) in partnership with Pacific Northwest National Laboratory (PNNL), a SuperCDMS collaborator. The proposed project has three primary objectives: 1) developing low-threshold ionization detectors for highly sensitive DM and neutrino detection, 2) evaluating crystal suitability for future SuperCDMS-style experiments by testing at least three detectors in the shallow underground laboratory facilities at PNNL, and 3) investigating low-threshold detectors with internal charge amplification to explore new avenues for achieving greater sensitivity in DM and neutrino detection. By achieving these objectives, the project aims to make significant contributions to the field of high-energy physics and our understanding of the universe's composition.

Project Description: The Demonstration of Home-Grown Crystals for Future SuperCDMS Experiment (DHGC-FSE) will use USD-grown Ge crystals fabricated into detectors to demonstrate charge-readout capability and the ability to achieve low-energy thresholds down to the sub-eV range for low mass DM searches. This collaboration will leverage the expertise, training capabilities, and world-renowned facilities of both institutions. The project entails growing high-quality Ge crystals using the Czochralski method, fabricating low-threshold detectors through sputtering techniques at USD, and testing the performance of the detectors at PNNL. The characterization of grown crystals will provide feedback for the growth process and determine if the crystals are of sufficient quality to be used in detector fabrication. Jointly, we will push detector performance toward sub-eV resolution to achieve lower-energy thresholds for low mass DM searches.

Potential Impact: The DHGC-FSE partnership aims to have both short-term and long-term positive impacts on the future of Ge-based experiments. In the short-term, the project's work will enable the scaling-up of the generation-two (G2) SuperCDMS detector payload to test low-mass DM detection using PNNL facilities as a testbed. In the long-term, DHGC-FSE will advance research in growing Ge crystals and fabricating large-size detectors (10 cm in diameter) suitable for beyond-SuperCDMS experiments in underground environments to minimize cosmogenic background interference. To cost-effectively and fully utilize the SuperCDMS detector volume, DHGC-FSE aims to develop a crystal defect profile metric that accurately predicts detector ionization collection performance. This will allow crystals to be screened before fabrication into detectors, ensuring that only suitable crystals are used in detector fabrication. DHGC-FSE will also position follow-on SuperCDMS experiments to address any potential DM detection cost-effectively. These follow-on experiments will require larger detectors to scale effectively to tens of kg-scale experiments and further reduce cosmogenic backgrounds by growing crystals and fabricating detectors in underground environments. This development will also have the potential to impact Ge-based low-energy neutrino experiments such as coherent elastic neutrino-nucleus scattering, neutrino magnetic moment, and mini-charge. The partnership aims to develop the necessary technology to pave the way for future Ge-based experiments in the search for DM and neutrino properties.

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

Investigating Large-Scale Models for High-Energy Physics Pattern Recognition

Dr. Alina Lazar,[1] Professor
Dr. Paolo Calafiura[2]
1: Youngstown State University Youngstown, Ohio 44555
2: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

The proposed work is focused on developing algorithms targeted towards scaling the training and inference of Graph Neural Networks (GNNs) for edge classification in the context of particle track finding for High-Energy Physics (HEP). Track reconstruction (tracking) connects the measured 3D points (hits) to reconstruct charged particle trajectories. Accurately identifying particle tracks from high-density particle hits datasets is essential for the next generation of HEP experiments identified as priorities by the P5 panel. However, the computational complexity of traditional tracking algorithms grows faster than linear with the number of tracking particles, making particle tracking a limiting factor, for example, for HL-LHC (High-Luminosity Large Hadron Collider) physics performance.

Graph representations of data are useful in many domains to capture complex relationships between data points. Graph Neural Networks (GNNs) are a popular subset of deep learning methods that leverage non-Euclidean structures to make accurate predictions at node, edge, and graph levels. However, training GNNs on large graphs with thousands of nodes and millions of edges is challenging due to long-range dependencies, over-squashing, and neighborhood explosion issues. To address these challenges, the proposed work will use an all-pair message-passing scheme and multiple sampling approaches to efficiently and accurately train GNNs on large-scale datasets. In addition, empirical optimization experiments will be used to find suitable sampling methods, optimal GNN architectures, and sets of hyperparameters for better edge and graph-level predictions.

To optimize the performance of GNNs on large graphs, increasing the model size and the number of hidden layers can be effective. However, large graphs do not fit into the GPU memory for training. Graph sampling methods can be used to break data into smaller subgraphs to mitigate this issue, but existing methods may not work well for edge prediction tasks. This project aims to scale the training and inference of GNN models for particle tracking in HEP datasets by designing new methods that scale well. The project will investigate sampling methods that select links or subgraphs instead of individual nodes before expanding the neighborhood to ensure that sampled subgraphs contain short-length random walks, which will help identify long-range dependencies or tracks.

We will test this combined approach on benchmark and realistic data. We expect it to work well because (1) of the success of sampling approaches on node-level tasks, and (2) the all-pair message passing scheme ensures that every pair of nodes is connected and exchanges messages even if they share no edge. Distributing graph mini-batches to train simultaneously across multiple GPU devices on the same node or across nodes will also reduce training times.

Besides increasing the physics reach and computing performance of HEP particle tracking algorithms, if successful, this project will develop methods to analyze the relations of noisy experimental 3D measurements that may be applicable to different contexts, from galaxy dynamics to scene reconstruction in self-driving car applications.

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

Wellesley / UTA Training and Growth in Underrepresented Groups

Dr. James Battat,[1] Associate Professor
Dr. Jonathan Asaadi[2]
1: Wellesley College, Wellesley, MA 02481
University of Texas, Arlington, TX 76019

This FAIR partnership between Dr. James Battat at Wellesley College (an Emerging Research Institution and a Women's College) and Dr. Jonathan Asaadi at University of Texas, Arlington (UTA, an R1 Minority Serving Institution) to construct and deliver early science from a cryogenic microelectronics test facility at Wellesley College. Cryogenic detectors (here meaning operation at 70-180 K) play a central role in frontier science in high energy physics in areas such as dark matter and neutrino detection, searches for neutrinoless double-beta decay, and other investigations into physics beyond the Standard Model. Our work aims to improve the sensitivity of detectors that use liquid noble elements like argon and xenon as their target material. The FAIR award would primarily fund infrastructure, equipment, and personnel/intellectual exchange. This project leverages existing resources at both institutions, as well as a long-standing collaboration between Battat and Asaadi to develop pixelated charge and light readouts for liquid noble detectors. The cryogenic facility will house two cryostats: a small one to support short (few-day-long) measurements, and a larger one for longer-term operation (weeks). The cryostats will house a time-projection chamber (TPC) filled with purified noble liquids using either a single-pass liquid purification column or a gas-based purification and recirculation system, all of which will be built under this award. This cryogenic TPC will serve as a test platform for novel pixelated charge and/or light readout systems. There has been a clearly articulated case for cryogenic detector development and "blue sky" R&D during the recent Snowmass planning process and the Particle Physics Projects Prioritization Panel (P5) meetings. The cryogenic facility proposed here aligns with that priority, and this FAIR award will build the associated research capacity, infrastructure and expertise at Wellesley College, an institution historically absent from the DOE SC funding portfolio.

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

Increasing Access to Radioisotopes by Advancing Radiochemical Training Capabilities

Dr. Melissa Deri[1], Associate Professor
Dr. Vanessa A. Sanders[2]
1: Lehman College of the City University of New York, Bronx, NY 10468
2: Brookhaven National Laboratory, Upton, NY 11973

This project aims to build high impact research capacity and infrastructure at Lehman College through equipping radiochemistry laboratory facilities. This will improve the research and training capabilities and enable more direct participation in isotope production projects. It will also further strengthen the existing collaborations between Lehman College and Brookhaven National Laboratory (BNL) through the expansion of our common efforts to advance radioisotopes of scandium for medical applications. The combined focus on the chemistry of titanium/scandium separations for target processing and generator design will expand the availability of radioscandium and highlight its utility within nuclear medicine.

Interest in radioisotopes of scandium (Sc), especially ^{44}Sc and ^{47}Sc, has only grown in recent years due to their individual and combined potential in nuclear medicine. ^{44}Sc is a positron emitting radionuclide with a half-life of 3.97 h that is well suited for positron emission tomography (PET) while ^{47}Sc has a half-life of 3.35 d and emits moderate energy beta particles suitable for targeted radiotherapy. This research investigates the isotope production, purification, separation, and radiochemical synthesis of both Sc isotopes as a method to both accelerate their development and availability for radiopharmaceutical use. The expertise from BNL will inform the development of complementary radiochemical facilities at Lehman College to assure a mutually beneficial research collaboration focusing on radioscandium production and chemistry. Non-radioactive, macroscopic synthesis and characterization as well as low activity radiochemistry work will be led at Lehman College, while target irradiations and processing as well as scaled up radioactive work will be carried out at BNL. This project aims to (1) develop improved accelerator production of ^{47}Sc through the ^{48}Ti(p,2p)^{47}Sc production route with a focus on optimizing post-irradiation separation chemistry, (2) investigate inorganic resin systems for use in a ^{44}Ti/^{44}Sc radionuclide generator to improve ^{44}Ti retention and generator lifetime, (3) demonstrate the utility of radioscandium isotopes by optimizing synthetic radiochemical protocols for labeling bioconjugates with radioscandium with established and novel chelating agents, and (4) expand these research capabilities to other radionuclides of interest, namely radio-lanthanides and actinides.

Enhancing Lehman's radiochemical research capacity will greatly increase the number and diversity of students who are able to participate in and be exposed to isotope production science. The existing collaboration with BNL has most directly impacted students who are able to travel there to conduct some radioactive experiments. Enabling those experiments to be done on campus at Lehman will allow for many more students to get involved which in turn will significantly increase the training and recruiting of students into nuclear science to enhance workforce development. Developing improved radiochemical separations for scandium and titanium will increase the availability of multiple isotopes of radioscandium with direct clinical relevance. Combined with optimized radiolabeling protocols, this will lead to a surge in radiopharmaceutical research. Furthermore, the fundamental chemistry developed can be translated to other tri- and tetravalent radiometals of interest within isotope production.

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

An Evaporatively Cooled Beamline Technology for the Project 8 Atomic Tritium Source

Dr. Ben Jones[1], Associate Professor
Dr. Brent VanDevender[2]
1: The University of Texas at Arlington, Arlington, TX, 76019
2: Pacific Northwest National Laboratory, Richland, WA 99354

The unknown absolute value of the mass of the neutrino is one of the most glaring holes in our understanding of the standard model of particle physics. The leading proposed method to advance the precision of neutrino mass measurements in the laboratory is cyclotron resonance emission spectroscopy of electrons produced in decays of atomic tritium. The international Project 8 collaboration is developing the technology needed to enable such a measurement, with realization of a high throughput atomic tritium source being one of its primary R&D goals over the next decade. Such a source is a necessity if target levels of neutrino mass sensitivity are to be reached, since previously used molecular tritium sources introduce irreducible systematic uncertainties associated with molecular final states. Our research supports University of Texas Arlington, a Minority Serving Institution and Emerging Research Institution to partner with Pacific Northwest National Laboratory to develop a critical yet un-demonstrated component of the Project 8 atomic source. A cooling stage is required that will accept tritium cracked from its molecular form and then partially cooled to 10 K, and emitting cold atoms that can be magnetically trapped in the sensing volume at 1 mK. This requires a fundamentally new technology: an evaporative atomic beamline that both cools and slows a high flux of light, magnetically trappable atoms. We will prove the concept of magnetic evaporative beamline cooling using a test segment fed with a Zeeman-slowed 6Li beam and validate a suite of detailed phase space simulations using its results. Our staged work plan involves the development of the partially cooled atomic Li source, implementation and optimization of the magnetic evaporation geometry, and then exploration of laser-less beam slowing techniques. The results of these experiments and simulations will inform detailed designs for the cooling segments of the Project 8 Atomic Tritium Demonstrator.

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

Bringing Experimental High-Energy Nuclear Physics to Navajo Nation

Dr. Abraham Meles[1], Associate Professor
Dr. Ceasar da Silva[2]
1: Navajo Technical University, Crownpoint, NM, 87313
2: Los Alamos National Laboratory, Los Alamos, NM, 87545

The novel nuclear physics project at Navajo Tech University (NTU) will address two main challenges in the Navajo community in a way that integrates culture and science: the need for the local workforce to deal with nuclear radiation contamination caused by abandoned uranium mineson Navajo soil and the formation of a diverse workforce for future Department of Energy (DOE) programs in nuclear physics. The project will equip NTU labs with radiation detectors for lab experiments and a detector assembly lab for a particle tracker to be installed in the Large Hadron Collider beauty (LHCb) experiment at CERN in collaboration with Los Alamos National Lab. The research project will also bring NTU to LHCb as the first indigenous college to participate in a big international high-energy physics collaboration. The combination of the research expertise of Los Alamos National Laboratory (LANL) scientists and an NTU professor specializing in Experimental Nuclear Particle Physics will enble the joint NTU-LANL team to develop nuclear physics lab setups at NTU. The team will undertake joint research projects that are feasible and possible. The project will enable the transfer of technology and expertise from LANL to NTU to establish a viable research effort that both attracts TU undergraduate researchers and allows access to a large class of experiments suitable for the research cadre of students at NTU. The project has four objectives: (1) Increase the number of Native Americans earning undergraduate degrees and entering graduate degrees in STEM fields equipped with hands-on training experience in scientific problem-solving and research skills. We expect at least one student participating in this program to enroll in a nuclear and particle physics graduate program, (2) Create a knowledge and technology transfer environment to establish a nuclear research infrastructure at NTU so that students and faculty can perform research within their own community. The goal on this task is to have students hired by local companies and/or National Labs engaged in studying the uranium contamination in the Navajo land and other nuclear physics efforts, which could benefit the Navajo Nation community and other DOE projects with a diverse workforce, (3) Establish NTU as a reliable player in nuclear and particle physics detector assembly. The intime assembly of good-quality components is a good metric for this evaluation. The panels should have a robust mounting, be light tight, and have scintillating light yield within 30% of the specifications. This target should be pursued during the course of the project given the time required for skill set development, (4) By the end of this project, NTU should have some visibility in the particle and nuclear physics field, putting this region of the US on the map of high-level research. The collaboration with big high-energy particle experiments such as LHCb and sPHENIX, participation in their data acquisition, and participation in conferences such as American Physics Society (APS) and Division of Nuclear Physics (DNP) are envisioned during the course of this project.

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

Enhancing Nuclear Data Measurements at the UMASS Lowell Research Reactor

Dr. Marian Jandel[1], Associate Professor
Dr. Shuya Ota[2]
1: University of Massachusetts, Lowell, MA, 01854
2: Brookhaven National Laboratory, Upton, NY, 11973

Neutron capture reactions play a central role in nuclear science that transcends the boundaries between engineering (reactors, homeland security, nuclear non-proliferation, and oil-welling) and academic sciences (astrophysics and planetary science). For all these needs, reliable knowledge of absolute cross sections and discrete gamma-ray transition scheme is essential, but their reliability is often taken for granted. In a recent gap/discrepancy analysis using various nuclear data libraries, we identified data on many isotopes, particular those measured with a single gamma-ray detector during 70-80's, in need of drastic revisions. Improving the data with modern gamma-gamma coincidence techniques to suffice the need is the basis for this research. Accurate production cross-sections for capture gamma-rays on some key isotopes of Cr, Ni, and Cu elements will be measured with the Mixed Array of Detectors (MAD) using a thermal neutron beam from the 1 MW Research Reactor at University Massachusetts at Lowell (UMass Lowell). The new data will be compared with previous data and ultimately replace those. Comprehensive thermal cross sections and gamma-decay data will be created through the nuclear data evaluation process by partnership with a National Nuclear Data Center (NNDC) staff scientist at Brookhaven National Laboratory (BNL). After establishing the training program through the partnership with NNDC, further work on measurements and evaluation of capture gammas of other isotopes can continue in a similar manner.

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

Towards Simulating Quantum Chromodynamics with External Electromagnetic Fields on Noisy Quantum Computers

Dr. Prabal Adhikari[1], Associate Professor
Dr. Meifeng Lin[2]
1: St. Olaf College, Northfield, MN, 55057
2: Brookhaven National Laboratory, Upton, NY, 11973

Quantum computing (QC) has been developing rapidly in the past decade and offers renewed hope for solutions to quantum many-body problems that appear in high-energy physics, in particular Quantum Chromodynamics (QCD), nuclear physics and condensed matter theory. The aim of this award is the development of a research group (at St. Olaf College) in collaboration with Brookhaven National Laboratory that will develop and implement QC algorithms. These are applicable to the study of strongly coupled theories such as QCD in a regime where classical lattice simulations suffer from the fermion sign problem and includes a wide range of physical systems including astrophysical objects (such as neutron stars) and heavy-ion collisions. In particular, the group will hire undergraduate students for a semester-long research program followed by a summer research program that will continue at Brookhaven National Laboratory, where students will work on real quantum devices. By providing students QC training, the participation of traditionally underrepresented students will be increased within the quantum workforce while working on meaningful research questions that will help develop quantum algorithms for studying open problems in QCD.

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

Precision Jet Drift and Energy Loss: An NMSU / LANL Partnership

Dr. Matthew Sievert[1], Associate Professor
Dr. Ivan Vitev[2]
1: The Regents of New Mexico State University, Las Cruces, NM, 88003
2: Los Alamos National Laboratory, Los Alamos, NM, 87545

When the jets of high-energy particles created in ultra-relativistic nuclear collisions propagate through matter, they carry a tomographic imprint of the medium they traversed. Traditional measures of the modification of jets in medium are energy loss, quantified by a nuclear modification factor, and transverse momentum broadening, quantified by two-particle azimuthal correlations. More sophisticated modern jet observables also include substructure, such as the radial distribution of energy within the jet, and the global distribution of energy throughout the event, such as angularities. More differential observables like jet substructure have the ability to constrain the microscopic mechanisms of energy loss and medium modification. The research seeks to leverage a new class of asymmetric jet-medium interactions termed “jet drift,” generated by the medium velocity and gradients to study jet tomography with new observables. Using event-by-event simulations which compute the bending trajectories of partons in the medium from first principles, the study will focus on the impact on both inclusive observables like hadron suppression and elliptic flow, as well as jet substructure and global event shapes. The physics of jet drift is interconnected with the physics of energy loss, and we will therefore couple their calculations in a self-consistent way to assess the feedback between these effects. Jet drift also exhibits interesting late-time contributions driven by the rising radial flow which suggest that nontrivial contributions may arise even during the hadron resonance gas phase. The team will construct novel potentials describing the interaction of a perturbative jet with a dilute hadron gas and use it to study the sensitivity of jet drift and energy loss to temperatures below freeze-out. The specific objectives of this project over a three year time period are: (1) to study the phenomenological consequences of velocity- and gradient-mediated jet drift on event-by-event heavy-ion collisions at sufficient precision to enable comparison to experimental data; (2) to determine the impact of these velocity and gradient effects on more differential observables like jet shapes and global event shapes; and (3) to study the role of late-time dynamics of jets in a flowing hadron gas. The theoretical methodology employed will be the opacity expansion approach incorporating the particular gradient and sub-eikonal corrections derived by the co-PIs. The expected deliverables of this project include the construction of new observables, models, and microscopic theories; quantitative predictions for RHIC and LHC; open-source simulation packages and analysis tools; and the advancement of student careers in high-energy nuclear physics.

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