Harnessing Nanotechnology for Fusion Plasma-Material Interface Research in an in-situ Particle-Surface Interaction Facility

Dr. Jean-Paul Allain, Assistant Professor
School of Nuclear Engineering
Purdue University
West Lafayette, IN 47907

The aim of this project is to utilize nanotechnology to address and improve plasma facing materials for use in a fusion device. The research intends to leverage advancements in nanotechnology and materials science of irradiation-driven nano-structured materials for a novel materials solution at the plasma-material interface (PMI) in fusion devices. Extensive work on conventional plasma-facing component materials such as graphite and tungsten and wall-conditioning strategies has been conducted in the past two decades. However, currently there is no viable materials alternative to tame the PMI for conditions found in a sustained burning fusion plasma devices. The work exploits an existing small experimental facility that is capable of not only characterizing new materials but, more importantly probing and manipulating materials at the nanoscale level while performing subsequent in-situ testing of their performance under simulated environments to discover new materials compatible with the PMI in burning plasma devices.

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

Studies of Nuclear Reactions that Drive Stellar Explosions and Synthesize the Elements

Dr. Daniel Bardayan, Research Staff Member
Nuclear Astrophysics Group
Physics Division
Physical Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

The origin of the elements in the cosmos, and the nuclear reactions that drive stars and stellar explosions, involve short-lived unstable nuclei not normally found on earth. Studies of these topics require accelerator-based experiments with exotic nuclei such as those available at the Oak Ridge National Laboratory's Holifield Radioactive Ion Beam Facility (HRIBF). This project will combine the exotic beams of HRIBF with a new high-density gas jet target using 3He and 4He to make direct studies of astrophysical reactions and nuclei that power stellar explosions and synthesize the elements. Such a measurement system will be unique in the world, and will greatly expand the ability to understand how stars and their spectacular explosions create the elements.

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

GENEVA: An NLO event generator for the Large Hadron Collider

Dr. Christian Bauer, Senior Research Scientist
Theory Group
Physics Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

The objective of this project is to develop software tools that are crucial for physics discoveries in hadron collider experiments, e.g., LHC, that probe the fundamental properties of Nature at the energy frontier. The project will improve on existing tools by implementing and incorporating the most accurate available theoretical calculations and predictions to simulate events that can be expected from the known Standard Model of particle physics. One can then search for new physics by comparing data with the expected events. Without such tools many signals of new physics (e.g., new particles, new fundamental forces, etc.) may not be revealed from the huge amount of data generated from these experiments.

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

Investigation of Fundamental Limits to Beam Brightness Available From Photoinjectors

Dr. Ivan Bazarov, Assistant Professor
Department of Physics
Cornell University
Ithaca, NY 14850

The objective of this project is to extend the fundamental understanding of high average current low emittance sources of relativistic electrons necessary for a new generation of coherent X-ray synchrotron radiation facilities. The proposal aims to perform experimental and theoretical investigations of the limits on beam brightness by focusing on photocathode sources and space charge effects in a systematic way, by measuring, analyzing, and investigating ways to reduce thermal emittance, and compensating emittance growth via laser pulse shaping and beam manipulations. Understanding these effects is an important step in producing high brightness electron sources for future light sources and electron diffraction applications. Better understanding of the associated physics and generation of a low emittance beam can lead to significant cost saving for future light sources.

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

Research and Development of Detection Systems for Neutron Imaging

Dr. Philip Bingham, Research and Development Staff Member
Image Science and Machine Vision Group
Measurement Science and Systems Engineering Division
Energy and Engineering Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

The objective of this project is to develop a high-resolution transmission imaging system for the simultaneous collection of neutron and x-ray computed tomographic projections using energy-dependent neutrons. Current state-of-the-art neutron radiography is reaching the 10-15?m resolution range with high cost detectors; however, typical resolutions are on the order of no better than 50?m today. The proposed development will result in an increased resolution using less expensive, lower resolution detectors through the use of a magnified detection system whose novel feature consists of combining neutron and x-ray transmission images. Together, the neutron and x-ray images provide complementary information due to the different mechanisms by which neutrons and x-rays interact with materials and their associated energy-dependent attenuation coefficients. By combining these distinct imaging modalities into a single system, different material properties can be quantified and higher resolution can be achieved.

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

Scaling Laws in Magnetized Plasma Turbulence

Dr. Stanislav Boldyrev, Assistant Professor
Department of Physics
University of Wisconsin
Madison, WI 53715

The objective of this research is to develop new analytic approaches, conduct numerical simulations with unprecedented resolution, and train students to carry out a comprehensive study of parameter-scalable regimes of magnetized-plasma turbulence. Plasma is a dynamically rich and technologically potent state of matter, beyond solid, liquid, and gas. A distinguishing property of plasma is its sensitivity throughout its volume to perturbations in density or velocity even in a small region. When embedded in an ambient magnetic field, the plasma can be sensitive also to perturbations in the magnetic field. Depending on the size of the plasma, this collective behavior can take place over lengths as small as a few centimeters, e.g., in laboratories, and as large as thousands of light years, e.g., in astronomy. Through the power of equations that express scaled relationships of parameters, a single mathematical model can predict the properties and dynamics of phenomena associated with almost any size and parameter value of the plasma. The magnetohydrodynamics (MHD) model is often invoked for this purpose because plasma behaves like an electrically conducting fluid embedded in a magnetic field. This model involves details, the appropriateness and microscopic level of which need to be customized for the specific laboratory or astronomical application, which are not always agreed upon by scientists and won't be until experiments can validate such details. In the meantime, the theories that describe these details sometimes lead to contradicting predictions, as the theories are typically empirical or phenomenological. Weak MHD turbulence, strong MHD turbulence, and magnetic dynamo action will be emphasized in the study.

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

Reliable High Performance Peta- and Exa-Scale Computing

Dr. Grigory Bronevetsky, Computer Scientist
Computer Science Group
Center for Applied Scientific Computing
Computation Directorate
Lawrence Livermore National Laboratory
Livermore, CA 94550

The goal of this research is to predict the effects of system faults and enable developers to protect their applications against the most likely and/or most critical errors. The project will develop statistical models that describe fault propagation through system modules and abstraction layers, synthesizing these models to create a full system model. The full model will be able to predict the effects of system faults, which will make it possible to develop vulnerability profiles for application and system software, which in turn will allow operating system developers to protect them against the most likely and/or most critical errors. The methodology will be applied to two major types of problems: component failures and performance degradations on MPI applications, and soft fault-induced data corruptions on numerical applications.

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

Ultrafast Electron Diffraction from Aligned Molecules

Dr. Martin Centurion, Assistant Professor
Department of Physics and Astronomy
University of Nebraska
Lincoln, NE 68588

The goal of this project is to capture the three-dimensional structure and dynamics of molecules with atomic resolution using ultrafast electron diffraction. Electron diffraction from molecules in the gas phase is a successful technique for determining the structure of isolated molecules. Due to the random orientation of molecules in a gas, only one-dimensional information such as bond lengths can be retrieved from the diffraction patterns. The experimental method proposed in this work solves this problem by combining electron diffraction with laser alignment. This will allow the retrieval of full three-dimensional images of molecular structure. A key to the success of this project will be the design and implementation of a new instrument to produce ultrafast pulses of electrons. After demonstrating the ability to record static images of small molecules, the method will be extended to more complex molecules such as biomolecules that cannot be crystallized. The method will also be extended to study the dynamics of molecules in space and time.

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

Sustainable Silicon - Energy-Efficient VLSI Interconnect for Extreme-Scale Computing

Dr. Patrick Yin Chiang, Assistant Professor
School of Electrical Engineering and Computer Science
Oregon State University
Corvallis, OR 97331

The objective of this research is to develop energy-efficient, VLSI inter-connect circuits and systems that will facilitate future massively-parallel, high-performance computing. The project will address critical barriers on the path to extreme-scale high-performance computing. The goal of the project is to improve energy-efficiency of off- and on- chip interconnects by more than an order of magnitude over conventional techniques by optimizing power consumption in global and local clock distribution to parallel links; understanding the theoretical and practical limits to fine-grain, instantaneous power gating of on/off links; exploring energy-efficient circuit topologies; and determining the limitations to using low-voltage swing for parallel interconnect such as core-core and crossbar links.

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

Superconducting Technology for Magnet Systems in Fusion Machines

Dr. Luisa Chiesa, Assistant Professor
Department of Mechanical Engineering
Tufts University
Medford, MA 2155

The objective of this project is to develop a fundamental understanding of the mechanical and material properties of superconductors. The aim is to understand the electromechanical behaviors of superconducting materials for both low (LTS) and high temperature superconductors (HTS). Superconducting magnets play a key role for the confinement of plasma in a large fusion energy device, providing magnetic fields high enough to confine the plasma and produce substantial fusion power density. The magnet components alone account for a considerable fraction (~30% for the International Thermonuclear Experimental Reactor (ITER)) of the investment in the fusion device (~50% of the magnet system cost is for superconducting materials). Low temperature superconductors, which are used both in current and near-term fusion devices, have showed unexpected sizable degradations compared to the expected currents estimated from single strand values. Those degradations are due to the inherent mechanical loads caused by thermal contractions and operational electro-magnetic forces. Understanding this behavior and designing around it will be extremely beneficial to the development of magnet technology for not only fusion but other magnet applications.

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

Thylakoid Assembly and Folded Protein Transport by the Tat Pathway

Dr. Carole Dabney-Smith, Assistant Professor
Department of Chemistry and Biochemistry
Miami University
Oxford, OH 45056

This project aims to better understand a critical protein transport pathway found in the chloroplasts of plants, bacteria, and some archaebacteria required for the assembly and maintenance of functional photosynthetic membranes. The proper assembly, maintenance, and function of the photosynthetic apparatus in the chloroplasts of green plants depend on three protein transport systems found in thylakoid membranes. The objective of this strongly-focused project is to better understand one of these three essential protein transport systems: the Twin arginine translocation (Tat) system. This transport system, also found in bacteria and some archaebacteria, is responsible for the proper location of ~50% of thylakoid lumen proteins. It is also rather unique in that it transports fully-folded and assembled proteins across ion-tight membranes using only three membrane components combined with the protonmotive force generated by photosynthesis. The successful completion of these studies will give us a better understanding of the biogenesis of photosynthetic membranes, and could provide the rationale as well as the means to engineer photosynthetic complexes into synthetic membranes for energy production.

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

Deformation and Failure Mechanisms of Shape Memory Alloys

Dr. Samantha Daly, Assistant Professor
Department of Mechanical Engineering
University of Michigan
Ann Arbor, MI 48109

The objective of this research project is to understand the fundamental mechanisms driving the deformation and failure of shape memory alloys. The project will seek to elucidate the mechanisms of shape memory behavior by developing and utilizing new methodologies to study the complex phase transformations that give rise to the unique properties of these materials. The investigator will conduct a comprehensive suite of experiments across multiple length scales and tie these results to theoretical and computational modeling. Linkages of atomic interactions, sub-granular transformation, intra-granular interactions, localized strain banding and macroscopic behavior in model Nickel-Titanium alloys will be made. Developing a fundamental understanding of the shape-memory behavior at small length scales can lead to improved vibration response in microscale energy harvesting devices.

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

Generation and Characterization of Ultra-short electron beams for xray free electron lasers

Dr. Yuantao Ding, Accelerator Physicist
Beam Physics Department
Accelerator Research Division
Accelerator Directorate
SLAC National Accelerator Laboratory
Menlo Park, CA 94025

The goal of this project is to develop mechanisms for generating ultra-short x-ray pulses that will enable the study of ultra-fast processes, such as electronic motions in atoms. This research will investigate ultra-short electron beam generation and characterization utilizing analytical, computational, and experimental methods. Free-electron lasers (FELs) are tunable, high power, coherent sources for short-pulse, short-wavelength radiation. Short x-ray pulses will enable the ability to photograph atomic motion or to trace the dynamics of molecular structure. The generation of even shorter x-ray pulses ("ultra-short") is a formidable challenge requiring theoretical and experimental breakthroughs. Shorter x-ray pulses, like a few femto-seconds or atto-seconds, will allow for the direct observation of electronic motion in an atom and enable many new ultrafast studies such as time-resolved electronic dynamics, with widespread applications in physics, chemistry and biology.

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

Directed Assembly of Hybrid Nanostructures Using Optically Resonant Nanotweezers

Dr. David Erickson, Assistant Professor
Sibley School of Mechanical and Aerospace Engineering
Cornell University
Ithaca, NY 14853

The goal of this project is to investigate the assembly of hybrid nanostructures using nanophotonically directed optical forces and to enable the directed assembly of nanostructures using nanophotonic optical devices that cannot be manufactured by other means. This approach offers a novel means to directly manipulate nanoscale matter, possibly down to the biomolecule level, for generating unique nanocomposites and ordered arrays and could usher in the development of new materials that harness or modulate energy. While the focus of this work will be on understanding some of the fundamental physics behind this new approach, the ultimate implementation of the technique as an optical nanofactory to fabricate unique high efficiency photoelectric or photo-thermal energy conversion devices is envisioned.

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

Model-Independent Dark-Matter Searches at the ATLAS Experiment and Applications of Many-core Computing to High Energy Physics

Dr. Amir Farbin, Assistant Professor
Department of Physics
University of Texas, Arlington
Arlington, TX 76019

Astronomical observations provide strong evidence that the Universe is dominated by two mysterious phenomena known as Dark Matter and Dark Energy. Both may be explained by new particles or forces which have yet to be discovered. The PI proposes to perform a first search for particle Dark Matter with the ATLAS detector at the Large Hadron Collider at CERN. To pursue the computationally intensive analysis techniques required by this proposal, the PI plans research into using General Purpose Graphical Processing Units (GPGPU), an emerging technology in which tens of thousands of simple processing units are marshaled in parallel to achieve orders of magnitude acceleration of certain calculations. This project will also explore other applications of GPGPU computing in High Energy Physics (HEP), including the most commonly used software tools in HEP, and finally tackle the very challenging areas of data reconstruction and simulation.

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

First Principles Modeling of Metal-Electrolyte Systems: A Novel Approach to the Study of the Electrochemical Interface

Dr. Maria-Victoria Fernandez-Serra, Assistant Professor
Department of Physics and Astronomy
Stony Brook University
Stony Brook, NY 11794

This project aims to computationally improve fundamental understanding of electrically induced chemical reactions in the condensed phase and at the liquid-metal interface. Improvement of future energy production and delivery systems - such as fuel cells, batteries, and next-generation hydrogen-production devices - require an unprecedented and detailed fundamental understanding of the interactions and processes occurring at the liquid-metal interface. The rate at which these processes occur ultimately determines the power of such systems. However, these rates are known to change as the system begins to deliver electricity and when the system is exposed to electromagnetic radiation such as sunlight. The power output is also strongly influenced by the very nature and peculiarities of the electrolyte. This works capitalizes upon a broad base of recent advances of quantum-mechanical computational methods to systematically understand how chemical reaction rates occurring at the liquid-electrode interface can be modified to optimize the system's power. Further it seeks to extend these capabilities so that simultaneous modeling and optimization of both the electrolyte and electrode can be realized in the first half of this decade. In addition to fuel cells and batteries, future technologies which depend on these fundamental advances include advances in photocatalysis, which will lead to solar induced water-splitting for hydrogen production and the eventual understanding of light-induced production of more complex fuels.

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

Chemical Frustration: A Design for the Discovery of New Complex Alloy and Intermetallic Phases

Dr. Daniel Fredrickson, Assistant Professor
Department of Chemistry
University of Wisconsin
Madison, WI 53715

The goal of this project is to test and develop the use of chemical frustration as a means of structural control in intermetallics. This research will determine whether the concept of chemical frustration, an incompatibility between different modes of packing or bonding of chemical components, can be used to create new intermetallic structures. Intermetallics are made up of two or more metals but whose properties are often intermediate between metals and ceramics, yielding unique properties for magnets, high temperature alloys, superconductors, and other applications. The program will develop and use theory and computational analysis to understand how chemical frustration impacts the electronic structures of synthesized materials. By coupling the synthesis of new materials with strong structural determination and theory, this work could produce the fundamental knowledge and guidelines needed to design intermetallics with optimum properties.

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

Molecular Transuranic Discovery Science: Underpinning National Energy Security and Waste Remediation Needs

Dr. Andrew Gaunt, Technical Staff Member
Inorganic, Isotope and Actinide Chemistry Group
Chemistry Division
Chemistry, Life, and Earth Sciences Directorate
Los Alamos National Laboratory
Los Alamos, NM 87545

The objective of this project is to gain a more complete understanding of the fundamental chemical bonding properties of uranium, plutonium, and related actinide elements to underpin the rational molecular design and development of novel, more efficient separation strategies for advanced nuclear fuel cycles, and to develop transformative knowledge about the extent to which covalent interactions control actinide bonding with complexants in advanced nuclear fuel cycles. The main components of all nuclear fuels are actinides. These radioactive chemical elements (such as uranium and plutonium) with many protons, neutrons, and electrons display unique chemical, nuclear, and materials properties. Waste-minimizing nuclear fuel cycles must recycle used nuclear fuel, requiring transformative chemical knowledge to develop advanced separation technologies. The focus of Dr. Gaunt's research will be to carry out chemical syntheses, coupled with structural, spectroscopic and theoretical analyses to determine the bond geometries and strengths between "soft donor ligands" (relatively covalently bonded complexants) with actinide ions that participate in nuclear fuel cycles. By carrying the investigation across the 5f series from thorium through curium, the research is expected to develop soft-donor ligands and bonding trends for all actinide ions in nuclear fuel cycles in all relevant oxidation states. The results will provide a foundation for design of advanced separation technologies in next generation fuel cycles. It is expected to show how basic chemical bonding principles such as structure, bond strength, covalency, and ligand donor type can achieve preferential bonding for actinide ions over lanthanide ions.

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

Investigation of the Role of Inhomogeneities and Phase Segregation on Correlated Electron Dynamics by Optical Spectroscopy and Nano-imaging

Dr. Adrian Gozar, Associate Physicist
Oxide Molecular Beam Epitaxy Group
Condensed Matter Physics and Materials Science Department
Basic Energy Sciences Directorate
Brookhaven National Laboratory
Upton, NY 11973

The objective of this project is to understand the role of intrinsic and extrinsic inhomogeneities at transitions between insulating, metallic and superconducting phases in strongly correlated electronic materials by using optical spectroscopy in the infrared and THz frequency ranges with nanometer spatial resolution. Through the combination of local probes with spectroscopy, the PI will develop a scattering-based scanning near-field microscopy system for the study of electron dynamics in metal-insulator and metal-superconducting transitions in correlated electronic systems and local electronic reconstructions at interfaces in transition metal oxide heterostructures.

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

Reducing Scale Dependence of Physics Parameterizations for Global Cloud Resolving Climate Models

Dr. William Gustafson, Scientist III
Atmospheric Chemistry and Meteorology Group
Atmospheric Sciences and Global Change Division
Fundamental and Computational Sciences Directorate
Pacific Northwest National Laboratory
Richland, WA 99352

The aim of this project is to increase the resolution of climate models by developing new parameterizations for processes such as clouds and radiation that are more adaptable to different spatial scales. The research will help address significant challenges in increasing the resolution of climate models, for example, from 100 to 1 km grid spacing. The research will help merge two different modeling cultures, one that has traditionally used coarse model resolutions integrated over long time periods for climate simulations versus one that has used high-resolution models for detailed studies of climate processes over shorter periods. The research will attempt to develop physics parameterizations for processes such as clouds, radiation, turbulence and other sub-grid phenomena that "sense" the underlying grid spacing and adapt accordingly or use assumptions appropriate for that resolution. A methodology will be adopted whereby individual parameterizations will be run at arbitrary resolutions compared to the remaining portions of the model, enabling determination of which parameterizations are most susceptible to scale issues. Based on those observations, targeted improvements to the parameterizations will be made with the goal of developing scale-adaptive parameterizations.

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

Diamond Pixel Luminosity Telescopes

Dr. Valerie Halyo, Assistant Professor
Physics Department
Princeton University
Princeton, NJ 8544

Proper monitoring and calibration of the instantaneous and integrated luminosity has direct input to almost all physics results for the Compact Muon Solenoid (CMS) Collaboration at the Large Hadron Collider (LHC) at CERN. The PI intends to use particle tracking telescopes based on single-crystal synthetic diamond detectors with the existing CMS pixel readout chip to provide an independent measure of luminosity with different systematic errors than the traditional calorimeter-based system. Diamond has a clear advantage over other technologies such as silicon in that it can be deployed without a complex cooling system and can thus be easily retrofit into the CMS detector. Diamond is also unique in its excellent radiation hardness, a requirement given the operating environment of the device at the LHC. Results from this project provide valuable experience in operating a detector in high radiation environment, leading to techniques involving the use of synthetic diamond detectors in High Energy Physics, dosimetry and space applications.

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

New States of Matter and Quantum Simulation with Ultracold Alkaline Earth Fermions

Dr. Michael Hermele, Assistant Professor
Department of Physics
University of Colorado
Boulder, CO 80309

This research project involves theoretical studies of strongly correlated systems realized with ultracold alkaline-earth atoms (AEAs) in optical lattice potentials. AEAs, which have shown the existence of strong correlation effects that are inaccessible in solid state materials, are expected to not only provide fertile ground for the realization of new states of matter but to also yield new insights into correlation effects more generally. Using analytical and numerical techniques of many-body and quantum field theory, the objectives will be to identify likely ground states to characterize their observable properties and devise schemes for their detection, and to develop an understanding of their phase diagram.

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

Neutrinos in the Universe

Dr. Patrick Huber, Assistant Professor
Department of Physics
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061

The primary objective of this project is to develop and advance theoretical tools to analyze and interpret data from neutrino experiments, the results of which will improve our understanding of neutrinos' properties and the role they play in the cosmos. Since the Standard Model of particles in its minimal version does not admit neutrino mass, the fact that neutrinos have mass suggests that neutrinos may be an important portal to new physics beyond the Standard Model. In addition to providing support for experimental projects such as the Daya Bay reactor neutrino experiment, this research will also use neutrinos as a tool for understanding high-energy and astrophysical phenomena, including ultra high energy cosmic rays and supernovae.

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

Introducing Enabling Computational Tools to the Climate Sciences: Multi-Resolution Climate Modeling with Adaptive Cubed-Sphere Grids

Dr. Christiane Jablonowski, Assistant Professor
Department of Atmospheric, Oceanic, and Space Sciences
University of Michigan
Ann Arbor, MI 48109

The objective of this effort is to develop a modern climate circulation model that enables computational resources to be focused on regions of greatest change. The research will develop a new atmospheric model appropriate for climate simulations that introduces state-of-the-art techniques for resolving multiple scales. These techniques, collectively known as adaptive mesh refinement, allow extreme-scale computational resources to be focused on spatial regions of greater interest, such as coastlines or mountain ranges, or on hard-to-resolve phenomena, such as cyclones. Success will result in more efficient climate simulations that capture more small-scale atmospheric phenomena than would otherwise be possible.

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

Theory and Simulation of Tailored Assembly in Rod-Coil Polymer Nanocomposites

Dr. Arthi Jayaraman, Assistant Professor
Department of Chemical and Biological Engineering
University of Colorado
Boulder, CO 80309

The objective of this research is to use theory and simulations to study tailored assembly within polymer nanocomposites in order to spatially engineer rod- coil polymer nanocomposites for photovoltaic devices. Theory and molecular simulations will be combined to study the morphology of conjugated rod-coil block copolymers, a type of polymer that is used in plastic solar cells. The impact that structure of the polymer molecules and the addition of spherical nanoparticles have on bulk and thin film morphology will be investigated with the aim of discovering the fundamental principles needed to tailor the nanocomposite properties. This work could have a significant impact on our understanding of how to design organic solar cells with higher efficiencies.

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

Nonequilibrium Physics and Phase-Field Modeling of Multiphase Flow in Porous Media

Dr. Rubin Juanes, Assistant Professor
Department of Civil and Environmental Engineering
Massachusetts Institute of Technology
Cambridge, MA 2139

Understanding complex flow physics remains a major challenge in geosciences, and in many other physical sciences and engineering sciences. Modeling subsurface flow patterns requires both improved experimental determinations and better theoretical constructs representing the critical relationships. The innovative new approach in this proposed effort has its origins in the mathematical description of solidification processes. An attractive aspect of the approach is that it lays out hypotheses that are nontrivial, and testable by carefully-designed laboratory experiments. This would be a very important result in soft-matter physics, and in a number of energy system problems such as improved oil and gas recovery, CO2 sequestration, improved efficiency in fuel cells, and improved designs for micro-fluidic devices, all of which depend on the formation and control of fluid-fluid instabilities.

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

Generation, Imaging, and Control of Ultrafast Electrical Currents and Radiation

Dr. Ki-Yong Kim, Assistant Professor
Department of Physics
University of Maryland
College Park, MD 20742

The goal of this research is to elucidate the underlying mechanisms in the production and control of ultrafast electrical currents and terahertz (THz) electromagnetic radiation by using ultra-short optical laser pulses. Various laser-matter interaction schemes will be explored for the ultrafast electrical current and THz generation. Ultrafast imaging techniques will be developed to visualize in time and space the propagation of excitations at metal-dielectric interfaces with femtosecond and micron resolution. The coherent control of electromagnetic radiation in the broad THz to extreme ultraviolet spectral range is expected to greatly benefit the ultrafast optical science community.

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

A Systems Biology, Whole-Genome Association Analysis of the Molecular Regulation of Biomass Growth and Composition in Populus deltoides

Dr. Matias Kirst, Assistant Professor
School of Forest Resources and Conservation
University of Florida
Gainesville, FL 32611

The goal of this research is to identify the genes that are the basis for the variation in biomass and biofuel productivity-related traits in the genus Populus (the poplar tree). Poplars are the principal woody crop species used for clean, renewable and sustainable fuels in North America because of their fast, perennial growth habit and wide natural distribution in a broad range of environments. This project will identify genes underlying bioenergy-associated traits in poplar using an innovative approach to map genome-wide changes related to lignocellulosic biomass formation. This novel method, that will use data from previously sequenced poplar cultivars to capture biomass-related genes in a poplar population, promises to reveal a much larger fraction of the poplar genetic diversity than previously possible. The results will help answer the very important question of which genes regulate biomass productivity and its composition.

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

Multifunctional Oxygen Evolution Electrocatalyst Design and Synthesis

Dr. John Kitchin, Assistant Professor
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

The objective of this project is to build a theoretical foundation for the molecular design of non-noble metal, oxide-based, catalysts for the electrocatalytic reduction of oxygen, and to synthesize and use stable and active electrocatalysts of tailored structure and composition. The efficiency of various energy technologies critically depends on the efficiency of oxygen evolution, yet detailed mechanistic understanding of such multielectron reduction is lacking for other than a few metal electrocatalysts. In particular, metal-oxide based electrodes (e.g., Ni oxide) are desirable for reasons of abundance when compared to noble-metal alloys, yet high-level electronic structure calculations of oxides under reaction conditions and of the organic or inorganic reactions catalyzed by them are rare. In this project, utilizing an atomistic thermodynamic framework based on density functional theory, the stability of nickel oxide surfaces under oxygen evolution conditions will be assessed as a function of the promoter transition metal oxide used. High surface area, mesoporous and promoted nickel oxide nanocatalysts will be synthesized and used as electrocatalysts for water electrolysis, for the purpose of testing and refining the theoretical methods.

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

Search for Time Reversal Symmetry Violation with TREK and J-PARC

Dr. Michael Kohl, Assistant Professor
Department of Physics
Hampton University
Hampton, VA 23668

The discovery of new sources of charge-parity (CP) violation is necessary to explain the observed matter-antimatter asymmetry in the current universe, which the current Standard Model fails to explain. This project will pursue the Time-Reversal Experiment with Kaons (TREK) at the Japan Proton Accelerator Research Complex (J-PARC) to measure the time (T) violating transverse muon polarization in decay of stopped charged kaons as a sensitive search for T-violation. A non-zero value of this observable would be the first observation of new physics in a T-violation experiment. Based on the CPT theorem, such an observation would be equivalent to CP-violation beyond the present accepted scheme of quark configuration mixing in the Standard Model and offer such a source CP violation. This project will design and build prototype detectors to be used in the TREK experiment, in anticipation that the experiment will be carried out in 2013, with the first results available before the end of the grant period.

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

Evaluating the Oxidative, Photothermal and Electrical Stability of Colloidal Nanocrystal Solids

Dr. Matthew Law, Assistant Professor
Department of Chemistry
University of California, Irvine
Irvine, CA 92697

This goal of this project is to bring a fundamental understanding to the degradation mechanisms of semiconducting nanocrystals (NCs) and to introduce new physical and chemical strategies in an effort to improve their operating lifetimes and overall performance in technological applications. The research will use field-effect transistors and solar cells as model systems to establish the degradation mechanisms and develop effective countermeasures. By revealing both how NCs degrade in response to environmental stresses (oxidative, photothermal, and electric) and identifying ways to prevent this degradation, the project will greatly improve our ability to develop new materials for applications from a broad range of nanoscale building blocks, including nanocrystals, nanowires and organic-inorganic hybrid structures.

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

Ton Scale Germanium: Beyond Zeptobarn WIMP Cross-section

Dr. Rupak Mahapatra, Assistant Professor
Department of Physics and Astronomy
Texas A&M University
College Station, TX 77845

The currently favored explanation for the invisible "Dark Matter" that holds galaxies together is a new kind of fundamental particle: a Weakly Interacting Massive Particle (WIMP). These particles may be produced and detected in high-energy particle collisions at the Fermilab Tevatron or the CERN Large Hadron Collider, but there are also many active searches underway to directly detect cosmic WIMPs interacting with normal matter. The extremely weak nature of the WIMP interaction dictates detectors that have extremely low naturally occurring radioactive background, a large active volume (mass) of sensitive detector material to maximize statistics, and a highly efficient rejection of any residual background. To fully explore the possible WIMP parameters we need to scale up from the current few kilogram experiment to few ton experiments. This proposal is a three-pronged, phased approach to address all these issues through the research work of the PI as a member of the Cryogenic Dark Matter Search (CDMS) collaboration, and the next generation proposals for 100kg-scale SuperCDMS and ton-scale Germanium Observatory for Dark Matter (GEODM) experiments.

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

Probing Neutrino Properties with Long-Baseline Neutrino Beams

Dr. Alysia Marino, Assistant Professor
Department of Physics
University of Colorado
Boulder, CO 80309

We know from other experiments that neutrinos have very small masses, come in three types and can undergo transitions from one type to another (often called "neutrino oscillations"). This phenomenon causes the disappearance of electron antineutrinos coming from the sun and muon neutrinos produced in cosmic ray showers in Earth's atmosphere. However, more precise measurements of neutrino properties require intense man-made neutrino sources, such as accelerator-produced neutrino beams, traveling through multiple detectors at different distances. The PI proposes a research program that will center on investigating neutrino oscillations with the high-intensity Tokai-to-Kamioka (T2K) accelerator neutrino experiment, and will also support preliminary design work for a potential future Long-Baseline Neutrino Experiment (LBNE) the US. The primary focus of this project will be measurement and analysis of neutrino beam data in the T2K experiment to understand the properties of the beam, and using this knowledge to inform design choices for LBNE.

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

An Experimental Research Program on Chirality at the LHC

Dr. Christina Markert, Assistant Professor
Physics Department
University of Texas at Austin
Austin, TX 78712

One of the main remaining topics in the nuclear evolution of the universe is a profound understanding of the phase transition from partonic (quark-gluon) to hadronic (nucleon) matter, which happened a few microseconds after the Big Bang. According to modern calculations, two fundamental symmetries of quantum chromodynamics, chirality and color and its deconfinement, are expected to be restored at the transition to the quark-gluon plasma. Experiments at the Relativistic Heavy Ion Collider have yielded evidence of color deconfinement, but it is conceivable that the facility is not energetic enough to populate the high mass resonance states relevant to studies of chirality. This project will develop and apply a new analysis strategy to study chirality using hadronic resonances detectable with the ALICE experiment at the very high energy Large Hadron Collider at CERN.

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

Predictive Modeling of Complex Physical Systems: New Tools for Uncertainty Quantification, Statistical Inference, and Experimental Design

Dr. Youssef Marzouk, Assistant Professor
Department of Aeronautics and Astronautics
Massachusetts Institute of Technology
Cambridge, MA 2139

The aim of this project is to develop rigorous mathematical formulations and scalable simulation approaches for quantifying uncertainties in large-scale simulations of complex systems. The research will focus on quantifying uncertainties that may arise due to incomplete knowledge of the phenomena, imprecise measurements, or insufficient computing power, when making predictions through modeling and simulation. Advanced mathematical and statistical techniques will be employed to develop tools for efficiently computing uncertainties in complex systems, test new techniques for using available observation data to improve models, build a comprehensive, scalable framework for automating the modeling and simulation-uncertainty quantification process, and demonstrate the utility of these tools through the modeling and simulations of combustion processes and subsurface flows. This research in quantification of uncertainties will allow scientists to understand how to use available knowledge to improve models of complex systems, effect sound management of limited resources in designing and conducting experiments, and make simulation-based predictions with increased confidence.

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

Design of the Near Detectors and Optimization of Water and Ice Targets for Fine-Grained Tracking Detectors for the Fermilab Long-Baseline Neutrino Experiment

Dr. Christopher Mauger, Physicist
Subatomic Physics Group
Physics Division
Associate Directorate of Experimental Physical Sciences
Principal Associate Directorate of Science, Technology and Engineering
Los Alamos National Laboratory
Los Alamos, NM 87545

The Long-Baseline Neutrino Experiment (LBNE) is actively being developed in the U.S. This project will employ a neutrino beam at Fermilab aimed at a far site -- most likely the proposed Deep Underground Science and Engineering Laboratory in Lead, South Dakota, (currently being developed by the National Science Foundation) -- to search for neutrino transitions from one type to another . LBNE will measure these transitions with unprecedented sensitivity, which will reveal key properties of these elusive fundamental particles. These experiments work by observing the rate of neutrino interactions in "near" detectors close to the beam and in "far" detectors 100's of kilometers away to see if any neutrinos appear (or disappear) in between; the (dis)appearance is evidence that the neutrinos oscillated from one type to another. The PI proposes to lead the development of the suite of near detectors required to optimize the sensitivity of the LBNE project. The PI will focus particularly on using the near detectors to measure neutrino processes that contribute to the background in the far detector. In addition, the PI will develop liquid and solid water targets for a fine-grained tracking near detector.

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

An Integrated Theory on the Mechanisms of Vegetation Survival and Mortality During Drought

Dr. Nathan McDowell, Staff Scientist
Earth and Environmental Sciences Division
Chemistry, Life and Environmental Sciences Directorate
Los Alamos National Laboratory
Los Alamos, NM 87545

The goal of this project is to develop and test a new and improved theory that describes the mortality and survival of vegetation during drought. Research will focus on understanding the impacts of climate change on terrestrial ecosystems with an emphasis on regional scale vegetation mortality during droughts. In particular, the research will attempt to address three significant knowledge gaps, including: 1) improved understanding and resolution of controversy over the specific mechanisms of vegetative mortality, 2) understanding the variability in vegetation mortality that, for unknown reasons, is correlated to plant size and 3) the role of moisture versus temperature as mortality drivers during drought. Research will use manipulative experiments to generate results and datasets that will be used to develop a new and improved mortality model that will be tested against independent field data. Vegetation will span a range from Arabidopsis to pine trees. Coordination with leading scientists in the molecular, ecological, and dynamic modeling fields will ensure maximum knowledge gain.

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

High Resolution Spectroscopic X-ray Detectors using Superconducting Sensors

Dr. Antonino Miceli, Assistant Physicist
Optics and Detectors Group
X-ray Science Division
Advanced Photon Source
Argonne National Laboratory
Argonne, IL 60439

The objective of this project is to develop spectroscopic x-ray detectors with high energy resolution using superconducting sensors that are optimized for high-count rate experiments. The research will focus on developing x-ray detectors using a promising new technology that measures the energy of the incoming photons and the consequent change in the properties of superconducting sensors. The current state-of-art spectroscopic x-ray detectors are semiconductor devices (e.g., silicon drift diodes) whose energy resolution is approaching their theoretical limit. The new detectors, called Microwave Kinetic Inductance Detectors (MKIDs), allow for the increased energy resolution necessary for high-intensity x-ray experiments including x-ray micro/nano-probes and x-ray absorption spectroscopy for biology and geophysical applications. By multiplexing the readout of arrays of MKIDs one can build detectors capable of high count rates. The research has the potential to impact the scientific output in several areas of x-ray spectroscopy.

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

Inorganic Nanocomposite Electrodes for Electrochemical Energy Storage and Energy Conservation

Dr. Delia Milliron, Staff Scientist and Facility Director
Inorganic Nanostructures Facility
The Molecular Foundry
Materials Sciences Division
Energy and Environmental Sciences
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

This project aims to develop a combinatorial approach to solution-processed inorganic nanocomposite materials as a new route to the complex physical properties required for efficient energy storage and conservation devices. The research will apply a new, general solution-processing approach to fabricate well-controlled, chemically and morphologically tunable inorganic nanocomposites for battery and electrochromic device electrodes. Modular combinations will be made of different nanoparticle compositions sizes, and of secondary phase materials (electronic insulators, semiconductors, and metals). From the ionic and electronic transport properties of the resulting composites, design rules will be derived to guide the development of highly efficient mixed ionic and electronic conductors. This nanocomposite platform will be further developed to resolve fundamental questions to guide the development of advanced battery and electrochromic device electrodes. Nanocomposite electronic materials will be then developed for applications in physics, chemistry and biology.

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

Viscosity and equation of state of hot and dense QCD matter

Dr. Denes Molnar, Assistant Professor
Department of Physics
Purdue University
West Lafayette, IN 47907

At the extremes of temperature and density, such as those that occurred during the early Universe, ordinary matter dissolves into its constituent quarks and gluons, creating a new state of matter called the quark-gluon plasma. One of today's main experimental efforts is collide energetic heavy ions with each other to create this new state of matter. This matter behaves like a fluid with very low viscosity, and theory should be able to verify predictions of its thermodynamic and transport properties, such as its equation of state and shear viscosity. However, major simplifications and shortcomings in current theoretical approaches prevent obtaining reliable constraints from the data. This work will significantly advance the theoretical description of collision dynamics through developments in covariant transport, causal viscous hydrodynamics, and the interface between these two approaches. The result will be the determination of the viscosity and equation of state off hot and dense quark-gluon matter with unprecedented accuracy from data obtained at present and future facilities.

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

New Experiments to Measure the Neutrino Mass Scale

Dr. Benjamin Monreal, Assistant Professor
Department of Physics
University of California, Santa Barbara
Santa Barbara, CA 93106

After eighty years of study, much is known about the neutrino's three family structure, its handedness, and fundamental role in the particle zoo. While the mass differences between neutrino types are known, the absolute masses themselves are not known. This project will make two major efforts at such a measurement: the European-American KATRIN experiment currently being fabricated and Project 8, a concept that shows promise for a very sensitive measurement. KATRIN will measure the effect of the neutrino mass on the rare end-point electrons in tritium beta decay; this experiment will have sensitivity to a neutrino mass of 0.2 eV. The Project 8 concept will exploit the very week microwaves emitted by low energy electrons as they traverse a strong magnetic field. This project will provide interdisciplinary research and a laboratory scale proof-of-principle for a possible neutrino mass measurement with a sensitivity down to about 0.05 eV.

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

Physics Analysis of Microwave Imaging Data from DIIID & KSTAR

Dr. Tobin Munsat, Assistant Professor
Department of Physics
University of Colorado
Boulder, CO 80309

The aim of this effort is to use advanced data analysis techniques to improve our fundamental understanding of turbulence and transport in tokamak plasmas. The research project will perform analysis of the core and edge plasma in the DIII-D and KSTAR tokamaks using data from the electron cyclotron emission imaging (ECEI) and microwave imaging reflectometry (MIR) diagnostic systems and a suite of original analysis algorithms. These diagnostics provide two dimensional images of temperature and density fluctuations in the tokamak plasma and the data is now detailed enough to challenge the most advanced computational models. Theory proposes that small-scale turbulence is a primary cause of anomalous thermal and particle transport in tokamak plasmas and advanced analysis of the spectral and velocity characteristics of these data holds the key to understanding the basic physics. Highly developed methods will be used for image interpretation, spectral analysis, wavelet-based processing, and velocity field analysis. The work will provide the critical link between theoretical models of turbulence behavior and experimental observation.

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

Integrated Analysis of Particle Interactions at Hadron Colliders

Dr. Pavel Nadolsky, Assistant Professor
Department of Physics
Southern Methodist University
Dallas, TX 75205

The objective of this project is to develop theoretical methods to help improve our knowledge about the internal structure of protons and other strongly interacting particles. Theoretically, the internal structure is coded into a set of parameters called the parton distribution functions. Detailed knowledge about these functions is necessary for proper interpretation of the data from high-energy collision experiments that probe the fundamental properties of matter.

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

Overcoming Photometric Redshift Systematics in Dark Energy Experiments

Dr. Jeffrey Newman, Assistant Professor
Physics and Astronomy Department
University of Pittsburgh
Pittsburgh, PA 15213

There are many operating or proposed experiments to study the mysterious Dark Energy pervading the universe which rely on estimates of the distances of astrophysical objects based only on their observed colors in imaging (commonly called "photometric redshifts"). However, any bias in the mean or scatter of these measurements must be extremely small (below 3 parts in 1000) for these projects' sensitivity to the properties of Dark Energy not to be overwhelmed by systematic errors in the photometric redshift. No calibration technique employed so far has come close to this limit; addressing this issue is one of the top priorities for future experiments, ranging from the Dark Energy Survey to LSST and JDEM. The PI has recently developed a new method of calibrating photometric redshifts which can avoid both the astrophysical systematics and spectroscopic requirements of current techniques. Using detailed studies of currently available datasets, this proposal will establish whether this method can in fact meet the stringent calibration requirements for future Dark Energy experiments.

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

Templating of Liquid Crystal Microstructures by Reversible Addition-Fragmentation Chain Transfer Polymerization

Dr. Jennifer O'Donnell, Assistant Professor
Department of Chemical and Biological Engineering
Iowa State University
Ames, IA 50011

The goal of this project is to develop the fundamental knowledge necessary for the design and synthesis of chemically and mechanically robust, internally-structured polymer nanoparticles. This research will focus on the underpinning science needed to make polymer nanoparticles with a predetermined internal structure. The project combines theory and chemical synthesis with characterization tools available at Ames Laboratory and neutron scattering at Oak Ridge National Lab. The knowledge will enhance our understanding of how to manipulate matter at the nanoscale and could impact the development of nanoreactors, bioelectrodes and sensors.

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

Integrative Molecular and Microanalytical Studies of Syntrophic Partnerships Linking C, S, and N Cycles in Anoxic Environments

Dr. Victoria Orphan, Assistant Professor of Geobiology
Division of Geological and Planetary Sciences
California institute of Technology
Pasadena, CA 91125

The objective of this research is to improve understanding of anaerobic methane oxidation (a potent greenhouse gas) by microbes, a globally significant biogeochemical process. Anaerobic methane oxidation results in the consumption of methane, a potent greenhouse gas, in numerous anoxic environments and is thought to have potentially global climate significance as a biogeochemical carbon cycle pathway. This research will focus on a metabolic partnership between sulfate-reducing bacteria and methane-oxidizing archaea that allows metabolism of methane for energy under anoxic conditions. The work emphasizes the optimization of new technologies for visualization of interactions between the partner organisms at the level of single microbial cells and the tracking of joint metabolic processes.

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

Self-Consistent Calculations of Pedestal Structure Modification by 3D Fields in Tokamaks

Dr. Jong-Kyu Park, Staff Physicist
Experimental Division
Princeton Plasma Physics Laboratory
Princeton, NJ 0

The objective of this research is to use advanced, state-of-the-art computational tools to understand off-symmetry breaking of the magnetic fields. Tokamaks are the most successful fusion devices and a critical feature that is central to their high performance is the symmetry of the magnetic field in the toroidal direction. However, in recent years experiments have uncovered the unexpected result that very small amounts of symmetry breaking in the magnetic field at the edge of the tokamak plasma can have surprising positive effects through the mitigation of damaging plasma instabilities. Because of this mitigation, the symmetry breaking has become a very important topic for the next generation of fusion devices such as ITER. A central part of the effort to understand this unexpected benefit from symmetry breaking is the development of methods of calculating the new plasma equilibrium in the presence of small symmetry breaking perturbations.

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

ReveR-SES: Reversible Software Execution Systems

Dr. Kalyan Perumalla, Senior Research Staff Member and Research and Development Manager
Modeling and Simulation Group
Computational Sciences and Engineering Division
Computing and Computational Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

The objective of this project is to develop novel software tools for increasing the efficiency and usability of codes on extreme-scale computing systems. The research will pursue new approaches for high-performance computing on extreme-scale systems. Challenges to high-performance include the high costs of coordination and synchronization on systems with potentially one million or more processor cores. This research effort is based on the development and use of a so-called reversible software execution paradigm that enables extreme-scale computations to proceed, but with the ability to dynamically detect and recover from transient hardware faults and other errors that are likely to occur in computing systems of extreme complexity.

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

Ultrafast electron transport across nonogaps in nanowire circuits

Dr. Eric Potma, Assistant Professor
Department of Chemistry
University of California, Irvine
Irvine, CA 92697

The objective of this project is to overcome the experimental challenges that have held back ultrafast, time-resolved optical experiments on single molecules. By zooming in on ultrafast timescales at which molecular motions are coupled to moving charges, the findings will ultimately guide the design of electronics components of relevance to many facets of energy generation and utilization, including solar energy conversion and energy storage. Detailed knowledge of how molecular structure relates to conductivity and charge storage is imperative to the design of devices at the level of a single molecule, and includes an understanding of how molecular orbitals participate in the electron transport, which structural changes occur during molecular charging, and what timescales are important for these processes. To this end, the field of molecular electronics will be combined with ultrafast microscopy to study electron transport in single molecules at ultrafast time scales.

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

Spatial and Temporal Proteomics for Characterizing Protein Dynamics and Posttranslational Modifications

Dr. Wei-Jun Qian, Senior Research Scientist
Biological Separations & Mass Spectrometry Group
Biological Sciences Division
Fundamental Computational and Science Directorate
Pacific Northwest National Laboratory
Richland, WA 99352

This project aims to develop a suite of quantitative proteomics technologies that enable spatially-resolved measurements of subcellular protein abundance changes and the dynamics of posttranslational modifications in environmental eukaryotes to gain understanding of the regulation of cellular function. The research will integrate subcellular fractionation, posttranslational modifications, and quantitative proteomics technologies to establish a general approach for enabling spatial and temporal proteomics. The effectiveness and utility of these technologies for biological applications will be demonstrated using the filamentous fungus Aspergillus niger, an organism that plays an important role in biofuel production and global carbon cycling, to attain a better understanding of how its morphology is regulated. The unique suite of technologies will have broad application in diverse studies of microbial and plant organisms and in systems biology studies aimed at better understanding of cellular machineries. Such capabilities not only provide core value for current systems biology efforts, but they also add unique datasets for refining gene models, genome annotation, and future predictive modeling.

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

Consolidating Biomass Pretreatment with Saccharification by Resolving the Spatial Control Mechanisms of Fungi

Dr. Jonathan Schilling, Assistant Professor
Department of Bioproducts and Biosystems Engineering
University of Minnesota
Minneapolis, MN 55455

The aim of this project is to characterize enzymatic mechanisms used by brown rot fungi to degrade woody biomass. The research will examine the enzymatic mechanisms used by Postia placenta, a brown rot fungus, to degrade woody biomass, since this fungus has already "developed" its own solution to the efficient use of lignocellulose for energy production. In particular, the work will address potential spatial partitioning of delignification reactions used by fungi to prepare the wood for digestion from final enzymatic deconstruction of cellulose, a natural analogue to the separate steps used in industrial biomass treatment processes. A combination of physical characterization of partially digested wood samples, microscopic examination of the wood/fungus interface, and analysis of gene expression will be used to address the study questions. The aim of the work is provide new mechanistic understanding of fungal processes that could be used to develop new approaches to consolidated, industrial bioprocessing for biofuels production.

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

Understanding Jets at the Large Hadron Collider

Dr. Matthew Schwartz, Assistant Professor
Department of Physics
Harvard University
Cambridge, MA 2138

The objective of this project is to develop new theoretical methods to help improve our understanding of the properties of particle jets that are produced in high-energy collisions. There is also a relatively new area of research on jet substructure that tries to identify characteristics of jets that allows one to distinguish jets produced by known particles from those produced by unknown new particles. Improved knowledge about jets and jet substructure will be very important for correctly interpreting the data from high energy experiments.

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

Enhancing the LHC Discovery Potential with Jets, Missing ET, and bit -tagging Physics Signature Reconstruction in ATLAS

Dr. Ariel Schwartzman, Assistant Professor
ATLAS Department
Particle Physics and Astrophysics Directorate
SLAC National Accelerator Laboratory
Menlo Park, CA 94025

One of the most important signatures in searches for new physics beyond the Standard Model at the LHC are events consisting of missing transverse energy (ET) and multiple jets originating from bottom or top (b/t) quarks. The PI intends to continue developing an optimized capability that utilizes the integrated capability of all ATLAS detector systems to enhance overall performance. Given the broad range of physics analyses that will benefit from improved jets, missing ET and b/t-jet tagging, the results of this research will impact most of the LHC physics program. The search for new physics in events rich in heavy flavor quarks (b/t) will help shed light on some of the most important questions in particle physics today, such as the structure of the electroweak symmetry breaking (Higgs boson), the hierarchy problem (neutrino mixing) and the origin of dark matter.

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

Origin of Superconductivity in Structurally Layered Materials

Dr. Athena Sefat, Wigner Fellow
Correlated Electron Materials Group
Materials Science and Technology Division
Physical Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

The goal of this project is to understand the fundamental mechanisms that produce superconductivity at high temperatures in structurally layered materials. The work will be focused on materials design and synthesis but will also include significant efforts in theoretical calculations and neutron scattering. Superconducting materials have the potential to impact a variety of energy relevant technologies, including power generation and transmission, particularly if materials can be found that can carry more current and operate at higher temperatures. Ultimately this research could lead to the discovery of new superconductors with superior properties compared to current materials.

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

Catalyst Biomimics: A Novel Approach in Catalyst Design

Dr. Wendy Shaw, Senior Research Scientist
Catalysis Science Group
Institute for Interfacial Catalysis
Chemical and Materials Science Division
Fundamental and Computational Sciences Directorate
Pacific Northwest National Laboratory
Richland, WA 99352

The objective of this project is to develop rationally designed proton channels for artificial homogeneous catalysts following principles derived from natural enzyme catalysis. Proton shuttling across or out of organic and/or inorganic molecules is fundamental to a number of energy-relevant reactions, such as hydrocarbon oxidation or hydrogenation and hydrogen production or water splitting. Using energy-minimized computational models of catalysts and reaction pathways, primary and secondary ligands to transition metal catalysts will be rationally designed to promote enhanced reaction rates for that type of reactions; molecular enzyme-mimic catalysts will then be synthesized and characterized; and uses of those novel catalysts in energy conversion and storage reactions will be explored.

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

Supersymmetry Breaking, Gauge Mediation and the LHC

Dr. David Shih, Assistant Professor
Department of Physics and Astronomy
Rutgers, The State University of New Jersey
New Brunswick, NJ 8901

The objective of this project is to advance theoretical understanding of a class of models that may provide a consistent framework to address how elementary particles acquire their mass. This class of models invokes a new symmetry called supersymmetry which has to be broken in some way at low energies. There are several proposed mechanisms for supersymmetry breaking. This project will focus on what is known as the gauge-mediation mechanism. Supersymmetric models suggest possible dark matter candidates and new particles that may be produced in hadron colliders such as the Tevatron and the LHC. This project will examine the phenomenological consequences of models with gauge-mediated supersymmetry breaking to aid the search for evidence of such models in collider and dark matter experiments.

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

Advancing our Understanding of Photonic Band Gap Structures for Accelerators

Dr. Evgenya Smirnova, Scientist IV
ISR-6
High Power Electrodynamics
International Space and Response Division
Global Security Directorate
Los Alamos National Laboratory
Los Alamos, NM 87545

The objective of this research is to advance photonic-band-gap (PBG) accelerator technology to a stage where it can be used in future particle accelerators for high energy physics or other science applications. In conventional accelerating structures, intense particle beams can excite undesired states in the structure -- called higher-order modes (HOMs) -- that in turn disrupt the beam. PBG structures, however, can be designed to contain the desired accelerating mode while transmitting HOMs out of the structure for disposal. Using PBG structures in particle accelerators could enable progress to significantly higher beam intensities, leading to a completely new generation of accelerator technologies.

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

Advanced High Heat Flux Divertor Program on the National Spherical Torus Experiment

Dr. Vsevolod Soukhanovskii, Physicist
DIII-D Group, Fusion Energy Program
Physics Division
Physical and Life Sciences Directorate
Science and Technology Principal Directorate
Lawrence Livermore National Laboratory
Livermore, CA 94550

The objective of this research is to investigate advanced divertor solutions, including the "snowflake" divertor configuration on the National Spherical Torus Experiment (NSTX). One of the grand challenges for magnetic fusion energy research is to develop innovative plasma-material interface solutions for high heat and particle fluxes incident on the first wall and divertor. To address this critical research gap, the project will entail an experimental and modeling program to investigate advanced divertor solutions including the "snowflake" divertor configuration on the National Spherical Torus Experiment (NSTX). The project is a study of divertor heat and particle transport in these advanced configurations, and prototype magnetic control and radiative divertor performance optimization with feedback. With the help of Thomson scattering diagnostic system for divertor electron temperature and density measurements, kinetic and multi-fluid one and two-dimensional transport models of the advanced configurations will be validated. Studying the high heat flux handling divertor solutions on NSTX and NSTX Upgrade will facilitate extrapolations to future spherical tokamak-based nuclear devices and tokamaks beyond International Thermonuclear Experimental Reactor (ITER), the international fusion research project.

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

Separating Algorithm and Implementation via Programming Model Injection (SAIMI)

Dr. Michelle Strout, Assistant Professor
Computer Science Department
Colorado State University
Fort Collins, CO 80523

The goal of this effort is to improve the programmability of extreme-scale computing systems, resulting in increased portability and transparency. The research will address the challenges of developing portable, high-performance scientific software for next-generation computing systems. These goals will be accomplished by developing a programming model that enables scientists to focus on algorithm development rather than the implementation details. This project will develop high-level scheduling abstractions, including the mapping of computation to processors; storage mapping abstractions; abstractions for scheduling how computation accesses data; and similar abstractions for programming models such as sparse computations, task graph computations, and look-up tables.

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

Technology Development Toward Very High-Gradient and High Quality-Factor Superconducting RF Cavities

Dr. Tsuyoshi Tajima, Research and Development Engineer 4 and Team Leader
Mechanical Design and Engineering Group
Accelerator Operations and Technology Division
Engineering and Engineering Sciences Directorate
Los Alamos National Laboratory
Los Alamos, NM 87545

The goal of this research is to produce a prototype multi-cell superconducting radiofrequency (SRF) cavity for particle accelerators that generates an accelerating gradient of 100 megavolts/meter (MV/m) or higher with a quality factor of 2E+10 or higher. Current niobium technology used in SRF cavities has a theoretical limit of 50-60 MV/m, and a new technology needs to be developed for advanced accelerators. This project will use a thin film technology to achieve the improvement taking advantage of the phenomenon that the lower critical field is increased for a thin-film superconductor material. If successful, the new cavity technology will enable smaller, more energy-efficient and cost-effective particle accelerators.

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

Early-Late Heterobimetallic Complexes Linked by Phosphinoamide Ligands: Tuning Redox Potentials & Small Molecule Activation

Dr. Christine Thomas, Assistant Professor
Department of Chemistry
Brandeis University
Waltham, MA 2454

The goal of this project is to increase our understanding of how interactions between early and late transition metals can be used as a strategy to control chemical transformations related to the clean production of fuels. Energy-efficient conversion of abundant small molecules such as CO2 and H2O into liquid fuels is both scientifically challenging and strategically important for society. Hetero-bimetallic complexes (of, for example, Co and Zr) where one metal is strongly acidic and the other strongly basic possess polar bonds and unusual reactivities. Such bimetallic interaction can be tuned and stabilized by means of phophino-amide ligands. Using complexes designed and synthesized at the molecular level, this project will generate better understanding of structure-activity relations and will lead to catalysts for low-temperature activation of CO2, O2, H2, and N2 and their conversion into liquid fuel precursors.

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

Linking Plant Stress, Biogenic SOA, and CCN Production - A New Feedback in the Climate System?

Dr. Timothy VanReken, Asssistant Professor
Department of Civil and Environmental Engineering
Washington State University
Pullman, WA 99164

The goal of this project is to improve understanding of how biogenic, volatile organic compound (VOC) emissions affect the climate system. The research aims to significantly improve our understanding of how biogenic VOC emissions influence secondary organic aerosol (SOA) formation and cloud condensation nuclei (CCN) production. There is particular focus on the SOA formation potential of real plant emissions, how the SOA formation potential changes in response to climate-induced plant stress and how biogenic SOA contributes to cloud condensation nuclei activity. The research is characterized by laboratory experiments on select tree species to determine how SOA formation is affected by emissions changes arising from plant stress, field experiments to determine how such SOA formation is affected by conditions in a natural forest, field observations of aerosol properties in a variety of environments, and studies to connect SOA formation to cloud condensation nuclei activity.

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

Diffusion on Complex Networks: Algorithmic Foundations

Dr. Anil Vullikanti, Assistant Professor
Department of Computer Science
Virginia Polytechnic Institute and State University
Blacksburg, VA 24060

The aim of this effort is to develop the mathematical and computational foundations for improving the robustness of complex network systems. The research addresses important mathematical and computational issues arising in the analysis of complex phenomena within extreme-scale network systems - such as the cascade of failures in a blackout across an electric power grid; the propagation of malware in wireless networks; the spread of an epidemic within social contact networks. This effort is motivated by the goal of fundamentally understanding the robustness of such complex systems in a systematic manner. Algorithms to detect vulnerabilities and improve robustness are investigated in order to address key concerns for network and policy planners. Realistic models and scalable, efficient simulation tools will be developed for understanding diffusion processes within complex network systems of importance to the Department of Energy.

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

Control Graphene Electronic Structure for Energy Technology

Dr. Feng Wang, Assistant Professor
Department of Physics
University of California, Berkeley
Berkeley, CA 94704

The goal of this research project is to develop a fundamental understanding of the electronic structure and the novel electrical, vibrational, and optical behavior of grapheme, a one-atom thick sheet of carbon that exhibits incredible structural flexibility, electrical transport, and optical properties. This understanding and control would enable the development of a number of novel graphene based devices that will impact a broad range of energy technologies ranging from thermal energy converters and low power electronics to fuel cells and solar energy harvesting.

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

Exploring New Physics Beyond the Standard Model

Dr. Lian-Tao Wang, Assistant Professor
Physics Department
Princeton University
Princeton, NJ 8544

The objective of this project is to explore new theoretical models that may lead to interesting signals in high-energy collision experiments and for developing techniques to help identify such signals from the data. It is widely expected that new physics beyond the Standard Model of particles exists around the TeV energy scale. However, it is anybody's guess what this new physics will turn out to be. This creates a serious challenge on what signals to look for in a given experiment. An important outcome of this project will be a set of search strategies that will increase our chance of finding new physics.

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

Methods for Decision Under Technological Change Uncertainty and Risk Assessment for Integrated Assessment (IA) of Climate Change

Dr. Mort Webster, Assistant Professor
Engineering Systems Division
Massachusetts Institute of Technology
Cambridge, MA 2139

The objective of this effort is to improve the way that technology and uncertainty are represented and treated in integrated assessment models (IAMs) of the coupled human-climate system. The research project will address key gaps in representing technological change and the treatment of risk and uncertainty within IAMs. Integrated Assessment Models contribute to our understanding of many issues in climate change, such as the development of internally consistent global emission scenarios and the exploration of economic, technological, emissions, and climate impacts of alternative mitigation strategies. Specific elements of this work will also contribute to improving the spatial and temporal resolution of IAMs for understanding climate impacts. The research will advance methods in three critical areas: 1) modeling of climate mitigation as sequential decisions under uncertainty, 2) modeling of uncertainty in technological change that represents structural uncertainty and 3) design of reduced-form models of complex earth systems processes to improve the ability to analyze the risks of climate change.

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

Chemical Control of Charge Trapping and Charge Transfer Processes at the Organic-Inorganic Interface within Quantum Dot-Organic Complexes

Dr. Emily Weiss, Assistant Professor
Chemistry Department
Northwestern University
Evanston, IL 60208

The objective of this project is to understand and control nanoscale structures for solar energy conversion. This research will pursue a fundamental understanding of how charge flows in and out of nanoscale spherical structures within hybrid organic and inorganic environments. The unique quantum behavior of light absorption in nanometer-sized spheres will be coupled with the chemistry of charge transfer to form the cornerstone of next generation solar cells with power conversion efficiencies that exceed present limitations. The research represents a unique combination of materials preparation, state-of-the-art instrumental analysis, and theoretical design and calculation.

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

Theoretical Investigation of Nucleon Structure

Dr. Feng Yuan, Physicist Division Fellow
Nuclear Theory Group
Nuclear Science Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

One focus of fundamental research in sub-atomic physics is the spin and gluonic structure of the nucleon. These studies are driving forces for experimental programs in these areas, and are key questions in current hadronic physics. This research will investigate nucleon structure, by developing the necessary theoretical framework and phenomenological techniques. The project will apply important aspects of perturbative Quantum Chromodynamics (QCD) theory, such as gauge invariance and QCD factorization, to extract the relevant nucleon structure from the various experiments. The studies will focus on important issues such as the difference and relevance of proton spin sum rules, and improving the description of transverse spin phenomena with the goal to extract information about the orbital angular momentum contribution to the nucleon spin.

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

Measurement of Parity Violation in Deep Inelastic Scattering and Studies of the Nucleon Spin Structure at Jlab 6 and 11 GeV

Dr. Xiaochao Zheng, Assistant Professor
Physics Department
University of Virginia
Charlottesville, VA 22904

This project will focus on two thrusts of nuclear science, a test of the Standard Model using measurements of the parity-violating asymmetry in deep inelastic scattering (PVDIS) of polarized electrons on deuterium, and the study of spin observables to address the structure of the nucleon. The project will conduct an exploratory PVDIS experiment using the 6 GeV electron beam at the Jefferson Laboratory that will provide the first precision data on selected coupling constants of the Standard Model. In addition, the project will develop a new large acceptance spectrometer called SoLID to be used with 11 GeV electron beams available by 2015 for both the PVDIS experiments and the study of the spin observables.

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