

## UC-National Laboratory Fees Research Program

Abstracts for Active Awards

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## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

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## **Point Defect and Short Range Order Kinetics in Concentrated Substitutional Alloys**

*Host Campus:* Berkeley

*Lead Investigator:* Anas Abu-Odeh

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 124,236

*Abstract:*

Compositionally complex alloys (CCA's), which contain multiple metallic elements with near equal proportions, have garnered much recent attention. These alloys can exhibit desirable combinations of properties, such as strength, toughness and corrosion resistance, which make them attractive for a range of potential applications in energy, transportation and national security sectors. Due to their composition, and the disordered nature of their atomic structure, these alloys display a statistical distribution of local atomic environments that underlie their ability to host a variety of different deformation mechanisms, and that can affect diffusive transport at high temperatures or under irradiation. An important issue for their design then becomes the exact nature of these statistical distributions, i.e., whether they are characteristic of perfectly random compositional disorder, or possess differing degrees of local atomic short-range order (SRO). Understanding the kinetic processes that govern the formation and destruction of SRO is necessary for optimizing properties in the processing of CCAs, as well as controlling their performance in extreme conditions. The proposed scope of this research is to use advanced atomistic computer simulations to investigate these questions surrounding the kinetics of SRO formation and its effect on diffusive transport of relevant point defects. A major limitation with current computer simulation methods at the relevant atomistic length scales is reaching diffusive timescales without simplifying assumptions that limit their accuracy and general applicability. Los Alamos National Lab (LANL) scientists have pioneered the development of a suite of tools to overcome this limitation, called Accelerated Molecular Dynamics (AMD). Working with LANL scientists, AMD methods will be applied to simulate the kinetics of SRO formation, and to understand its impact on point defect diffusion. The work will focus initially on a concentrated Ni-Cr alloy, a material central to LANL's Fundamental Understanding of Transport Under Reactor Extremes (FUTURE) project. Results obtained spanning simulation parameters of temperature, solute, and defect concentration will allow for the development and validation of theoretical models that can predict transport kinetics in systems with SRO, thus opening this analysis to CCA materials more broadly.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### **Novel image analysis and neural network techniques for observing Earth's surface water dynamics**

*Host Campus:* Los Angeles

*Lead Investigator:* Bohan Chen

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2021    *End Date:* 3/31/2024    *Amount:* \$ 206,496

*Abstract:*

One of the major hurdles toward developing robust machine learning models for remote sensing image analysis is the difficulty in collecting large amounts of quality training data. This project proposes to tackle this issue by exploring how generative adversarial neural network (GANN) models can be used to maximize the utility of already-existing and often too-small training datasets through novel transfer learning techniques. UCLA Ph.D. student Bohan Chen will undertake dissertation research at LANL, advised by Dr. Jon Schwenk and also Drs. Cristina Garcia-Cardona and Brendt Wohlberg. His Ph.D. advisor, Andrea Bertozzi, has prior joint work with Dr. Garcia-Cardona and has had a prior UC Lab Fees joint research project with Dr. Wohlberg. This is the first time for a joint collaboration between Dr. Schwenk's group and Dr. Bertozzi's group. The GANNs allow us to generate synthetic images by superimposing qualities learned from other images, e.g. adding clouds and noise to existing training data. GANNs will also be used to create additional training data by acting as a translator between sensor types, e.g. transforming cloud-penetrating radar images to Landsat-like optical images. The new machine learning techniques developed will support ongoing work at LANL that seeks to automatically identify surface water from remotely-sensed imagery. Understanding surface water dynamics is crucial for water security, including reservoir monitoring and estimating freshwater abundance. Preliminary research at LANL to detect waterbodies in Landsat imagery shows that a convolutional neural network method outperforms the state of the art Global Surface Water data product. Dr. Schwenk's group has created an abundant high-precision training data set for arctic river waters, but have found that models trained with this data transfer poorly to other regions. Through GANNs and new transfer learning techniques, this project will develop a surface water detection model with a global application based on arctic training data. In addition to data generation, the research will develop hybrid algorithms that combine image segmentation methods with convolutional neural network methods. This project will enable anticipation and mitigation of water security crises via cutting-edge image analysis techniques to estimate water availability without on-the-ground observations.

## **Scalable Fabrication of Ultra-Strong and Stiff Hierarchical Syntactic Nanofoams**

*Host Campus:* Irvine

*Lead Investigator:* Cameron Crook

*Graduate Fellowships*

*Collaborating Sites:* Livermore

*Start Date:* 4/1/2021      *End Date:* 3/31/2023      *Amount:* \$ 139,536

*Abstract:*

Architected materials have garnered intense interest over the past two decades for their desirable combination of otherwise mutually exclusive properties, such as high strength and low density. This is further driven by two recent advances, namely new plate/shell-based lattices with superior properties to beam-based lattices, and the “smaller is stronger” design paradigm, wherein nearly defect-free nano/micro-sized constituent materials enhance strength. As detailed in a recent report on Metamaterials Manufacturing (authored by the mentor, Spadaccini), despite their demonstrated exceptional performance, architected materials have extremely limited industrial penetration, largely due to the lack of scalable manufacturing processes. Furthermore, key high temperature applications require chemical inertness, high strength and stiffness and high temperature resistance, which are mostly associated with undesirably brittle ceramic constituent materials.

We propose to address these two challenges with a research proposal aimed at the introduction, modeling and optimal design of a novel closed-cell architected nanofoam topology with properties approaching the theoretical upper bounds for isotropic materials, and the development of a scalable self-assembly process to produce the aforementioned topology. The proposed topology comprises a hierarchy of micron-sized spherical voids with increasingly small diameter, and will be manufactured by dispersing well controlled hollow alumina spheres in an alumina slurry, producing an ink for direct ink writing (DIW), followed by DIW of hierarchical architected materials with macroscopic geometry and nanoscale-strengthened “constituent materials.” If successful, this work will result in a nanoarchitected ceramic material with exceptional mechanical properties which can be manufactured at the scale and throughput required by structural applications. The proposed research work will capitalize on ink development expertise, DIW equipment, and large area projection and Nanoscribe systems available at the Center for Engineered Materials and Manufacturing at LLNL, in addition to ancillary equipment at the Advanced Manufacturing Laboratory. The dissertation advisor and the lab mentor have been collaborating on a number of initiatives in the area of architected materials for nearly a decade and fully support this application.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Controls of Methane Dynamics in Tropical Peatlands

*Host Campus:* Los Angeles

*Lead Investigator:* Alexandra Hedgpeth

*Graduate Fellowships*

*Collaborating Sites:* Livermore

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 139,536

#### *Abstract:*

Rising atmospheric methane (CH<sub>4</sub>) levels since the early 2000s are likely related to changes in efflux and/or sink strength in terrestrial ecosystems. Much of this increase in atmospheric CH<sub>4</sub> has been attributed to greater inter-annual and seasonal variability in climate and water table in tropical wetlands. Tropical ecosystems are projected to undergo large changes in precipitation, which may lead to even larger changes in atmospheric CH<sub>4</sub>. There are significant gaps in global carbon budgets and climate predictions due to the lack of carbon cycling data from tropical wetlands. Filling in these gaps will help better predict how the large carbon stocks in these soils will respond to future environmental change. The goal of this proposed work will be to assess the environmental controls on methanogenesis and methanotrophy in deep soil profiles across tropical wetland ecosystems where 104 Gt of global carbon is stored. Specifically, we will examine surface and soil profile flux to accurately predict changes in future CH<sub>4</sub> efflux. This will be the first assessment of CH<sub>4</sub> dynamics in tropical wetlands below 1m, where the majority of CH<sub>4</sub> is produced. This project will measure radiocarbon using Accelerator Mass Spectrometry (AMS) to determine source of CH<sub>4</sub> from tropical wetlands. The PhD student, Alexandra Hedgpeth, has previously worked at LLNL's Center for AMS and is proficient in sample preparation and graphitization. As such, training will focus on AMS runs, and modeling and interpretation of data under the mentorship of Dr. Karis McFarlane. There is a significant lack of CH<sub>4</sub> flux data and a large sampling bias towards Indonesia and Malaysia due to the difficulties associated with field work in these regions. We will conduct the proposed research in a Panamanian wetland site previously established by Alexandra Hedgpeth to add needed data from other tropical wetland regions to provide a more extensive understanding in the spatial pattern of CH<sub>4</sub> flux. We hypothesize that the results of this study will demonstrate that in tropical wetlands rapid drops in water table lead to short-lived but large CH<sub>4</sub> release from anaerobic subsoils to the atmosphere. We expect that decreased moisture and water table together suppress methanotrophy increasing CH<sub>4</sub> efflux.

## **Interactive Visual Analysis of Data Movement in Heterogeneous Computing Architectures**

*Host Campus:* Davis

*Lead Investigator:* Suraj P. Kesavan

*Graduate Fellowships*

*Collaborating Sites:* Livermore

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 139,536

*Abstract:*

With the end of Moore's law in sight, High-Performance Computing (HPC) has increasingly focused on heterogeneous architectures to meet the exascale computing goals. Leading supercomputers provide unprecedented capabilities through a combined prowess of large multi-core CPUs and several high-performant GPUs on each computational node. While heterogeneous architectures have demonstrated effectiveness in solving large and complex scientific problems, there still exist many opportunities to improve the returns on investments in this relatively new paradigm.

In particular, although significant speedup can be reaped by porting the computationally expensive operations to the GPUs or by using dedicated I/O nodes, the corresponding data movement costs may substantially compensate for the overall gains. Identification of such data movement penalties, in particular, to and from I/O nodes, between CPUs and GPUs, and across memory hierarchies, can shed new light on the associated bottlenecks, leading to development of new ways to improve the utilization of these architectures.

We propose to develop new visual analysis techniques to enable a detailed investigation of data movement costs and investigate their impact on the application's performance. We will develop a new framework to allow holistic exploration of data movement to satiate the need for large-scale heterogeneous computing. Focusing on the need for in-situ exploration, e.g., for understanding the data costs of training deep neural networks, we will visualize streaming performance data enabling real-time exploration for applications on heterogeneous machines.

Although one may use known metrics to analyze the performance of applications, such an approach is primarily useful for validating/invalidating their hypothesis. Whereas developing new conjectures about the causes and potential solutions to performance problems is typically not possible. Our framework will inform code developers, computational scientists, and HPC researchers of possible ways to improve machine utilization and efficiently run larger and communication-demanding applications, e.g., by identifying incompatible job placement, and hardware latencies and communication patterns. Overall, our approach can help in narrowing the growing gap between the computing power of processes and data bandwidth at various levels of granularities.

## **Exciton Transport in 2D and 3D Halide Perovskite Materials**

*Host Campus:* Davis

*Lead Investigator:* Luke McClintock

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2021     *End Date:* 3/31/2023     *Amount:* \$ 139,536

*Abstract:*

Excitons have significant effects on the photoinduced response of halide perovskites - materials that promise revolutionary advances in optoelectronic and spintronic technologies. Despite intense efforts, the formation, transport, and spin polarization mechanisms of these excitons are not well understood. My dissertation is focused on understanding exciton behavior in halide perovskites through a wide variety of transport and spectroscopic experimentation coupled to theoretical simulations. Recently, we developed unique fabrication procedures that allow for the novel study of exciton transport under a wide range of temperature and charge density conditions in single crystalline perovskites. We also revealed indirect signatures of excitonic dominance over charge diffusion in perovskites up to technologically relevant temperatures. This Fellowship will allow me to leverage these breakthroughs and visualize exciton dynamics under several key experimental avenues - space, time, spectrum, and dimensionality (3D bulk to 2D molecular layers), with an aim of understanding and manipulating excitonic responses. Through a combination of spatially, temporally, and spectrally resolved temperature-dependent fluorescence and absorption microscopies, we will reveal an increasing excitonic population at low temperatures and provide direct evidence of its connection to enhanced photoinduced carrier diffusion behavior. Furthermore, we will utilize LANL's ultrafast optical microscopy facilities to study the formation and recombination dynamics of the excitons in 2D and 3D samples, thus validating dimensionality as an important tuning parameter for their photovoltaic response. Overall, this work will provide better understanding of the interplay among free carriers, excitons, phonons, and spins and allow us to harness these interactions for creating new materials with enhanced optoelectronic and spintronic properties. Working under joint supervision from Dr. Yarotski (LANL) and Prof. Yu (UCD) will allow me to benefit from their expertise of photovoltaic materials, as well as nanoscale and ultrafast optical and transport techniques. The results of this work will lead to many high-profile publications that will be of great interest to a broad community of researchers in condensed matter physics, optical science, and related fields.



## **Unraveling the Dark Side of Marine Biotoools: Development of Lightweight & Radioprotective Composites**

*Host Campus:* Berkeley

*Lead Investigator:* Katerina Gensila Malollari

*Graduate Fellowships*

*Collaborating Sites:* Livermore

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 139,536

*Abstract:*

In nature, the primary reinforcing elements of structural tissues are almost always inorganic minerals. However, this is not the only blueprint for achieving rigidity, high strength, and abrasion resistance in composites. The Humboldt squid and several carnivorous marine worms have "biotoools" (beaks, jaws or teeth) that exhibit impressive mechanical performance yet contain little or no inorganic mineral content. The bloodworm *Glycera dibranchiata* offers an interesting example, as its load- and impact-resistant jaws are comprised of a network of proteins, mostly unmineralized copper and melanin. The use of melanin as a structural component is a unique design concept not found elsewhere, as the typical biological roles of melanin are pigmentation and photoprotection. Limited prior studies of *Glycera* jaws revealed hard, strong, and tough mechanical properties- on par with or even exceeding human bone- despite minimal degree of mineralization (<1%). However, the formation of these biocomposites, the exact role of melanin, and the synergy among the various components in the *Glycera* jaw remain poorly understood. The principal objectives of this research are to elucidate the structure-property relationships of melanin, proteins, and metal building blocks in the jaw and to use this information to inform the design of future lightweight high-performance composites. To unravel this mystery, we will investigate the jaws' molecular and nanoscale mechanics, the morphology and structure of melanin, and the interactions among individual constituents in *Glycera* jaws by leveraging state-of-the-art 4D scanning transmission electron microscopy (4D-STEM) and single-molecule force spectroscopy (SMFS). In addition, since melanin is known for its extraordinary radioactive shielding properties in organisms exposed to high background radiation levels, we will investigate whether these biocomposites exhibit any radioprotective capabilities. New information regarding the relationship between biochemical structure and mechanical behavior of the various components will be coupled with bioinspired materials processing and the unique capabilities of LLNL on advanced manufacturing processes as well as materials characterization to support the fabrication of biomimetic lightweight yet strong melanin composites, with potential applications as structural and radiation shielding materials.

## **Probing spin transport in many-body entangled quantum magnets under extreme conditions**

*Host Campus:* Berkeley

*Lead Investigator:* Vikram Nagarajan

*Graduate Fellowships*

*Collaborating Sites:* Livermore

*Start Date:* 4/1/2021    *End Date:* 3/31/2024    *Amount:* \$ 185,795

*Abstract:*

The many-body problem is at the root of some of the biggest open questions in physics, including understanding the nature of high-temperature superconductivity, or the fate of quantum information in a black hole. The challenge, simply described, is that the properties of such systems are intrinsically collective and cannot, in general, be framed in the familiar language of a single particle quanta like spin, charge or momentum. Rather, these systems are characterized by emergent quantum numbers which may not take on conventionally quantized values. In this proposal, we suggest a new experimental approach aimed at identifying the underlying characteristics of the collective objects resulting from many-body physics. Our strategy uses state-of-the-art nanofabrication techniques to inject spin into a material, and probe the non-local response carried by these collective objects. Essential to this approach is the ability to tune the system from one many-body state to another, in order to probe the evolution of the collective response. We achieve this by applying extreme pressures, a unique capability developed at Lawrence Livermore National Lab. We focus on a specific class of materials known as quantum spin liquids, a family closely related to high temperature superconductors and theoretically contain emergent spin quanta. Our experiment will reveal how these particles transport information and energy, and demonstrate a path to extending these techniques to answer long standing questions in exotic materials.

## **A Submerged Wireless Imaging beam Monitor Diagnostic Development for High Rep-Rate Accelerators**

*Host Campus:* Santa Cruz

*Lead Investigator:* Nora Norvell

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 139,536

*Abstract:*

With the push towards higher rep-rate accelerators to drive particle physics and photon science research, diagnostic systems need to keep up with the influx of signal data as well as be able to withstand increased radiation damage. The guiding goal for this proposal is to develop a profile monitor for these high-repetition machines that can measure pulse by pulse beam metrics such as beam shape, position, bunch length, flux and timing within the pulse train. Knowing these beam metrics is essential to be able to properly tune next-generation X-Ray free electron lasers and particle beam experiments and be able to distinguish what is just an isolated pulse abnormality versus a chronic problem with every pulse. This proposal would generally advance R&D for pulse by pulse, radiation tolerant and effective beam diagnostic profile monitors by specifically focusing on dramatically speeding up and improving how the proton beam at LANL's Isotope Production Facility (IPF) beam line is imaged and tuned. IPF is a critical beam line that produces much of the United States' supply of medical radioisotopes but currently the beam line has a slow and tedious tuning process. I propose to use these fellowship funds to join the Los Alamos Accelerator Operations and Technology group. With Deputy Group Leader Dr. John Smedley, I propose to lead the development of a wireless pulse-by-pulse profile monitor for the IPF beam line. We will design and fabricate a diamond detector to both document the capabilities of diamond detectors on proton beams for pulse by pulse beam characterization as well as significantly speed up the tuning time for IPF. To meet both the needs of the IPF beam line and the diamond detector research community, we propose here a diamond Submerged Wireless Imaging Monitor (SWIM) for the Isotope Production Facility.

## **The response of Arctic delta morphology and dynamics to permafrost loss and hydrological change**

*Host Campus:* Irvine

*Lead Investigator:* Lawrence Vulis

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 120,190

*Abstract:*

River deltas ringing the Arctic Ocean coastline are unique landforms shaped by both highly seasonal cold region hydrology and permafrost features such as thermokarst lakes. These lakes trap, store, and modulate the timing and magnitudes of riverine freshwater, sediment, and nutrients normally routed directly to the ocean through a distributary delta channel network (DCN). Future climate warming is expected to thaw permafrost, modifying lake coverage and therefore riverine flux delivery to the Arctic Ocean, as well as release large quantities of previously frozen carbon into the atmosphere. How and where thermokarst lake coverage on deltas will change, and how these changes will impact sediment and nutrient transport to the coast, remains highly uncertain. We propose a two-pronged approach towards building an understanding of delta lake cover response to warming by: (1) performing a data-driven multiscale analysis of lake sizes and lake and channel network spatial patterns on arctic deltas using satellite imagery and graph theoretic techniques; and (2) developing a simplified modelling approach to project lake cover changes and associated changes to delta riverine fluxes. For (1) we are developing a novel technique to study lake spacing using Voronoi tessellation and then harnessing tools from biology for quantifying multiscale organization of cells in leaves to study the tessellation of lakes on deltas. Our work is expected to discover relationships between lake size and spacing patterns and climate variables which can guide physically-based models upon which future projections can be made. For (2) we will couple a regional thermokarst lake generation model with a reduced complexity model for delta evolution (DeltaRCM), which Dr. Joel Rowland's group at LANL recently introduced ice and permafrost representation into. We will use this to quantify how lake coverage will respond to warming, and how changing lake coverage will modify sediment and nutrient delivery to the coastline. The proposed work builds on an existing NSF Collaborative Project between Prof. Efi Foufoula-Georgiou's group at UCI and Dr. Rowland's group at LANL on analyzing DCN geometry and topology using graph theoretic approaches, and contributes to cross-cutting question #2 of the DOE InterFACE (Interdisciplinary Research for Arctic Coastal Environments) project of Dr. Rowland at LANL.

## Heterogeneous 2D Lamellar Membranes for Improved Separation in Water Purification

*Host Campus:* Berkeley

*Lead Investigator:* Monong Wang

*Graduate Fellowships*

*Collaborating Sites:* Livermore

*Start Date:* 4/1/2021    *End Date:* 3/31/2023    *Amount:* \$ 139,536

*Abstract:*

Membrane technology has played a key role addressing global freshwater scarcity, providing additional water supplies such as desalination and water reuse. Lamellar membranes based on homogeneous 2D-materials have demonstrated intriguing performance for water treatment, but suffered from poor selectivity, membrane swelling, stacking defects, or poor stability. To address these problems, I propose to develop heterogeneous lamellar membranes by combining Graphene Oxide (GO) with porous nanosheets such as Zeolite and MoS<sub>2</sub>. Heterogeneous stacking of GO-Zeolite/MoS<sub>2</sub> nanosheets can minimize membrane swelling by rebalancing the attractive and repulsive forces between layers, thus improving stability of the interlamellar spacing and membrane selectivity. In-plane pores on porous nanosheets and the interlamellar nanochannels provide hybrid transport pathways for molecules, which could be exploited to transcend the permeability-selectivity tradeoff of conventional membrane materials. Together with swelling control, a major goal of my study is to understand the hybrid transport mechanisms in the heterogeneous membranes to achieve high separation performance. I propose to incorporate 2D nanosheets onto a single-nanopore substrate and investigate ion transport using patch clamp technique. This analysis will isolate the molecular transport through in-plane pores and nanochannels by altering substrate pore size and thickness of deposited nanosheets. Molecular transport will be likely dominated by in-plane pores when the substrate pore is small, while transport through nanochannels will be more pronounced with larger substrate pore and thicker nanosheets deposition. TEM-compatible, single-pore silicon nitride membrane will be used as membrane substrate to facilitate device imaging and characterization. This work will leverage the LLNL mentor expertise in nanofluidics and ion/water transport, as well access to LLNL tools for single nanosheet (Axopatch patch clamp and Keithley instruments) and centimeter-scale membrane transport (RO and diffusion cells) characterization. With combined structural and chemical control in 2D membranes and selective characterization of the transport pathways, this research will ultimately provide fundamental knowledge required to develop lamellar membranes meeting the demanding performance metrics for efficient water purification and desalination.

## **From adhesion to thermodynamics and kinetics of polymers**

*Host Campus:* Davis

*Lead Investigator:* Michael Bull

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2020      *End Date:* 3/31/2022      *Amount:* \$135,216

*Abstract:*

Polymer mixtures and composites are essential to a wide array of applications. However, these systems are difficult to model and can be prone to phase separation and slow, diffusion-driven degradation. Polymer Bonded Explosives (PBXs) are a particularly challenging class of nanocomposites. PBXs use polymers that thermodynamically prefer phase separation but need to remain mixed for long periods and variable environmental conditions. Some major obstacles to improving PBXs (and polymer mixtures in general) are that (1) their mixing thermodynamics are highly complex; (2) they are usually processed into kinetically trapped states; (3) experiments and simulations have difficulty identifying free energy contributions with sufficient accuracy; as a result (4) aging of nanocomposite materials is difficult to predict from short time experiments or simulations. My research will study the interfacial properties and microstructure of PBXs (and proxies of PBXs) by combining high accuracy adhesion measurements with neutron scattering experiments. The proposal has three goals: (1) develop an improved adhesion measuring device based on the Surface Force Apparatus (SFA) for studying PBX interfacial energies; (2) pair interfacial energy investigations with Small Angle Neutron Scattering (SANS) and Ultra-Small Angle X-ray Scattering (SAXS) to quantify how interfacial properties affect PBX microstructure; and (3) explore novel applications of the new device to PBX science. I am fully trained on the SFA (under Prof. Tonya Kuhl), and my training with scattering has already started through graduate classes and the National School on Neutron and X-ray Scattering. Further training in SANS and SAXS will take place at LANL under my National Lab supervisor Dr. Erik Watkins. The expected scientific outcomes of the proposed work will be (1) accurate measurements of interfacial energies between PBX components and improved models of PBX behavior; (2) a detailed understanding of the effect of interfacial energy on PBX initial microstructure. My research will benefit from living on-site at LANL through access to neutron beam time, PBX resources (materials, literature, expertise, processing facilities, etc.), collaboration with LANL groups, and the mentorship of Dr. Watkins.

## **Langevin Methods for Quantum Electron-Phonon Simulations**

*Host Campus:* Davis

*Lead Investigator:* Benjamin Cohen-Stead

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2020    *End Date:* 3/31/2022    *Amount:* \$135,216

*Abstract:*

Electron-phonon interactions underlie some of the most exciting emergent phenomena observed in modern condensed matter physics research. Numerical methods, especially Quantum Monte Carlo (QMC), are playing an increasingly crucial role in their investigation. However, despite much progress, QMC remains computationally expensive; hence algorithm development remains a forefront problem in the evolution of the field. Langevin-based algorithms are key prospects for a breakthrough as they offer the possibility of improving the scaling of QMC from cubic to linear in the number of electrons. Although widely successful in lattice gauge theory (LGT), Langevin methods are less established in condensed matter physics, and have only recently been applied to simulating electron-phonon interactions. Working with Staff Scientist Kipton Barros at LANL, UC Davis Professor Richard Scalettar's graduate student Benjamin Cohen-Stead will build on this initial success. The proposed research will have two broad foci. First, Ben will work on further improving the effectiveness of Langevin methods as applied to electron-phonon systems by investigating algorithmic improvements, including machine-learned preconditioners that reduce the number of matrix-vector multiplications needed in simulations, developing better estimators for physical observables, and using GPU units to accelerate the core linear algebra operations. Second, he will apply these newly developed Langevin methods to simulating interacting electron-phonon systems that were previously intractable, with the promise of uncovering novel emergent physics. One key objective will be the first large-scale, low temperature calculation of the phase diagram of a model which combines electron-phonon and electron-electron interactions. By collaborating with Kipton Barros at LANL, Ben will be able to benefit from his mentors' complementary expertise in quantum simulations techniques, while developing dynamic codes capable of exploiting the substantial computing resources at LANL. Both the algorithmic improvements made to the Langevin method, and the resulting simulation studies of electron-phonon systems will result in publications that are relevant to a broad community of researchers in condensed matter physics, quantum simulation, and related fields.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Privacy Risks, Thoughts, Actions, and Regulations

*Host Campus:* Berkeley

*Lead Investigator:* Naniette Coleman

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2020    *End Date:* 3/31/2023    *Amount:* \$200,016

*Abstract:*

My research examines privacy at the individual and organizational level. The individual focused component interrogates how our personal privacy protection thoughts and actions differ. At the organizational level, my work examines how different organizations assess risk, make decisions, respond to data breaches, and work towards compliance within an increasingly complex web of state, federal, and international privacy laws. The benefits and outcomes of spending 6-months (or more) at Los Alamos National Lab include: 1) thinking more broadly by engaging in unexpected, innovative, interdisciplinary exchanges that expand my theoretical and methodological reach. I expect these will occur every day at the Center for Nonlinear Studies where I have been offered office space should my proposal be selected; 2) digging deeper via hands on work with privacy and cybersecurity content experts who are engaged with the analysis of the exact kinds of data transactions I consider in my work and the creation of IS&T tools. There are, for example, data sharing possibilities between healthcare providers and insurance companies, which will receive greater scrutiny under our new regulatory reality; 3) engaging decisively with my mentor, a statistician who has offered regular consultation as I do battle with the strategic thinking and analytical labor required to thoughtfully process and present findings on the myriad intertwining large data sets I have already collected to answer my research questions; and finally, 4) connecting and building relationships between my new colleagues at LANL and other entities with whom I have formal affiliations (e.g. Berkman Klein Center) for the purposes of expanding our audiences and deepening ties and growing research opportunities. Taking time to reflect is a driving force behind my desire to affiliate with LANL because the outcome of my work on individuals may have workforce implications and my work on organizations may lead to institutional changes. I expect my findings will shift how organizations think about who should have access to private or classified information, what a commitment to guarantee the protection of that information really means, how often that commitment should be reassessed or tested, and how.



## **Perovskite Quantum Dot Single Photon Emitters**

*Host Campus:* Merced

*Lead Investigator:* William Delmas

*Graduate Fellowships*

*Collaborating Sites:* Lawrence Livermore

*Start Date:* 4/1/2020    *End Date:* 3/31/2022    *Amount:* \$135,216

*Abstract:*

With the recent developments in the field of quantum information, it is more important than ever to develop stable and high-quality single photon emitters (SPEs). SPEs are essential for the development of quantum encryption devices, as well as fundamental investigations into quantum mechanical phenomena. In the past decade, several different systems have shown promise as SPEs including defects in diamond, hexagonal boron nitride and several different 2D materials. In addition to the defect-based emitters, quantum dots (QDs) have shown promise as strong SPEs at low temperatures. QD emitters are considerably easier to fabricate and achieve precise placement than defect-based emitters but so far have only worked at cryogenic temperatures. In collaboration with LLNL, we propose to investigate organo-metallic hybrid perovskite QDs as SPEs with the goal of stabilizing their emission through chemical, electromagnetic and plasmonic tuning to make a room temperature SPE. By collaborating with Dr. Ted Laurence at LLNL for his spectroscopy expertise, I hope to gain more insight into advanced time-resolved spectroscopies, such as photon correlation Fourier Spectroscopy techniques, that will measure the quality of our SPEs. We have previously shown that we can chemically tune our QD emission characteristics by changing the ligands that functionalize their surface. In collaborating with LLNL and with Dr. Tiziana Bond, specifically for her expertise in photonic materials as well as in modeling and fabricating plasmonic structures, we hope to use plasmonic structures to increase the SPE emission and tune their spectral properties via plasmonic coupling. LLNL fabrication capabilities with electron beam lithography and gold deposition and their Transmission Electron Microscope for structure characterization will also be of great assistance. The goal of this proposed thesis work is to make advancements in organo-metallic hybrid perovskite QD room temperature SPEs by making strides in our understanding of how to tune and manipulate these devices.

## **3D Printing with Acoustophoresis for Microstructure Control**

*Host Campus:* Santa Barbara

*Lead Investigator:* Drew Melchert

*Graduate Fellowships*

*Collaborating Sites:* Lawrence Livermore

*Start Date:* 4/1/2020      *End Date:* 3/31/2022      *Amount:* \$135,216

*Abstract:*

The goal of this project is to use acoustic fields during 3D printing to manipulate the microstructure of the printed material, thereby controlling the material properties in printed components. This method will enable printing of components with novel functional properties, such as embedded electrical circuits or thermal dissipation networks. Functionalities like these are in high demand, since the properties of feedstock material is currently the main limitation of 3D printing. Composite material consisting of filler particles in UV-cure polymeric matrices, will be patterned with pressure fields before it's cured into a solid material. This will be done within a stereolithography printing reservoir so that each layer of the printed component has user-defined microstructure. Thus, as the component is printed layer by layer, the material is patterned to have certain material properties in desired locations within the component. One especially promising application of this technology is embedding bundles of aligned, electrically conductive fibers which act as electrical interconnects in components. Another is assembling thermal transport pathways in boron-nitride-based composites for cooling electronics. This project relies on expertise in particle assembly, which will be provided by our group at UCSB, as well as expertise in 3D printing, which will be provided by Dr. Spadaccini at LLNL. Work completed in the first three years of the applicant's PhD has demonstrated that acoustic focusing effectively controls the microstructure of composite materials. With this method we've controlled functional properties like electrical conductivity, increasing it by an order of magnitude and modulating it spatially (e.g. between conductive and insulating states). Dr. Spadaccini will provide the resources and expertise needed to integrate this technology into 3D printing. In addition to providing a stereolithographic printer dedicated to modification for acoustic focusing, Dr. Spadaccini has valuable expertise in developing ink chemistries, particle dispersion, and high-resolution UV-curing techniques. In addition, resources at LLNL for X-Ray tomography and design optimization make this in-residence fellowship an excellent opportunity for investigating this problem and building a collaborative relationship between groups at UCSB and LLNL with shared research interests.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Environmental drivers of desert microbial nitrogen cycling

*Host Campus:* Riverside

*Lead Investigator:* Hannah Shulman

*Graduate Fellowships*

*Collaborating Sites:* Lawrence Livermore

*Start Date:* 4/1/2020    *End Date:* 3/31/2022    *Amount:* \$135,216

#### *Abstract:*

For this proposed research, I will determine how chronic exposure to atmospheric nitrogen deposition (N-dep) impacts microbial nitrogen (N) cycling in desert systems. I propose to investigate taxa responsible for N transformations and their functional genes that catalyze N turnover. I will target these N cycling microbes through shotgun metagenomic analysis of  $^{15}\text{N}$  enriched environmental DNA obtained with quantitative stable isotope probing (qSIP). Additionally, by using this qSIP-targeted metagenomics approach, I will aim to characterize genes associated with assimilation of nitrogen into microbial biomass. I have identified Dr. Steven Blazewicz at Lawrence Livermore National Lab as a collaborating scientist for my research goals. Dr. Blazewicz's expertise in developing qSIP methods to study microbial processes responsible for soil rewetting dynamics make him an ideal collaborator and mentor for this project. We will take advantage of LLNL's recently built semi-automated qSIP-metagenomics pipeline that uses robotics to speed processing of SIP samples by an order of magnitude, making well-replicated qSIP experiments tractable. The uniting research objective of this project is to couple this regional field site design to functional metagenomic analysis of the soil microbiome to characterize a key aspect of the nitrogen cycle as well as the influence of nitrogen deposition on strategies of microbial nitrogen assimilation. These findings will address pivotal questions in the field of microbial ecology: By focusing on the functional genes associated with nitrogen assimilation, we are contributing to a mechanistic understanding of how microbial processes immobilize soil nitrogen, an area that is of current interest in soil microbial ecology. Additionally, these data will provide resources for soil biogeochemistry in arid systems. By performing metagenomic analysis on DNA from the qSIP fractions exposed to  $^{15}\text{N}$  after drought, we hope to identify functions which may be contributing to rewetting pulses of N.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Exploring the new state of matter of the early universe

*Host Campus:* Los Angeles

*Lead Investigator:* Jared Reiten

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2019    *End Date:* 3/31/2021    *Amount:* \$135,216

*Abstract:*

This project explores the very first moments of our universe's history. A few microseconds after the Big Bang, the entire universe was permeated with an astonishingly hot (at a temperature of a trillion degrees), dense soup of fundamental particles called quarks and gluons, which interact through the strong force that binds together nucleons and nuclei. This new state of matter, dubbed the quark-gluon plasma (QGP), can be recreated in powerful accelerators by clashing two opposing beams of massive ions traveling at nearly the speed of light. Measurements at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory and the Large Hadron Collider at CERN have verified the existence of the QGP. However, none of the current experiments have revealed its microscopic structure, thus motivating a new experiment named sPHENIX. The fact that QGP is transient and lasts for just a few yoctoseconds ( $10^{-24}$  s) makes the determination of the QGP properties extremely challenging. To overcome this difficulty, one uses probes with large momentum (called "jets") or with large mass (called "bottom quarks") that are produced simultaneously with the QGP in heavy ion collisions. The heavy ion experimental group at Los Alamos National Laboratory (LANL) is currently leading the effort to build a Monolithic Active Pixel Sensor tracking detector for the first bottom quark measurements at sPHENIX. To interpret the eagerly-anticipated results, the vast international scientific community calls for state-of-the-art first-principles theory that describes the interactions between the QGP and jets or bottom quarks – a theory that is now being developed for the first time. The LANL nuclear theory group is a recognized world leader in this endeavor. From the start of my graduate career, I have been working on the development of this new theoretical formalism with Dr. Ivan Vitev and my advisor, Prof. Zhongbo Kang of UCLA. The UC Laboratory Fees Research Program will give me the unique opportunity to work closely with the experts at LANL, developing such a theory and leveraging the laboratory's superior computing resources. It will allow me to make a lasting contribution to science and to the sPHENIX program, which is of the highest priority in the Nuclear Physics Long Range Plan of the US Department of Energy.

## **High resolution paleoclimate reconstruction using NanoSIMS**

*Host Campus:* Irvine

*Lead Investigator:* Kevin Wright

*Graduate Fellowships*

*Collaborating Sites:* Lawrence Livermore

*Start Date:* 4/1/2019     *End Date:* 3/31/2022     *Amount:* \$200,016

*Abstract:*

Variations in precipitation in northeast Mexico can have powerful impacts on agriculture, industry and ecosystems in the region. However, it is uncertain how regional hydroclimate will be affected by climate change due to the short instrumental record and the paucity of paleoclimate records from the region. We propose to utilize geochemical variations in speleothems (cave calcite deposits) collected from NE Mexico, which span the last ~60,000 years, to investigate the timing and mechanisms of past hydrologic change over a range of timescales. Speleothems are unique paleoclimate archives in that they contain multiple climate proxies, can be precisely dated with U-series methods, and can cover seasonal to orbital timescales. The isotopic and elemental composition of speleothem calcite are widely utilized as paleoclimate proxies. However, interpretation is often complicated since multiple processes, from atmospheric to within cave, can influence the geochemical signal. Through collaboration with Dr. Peter Weber, we aim to integrate our long-term speleothem stable isotope and trace element (TE) data collected at UC Irvine, with high-resolution measurements conducted with the NanoSIMS instrument at LLNL, with the goals of improving our understanding of TE incorporation in speleothem calcite, identifying annual lamina for age model constraints, and testing for proxy evidence of extreme hydrologic events, such as droughts and hurricanes. NanoSIMS will allow us to spatially map TEs in key intervals to determine if they are uniformly distributed in calcite or associated with impurities, which has implications for their use as paleo-proxies. The high resolution of SIMS will also allow us to track seasonal changes in speleothem geochemistry, which may reveal annual cycles that could be utilized for age control, as well as for seasonal resolution paleoclimate reconstruction. Finally, annual droughts and extreme precipitation events may not be captured by other analytical methods due to their fast onset and brief duration. High resolution SIMS can potentially be used to identify previously unresolved events and develop new proxies for past tropical cyclones. We will also seek to collaborate with other LLNL scientists on this project, for instance through complementary analyses via SEM/TEM/ICPMS and through seeking collaborations with the E3SM climate modeling groups.

## **Climatic Controls on Subsoil Organic Carbon Dynamics**

*Host Campus:* Merced

*Lead Investigator:* Kimber Moreland

*Graduate Fellowships*

*Collaborating Sites:* Lawrence Livermore

*Start Date:* 4/1/2018      *End Date:* 3/31/2020      *Amount:* \$135,216

***Abstract:***

Research: Our understanding of the amount, chemical composition, stability, and stabilization mechanisms of soil organic matter (SOM) stored in deep soil layers and its vulnerability to changes in climate is, at best, incomplete. The goal of this proposed study is to investigate how climate regulates subsoil organic carbon (C) storage, chemical composition, stability, and stabilization mechanisms along the southern Sierra Climosequence, within the Southern Sierra Critical Zone Observatory (SSCZO). Specifically, we will examine how the concentration and chemical composition of bulk C and C in different soil fractions relates to atmospheric and soil microclimate, its stability (i.e. mean residence time), and mechanisms of stabilization through physical and chemical organo-mineral associations. Training plan: This project relies on the use Accelerator Mass Spectrometry (AMS) to employ radiocarbon to determine MRT of deep vs. near-surface soil C, including carbon that is stored in 10m weathered bedrock or saprolite. As such, training plan will focus on training on sample preparation, graphitization, AMS runs, and modeling and interpretation of data under the mentorship of Dr. Karis McFarlane at LLNL's Center for AMS. The collaboration with LLNL would allow hands-on experience for a PhD student. The education and training of the junior scientist is the core mission of the proposed mentorship plan. The applicant mentorship plan emphasizes scientific and technical skills, career planning and professional development, communication skills, and networking. Scholarly contributions: To our knowledge, this study is the only one of its kind with a potential to accurately determine stock and stability of deep soil C, from topsoil all the way down to bedrock contact that is at times below 10 m below the soil surface. These unique samples were acquired through our collaborative project with a large interdisciplinary group working in the SSCZO. Adding a collaboration with LLNL/DOE scientists is key to allow sufficient time and resources to develop the methodology needed to analyze samples that have wide variability in C concentrations, speciation, and mineral-associations. Expected Outcomes: We expect that results of this study will demonstrate that up to 2/3rd of soil C is in the subsoil, with up to 1/3 below 1m soil depth in saprolite and that the stability of soil C will increase in the subsoil (as indicated by increased contributions of mineral-associated, aromatic C functional groups, and <sup>14</sup>C turnover times).

## **Strongly Coupled Atomtronics**

*Host Campus:* Riverside

*Lead Investigator:* Shane Kelly

*Graduate Fellowships*

*Collaborating Sites:* Los Alamos

*Start Date:* 4/1/2017      *End Date:* 3/31/2020      *Amount:* \$200,016

*Abstract:*

The high controllability of cold atom systems has led to new devices and new possibilities for quantum computing as part of the emergent field of atomtronics. We propose a joint investigation between Shane Kelly(SK)(UCR), Dr. Eddy Timmermans(ET)(LANL) and Prof. Shan-Wen Tsai(SWT)(UCR) into a study of strong interaction effects in ultra cold atoms and their potential applications to atomtronics. By the start of this collaboration, next spring, Shane will have completed the fundamental courses, advanced to candidacy, and finished a renormalization-group(RG) study of strongly interacting Fermi systems. Training at LANL will begin with learning about cold atom physics and atomtronics. Specifically, by investigating bosonic systems, superfluidity and its application to Laser Painted Josephson Junctions, a unique cold-atom set-up pioneered by Dr. Malcolm Bolshier at LANL, whom SK will be able to interact closely with during his research at LANL. Moving on to strongly interacting systems, we will begin an investigation on Many Body Localization(MBL). MBL states have non-trivial properties, and, in cold atom systems, are highly controllable. Thus, they yield an interesting possibility for atomtronic devices. ET has previously investigated localization and found the possibility of a new type of polaron regime in cold atom systems. SK will use his experience studying fermionic systems with RG to build off of this work, investigating its extension to fermionic systems and the possibility of new devices in both fermionic and bosonic systems. Scholarly contributions will include scientific publications and presentation, and an open source numerical FUnctional RG LIBrary, fuRGlib, developed by SK throughout this process. ET, an expert in cold atom systems, and SWT, an expert in condensed matter systems and RG methods, have in the past combined their expertise studying narrow Feshbach Resonances and how their unique features affect many-body physics. With this grant, they will be able to again collaborate and together provide mentorship for SK. Concurrently, SK will gain invaluable exposure to state of the art cold atom experiments, a broad research background, and experience exploring the synergies between condensed matter, many body and cold atom physics. With this grant, SK will be able to do a multidisciplinary PhD. project that would not be possible otherwise.

## **Modeling Tropical Carbon Fluxes via Carbonyl Sulfide Uptake**

*Host Campus:* Merced

*Lead Investigator:* James Stinecipher

*Graduate Fellowships*

*Collaborating Sites:* Lawrence Livermore

*Start Date:* 4/1/2017    *End Date:* 3/31/2020    *Amount:* \$200,016

*Abstract:*

The feedbacks between climate and gross primary production (GPP) are the largest and most uncertain of terrestrial biogeochemical feedbacks and, as such, are crucial for understanding the cycling of carbon between the atmosphere and the biosphere. Competing signals of photosynthesis and respiration subject large-scale estimates of gross primary production to considerable uncertainty. The proposal at hand seeks to fill this critical knowledge gap by leveraging atmospheric carbonyl sulfide (COS) as a tracer for photosynthesis. Carbonyl sulfide is taken up by plants concurrently with CO<sub>2</sub>, but, whereas CO<sub>2</sub> is also respired, COS is irreversibly transformed. As such, the magnitude of COS uptake over land can serve as a proxy for gross primary production. In order to accomplish this, I propose to modify the Sulfur Transport Eulerian Model (STEM) to model the transport and photosynthetic drawdown of COS over the Amazon basin. This approach has been successfully applied over North America and, with recent large-scale COS data collection campaigns beginning in the Amazon, now is an ideal time to apply the method to the tropics. These data will be used in the inverse component of STEM to better constrain surface fluxes. In addition to being optimally timed for data collection, the proposed research can also inform and use results from the ongoing Accelerated Climate Model for Energy project to which LLNL is a large contributor. The ACME model can be used to provide dynamic boundary conditions for regional-scale simulations, while results from STEM can provide high-resolution information about plant-related surface fluxes, consistent with ACME's focus on biogeochemical and water cycles. Further work in both models is also needed to accurately model oceanic emissions of COS. Harnessing these models in tandem will allow for better understanding of the transport of COS and, by proxy, atmosphere-biosphere CO<sub>2</sub> interactions. These results could be further incorporated into diagnostics like those in the International Land Benchmarking (ILAMB) Project to provide a metric for GPP suitable for model intercomparison. In this way, results from this work will help fill a crucial knowledge gap, while also providing valuable constraints for other models.



## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Topological materials for Majorana-based quantum information

*Host Campus:* San Diego

*Lead Investigator:* Monica Allen

*Collaborative Research and Training Awards*

*Collaborating Sites:* Davis, Los Angeles, Santa Barbara, Los Alamos

*Start Date:* 3/1/2020    *End Date:* 2/28/2023    *Amount:* \$3,440,222

*Abstract:*

Topological materials offer a route to circumvent environmental perturbations that have hindered the scalability of conventional quantum computing architectures. The Majorana mode, which can be artificially engineered in hybrid devices that couple superconductors with topological materials, constitutes a key building block for a fault-tolerant quantum computer. Manipulation of such particles in complex device networks could enable a more robust paradigm for quantum information. We propose a comprehensive, multi-disciplinary program to synthesize and characterize an emerging class of topological superconducting materials posited to host Majorana modes. The overarching goal is to understand the fundamental physics while evaluating the feasibility of prototype devices that may enable braiding of particles in two dimensions. This program will leverage the broad expertise of a diverse team of scientists in materials synthesis, microscopy, device nanofabrication, quantum electronic transport, unconventional superconductivity, and high magnetic field measurements. It consists of three main research thrusts: (1) prediction and synthesis of emerging quantum materials, (2) characterization of topological phases and emergent phenomena in exotic superconductors and other platforms for Majorana modes, and (3) local interrogation and manipulation of topological states in mesoscopic devices. Bulk crystals and thin films will be synthesized at UCSB, UCD, and LANL, and state-of-the-art epitaxy of superconducting films on semiconductor materials will enable production of hybrid material systems with unprecedented interface quality. Upon integration of the materials into device structures, an array of quantum transport measurements will be performed to unequivocally identify Majorana modes, including tunneling spectroscopy and superconducting interferometry. To complement these efforts, we will employ milliKelvin microwave impedance microscopy measurements to achieve the first real-space visualization of Majorana modes in devices. The proposed work will lay the groundwork for the creation of scalable networks of devices for Majorana-based quantum computation. Graduate students and postdoctoral fellows will benefit from training on state-of-the-art facilities and collaborations at LANL, and periodic meetings will bring together scientists across career stages.

## **Transforming prescribed fire practices for California**

*Host Campus:* Irvine

*Lead Investigator:* Tirtha Banerjee

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Riverside, Los Alamos

*Start Date:* 3/1/2020    *End Date:* 2/28/2023    *Amount:* \$3,600,000

*Abstract:*

Widespread recognition of the importance of low intensity fires to reduce the frequency and severity of future megafires has prompted California to allocate more than \$1 billion over the next five years to support prescribed fire (Rxfire) activities. However, several factors limit Rxfire usage at sufficient scales to effectively minimize the risk of future catastrophic fires: e.g. narrow burn windows, air quality concerns, public perception, personnel training, and liability constraints. To address these urgent needs, our interdisciplinary team will develop technological and operational tools to facilitate the expansion of Rxfire in CA. Our effort will leverage unique multi-fidelity wildfire modeling capabilities, FIRETEC and QUIC-Fire, to assess the effects of (1) heterogeneous fuel structure on fire and smoke behavior; (2) CA and site-specific complex topography, flammable vegetation, micrometeorology and wind patterns; (3) novel ignition strategies e.g., aerial ignitions; (4) complex wildland-urban interface; (5) extents of pollutant formation and transport. Moreover, we will develop technologies/tools that can facilitate communities' understanding of Rxfire. Model ensembles will be aided and calibrated by sensors (in situ and mobile) that capture air quality, visibility, smoke, acoustic signatures, and imagery/video; while UAVs equipped with LIDAR and thermal cameras can further guide sensing. This information in conjunction with community crowdsensing will help map fuels at fine resolutions, monitor Rxfire progress, detect hotspots and quantify community impact. The use of data analytics and machine learning techniques trained by models on real time sensor data will help manage uncertainty in data, detect anomalous behavior rapidly, identify the source locations and potential abort points. The decision support and operational tools will be tested during actual Rxfires in collaboration with US Forest Service, Cal Fire and UC ANR, thus providing publishable data, training for students and postdocs as well as engaging fire practice professionals to develop and test the new tools. The multi-fidelity approach will foster collaborations between UC Irvine (fire modeling, IT decision support), UC Riverside (smoke chemistry and transport), UC Berkeley (experimental Rxfire operations at Berkeley forests) and LANL (model development, high performance computing).

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Assessment and mitigation of wildfire-induced air pollution

*Host Campus:* Davis

*Lead Investigator:* Michele Barbato

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Irvine, Los Angeles, Merced, Lawrence Livermore, Los Alamos

*Start Date:* 3/1/2020    *End Date:* 2/28/2023    *Amount:* \$3,749,855

*Abstract:*

Wildfire smoke threatens the health and quality of life of millions of people (especially Californians) every year. We propose an innovative, scalable framework for assessment and mitigation of wildfire-induced air pollution under climate change. For the first time, we will develop wildfire forecast tools that link statistically-based regional forecasts spanning multiple decades with short-term physics-based fire propagation models that can accurately forecast individual wildfires. Our innovative approach will predict fuel loads using a semi-dynamic vegetation ecology model in order to estimate future wildfire emissions. Emissions of potentially harmful wildfire particulates will be characterized through laboratory tests of mixed fuel loads (i.e., forest and buildings) typically found in the wildland-urban interface. The results of these experiments will inform: 1) new models of smoke plume transport and chemical transformation, which will be validated using satellite imagery; and 2) a novel high-throughput screening method to assess wildfire smoke toxicity. The toxicological study results will inform epidemiological analyses to estimate the association of wildfire smoke on human health. The health effects of four distinct mitigation strategies (i.e., urban growth policy, vegetation management, prescribed burns, and use of fireproof building materials) will be assessed in conjunction with issues of policy design, regulatory assessments, program monitoring/evaluation, financial feasibility, and social impact. Finally, the project results will be made public on the Cal-Adapt web platform. The proposed research activities will: 1) leverage the strengths of 5 UC campuses and 2 national labs; 2) engage multiple faculty, postdocs, and graduate students across disciplines in mutually beneficial new collaborations; 3) position our team members as international leaders on a timely topic of critical importance with significant potential for extramural funding; and 4) produce considerable societal benefits. This project will support valuable training/exchanges of students/postdocs among collaborating institutions, and structured mentorship/professional development activities for early career UC faculty and lab researchers. Finally, the Electric Power Research Institute plans to collaborate on this project and provide internship opportunities for student training.

## **Enabling Scalable Quantum Computing**

*Host Campus:* Riverside

*Lead Investigator:* Boerge Hemmerling

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Los Angeles, Santa Barbara, Lawrence Livermore

*Start Date:* 3/1/2020     *End Date:* 2/28/2023     *Amount:* \$3,750,000

*Abstract:*

Quantum computing is poised to drive the next technological revolution. Driven by the need of system integration and scalability today's quantum computing processors are based on 2D architectures. However, the 2D approach comes at the cost of increased gate errors and reduced connectivity. Here we break with this paradigm and propose to leverage novel 3D printing capabilities with sub-micrometer resolution to develop a scalable 3D-architecture based on trapped ions that will enable extensive quantum calculations with thousands of qubits in the near future. Implementations using traditional 3D Paul traps have already demonstrated memory times of several minutes, extremely low gate errors, and advanced quantum calculations. Moving to a scalable 3D-geometry will increase the confinement by about a factor of three to six and create traps up to 100 times deeper than what is feasible with 2D-fabrication. This is expected to reduce multi-qubit gate error rates by more than an order of magnitude. These advances will also enable novel approaches to quantum computing such as using trapped electrons or molecules, which share the same advantages as trapped atomic ions, while reducing the optical technology overhead. For this research program, we plan to leverage the existing infrastructure and expertise in two-photon 3D-printing and materials science at LLNL and combine that with world-leading expertise in ion-trap quantum information systems within the UC system. Groups at UCLA and UCB have established efforts in trapped-ion quantum computing, with demonstrations of the highest-fidelity single qubit, deep experience with multi-qubit entangling gates and the materials issues related to scalability. Groups at UCSB and UCR have extensive experience in microwave engineering, cryogenics and quantum simulation and work on establishing qubits based on molecules. Through this project, we will design, simulate, and test miniature scalable traps fabricated using 3D-printing methods and show their superior performance compared to current microfabricated traps. We anticipate record-setting error rates, long ion lifetimes and a path to scalability for quantum computing. If successful, this project will solve the most important problem of the scalability of quantum computing architectures and transform the field of quantum information science from within the UC system.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Mitigating and Managing Extreme Wildfire Risk in California

*Host Campus:* Santa Barbara

*Lead Investigator:* Charles Jones

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, San Diego, Lawrence Livermore, Lawrence Berkeley

*Start Date:* 3/1/2020    *End Date:* 2/28/2023    *Amount:* \$3,307,845

*Abstract:*

The recent tragic examples of wildfires in California underscore the importance of understanding the relationships among climate, extreme fire-weather, fire ignitions by electric powerlines and vegetation management. This proposal assembles a multidisciplinary team to investigate the interactions among four research themes —climate change and fire-weather, vegetation management, the electric power grid and associated policies — and their influences on wildfires. To make groundbreaking discoveries, this proposal will investigate a series of critical questions: what is the nature of changes in extreme fire-weather behavior in recent years? What factors interact with electric power system infrastructure to increase wildfire risk in California? How do trade-offs between reliability of energy supply and wildfire risk vary across alternative de-energizing protocols? Can cost-effective investments be implemented in the near future to minimize fire-risk associated with vegetation management and electric power grid infrastructure? The project consists of five interconnected objectives that will foster collaborations among 3 UC campuses and 2 national labs. Objective-1 will use a broad array of observations, global and regional climate models to investigate the problem of climate change and potential changes in fire-weather regimes in California. Objective-2 will use the unique database of high-resolution fire-weather regimes (Objective-1) to determine fire-risks associated with high winds and electric powerlines ignitions. Objective-3 will develop a model of de-energization rules applicable to the electric power grid under high winds and re-estimate fire-weather risk. Objective 4 will evaluate the reliability implications of alternative de-energization rules and contrast these with estimates of the economic impacts of mitigating increased fire risks (Objective 2). Objective-5 will analyze observations and model simulations to determine fire-spread and economic impacts of vegetation management strategies near power lines. The project will combine a wealth of educational and mentoring activities across an innovative and diverse team of undergraduate and graduate students, and postdoctoral scholars on four UC campuses.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Advanced Detectors for XFELs and Proton Accelerators

*Host Campus:* Davis

*Lead Investigator:* Eric Prebys

*Collaborative Research and Training Awards*

*Collaborating Sites:* Irvine, Santa Barbara, Santa Cruz, Los Alamos, Lawrence Berkeley

*Start Date:* 3/1/2020    *End Date:* 2/28/2023    *Amount:* \$3,745,225

*Abstract:*

As accelerator laboratories around the world aspire to create beams with ever-increasing repetition rate and intensity, there is a need to develop fast, radiation-hard detection technologies to provide critical real-time beam diagnostics. Los Alamos National Laboratory (LANL) is engaged in multiple accelerator (proton and photon) projects to meet mission needs, including those which require diagnostic capability beyond the current state-of-the-art. Solid-state sensors, such as those based on diamond and silicon, feature fast saturated drift velocities and collection dynamics that make them natural choices to explore for development of high-speed devices. In addition to these “front end” technologies, it will be essential to develop highly-granular high-speed electronics – for both amplification and data-handling – to achieve the required spatial and temporal precision. This project will bring together expertise in accelerator and high-energy physics sensor development with electrical engineering expertise to develop prototype systems at the forefront of accelerator beam detection technology. The collaboration will be led by Eric Prebys, Director of the Crocker Nuclear Laboratory at UC Davis, and consist of three interrelated thrusts: R&D on diamond sensors (primarily LANL and UC Davis), silicon diode sensors (primarily UCSC and UCSB) and enabling electronics and readout (primarily UC Irvine and LBNL). However, as each institution has broad expertise in instrumentation development and specialized capabilities in sensor fabrication and readout development, all six institutions will contribute in some measure to all three areas. Crocker Lab and LANL also provide accelerator (cyclotron, LANSCE) facilities well-suited to the validation and characterization of the prototype detection systems developed by the collaboration. UC students will be involved in design, fabrication, testing and data analysis aspects of the project, and will be provided an opportunity to spend a period of time in residence at LANL. Project progress will be disseminated through seminars at member institutions, workshops, presentations at national and international conferences and publications. The project will create strong collaborative ties (both intra-UC and UC-LANL) that will position the group to establish leadership in the area of advanced detection technologies for accelerators.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Great Power Competition in the 21st Century

*Host Campus:* San Diego

*Lead Investigator:* Tai Ming Cheung

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Irvine, Los Angeles, Lawrence Livermore

*Start Date:* 3/1/2018      *End Date:* 2/28/2021      *Amount:* \$3,724,742

*Abstract:*

Great power strategic competition has returned to the global stage and the consequences for international peace, stability, and prosperity will be profound. The contours, dynamics, and characteristics of this new strategic rivalry, primarily between the U.S., China, and Russia, but also to a lesser extent with other emerging power centers, will be very different though to what took place in the 20th Century. Confrontation will not be through massed armies in Europe or nuclear arsenals on trigger alert but will occur more indirectly and in more non-military domains. Strategic rivalry is taking place in the pursuit of technological innovation, in disputes below the threshold of full-scale war, and in trade, investment, industrial, and economic competition. This project examines the rise of 21st Century great power competition that is especially focused on the intersection between economics, strategy, security, technology, and politics. The project revolves around four themes each led by a University of California (UC) campus: 1) competition in security, technology, innovation, and strategy (UC San Diego); 2) economic strategic rivalry in trade, investment, and industrial policy (UC Berkeley); 3) the role of design and production networks in East Asia's regional relations and US-China cooperation and competition (UC Irvine); and 4) the international dynamics and domestic politics of great power security competition (UC Los Angeles). This project brings together scholars from political science, international relations, security studies, political economy, and area studies from these four UC campuses as well as Lawrence Livermore National Laboratory. While scholarship on great power competition is beginning to emerge, much of the work is on military, diplomatic, and hard power aspects and little attention has so far been paid to the technological, economic, and domestic dynamics. Opportunities for students to participate in collaborative research and training activities include: 1) the ability to take part in research teams that will write conference papers; and 2) taking part in a summer training workshop on great power competition that will be conducted in the second and third years that will examine the security, economic, political, and geostrategic dimensions of great power competition.

## **Headwaters to groundwater: Resources in a changing climate**

*Host Campus:* Santa Barbara

*Lead Investigator:* Jeff Dozier

*Collaborative Research and Training Awards*

*Collaborating Sites:* Davis, Irvine, Los Angeles, Merced, Lawrence Livermore, Lawrence Berkeley

*Start Date:* 3/1/2018      *End Date:* 2/28/2021      *Amount:* \$3,716,025

*Abstract:*

Climate change and greater water demand pose new challenges for managing water resources. To enable California to optimize future water infrastructure, legislation, and economy, scientists at 5 UC campuses, LLNL, and LBL will measure and model water from headwaters in the Sierra Nevada, through rivers, reservoirs, and groundwater in the Central Valley. The approach is to examine hydrologic sensitivities to changing climate and water demand through models and the historical record. The goal is to provide information to optimize water storage, quality, and groundwater sustainability as precipitation varies, temperatures warm, and population grows. To consider the range of headwater-to-groundwater systems, we focus on three river basins comprising different climatic, geologic, and socio-economic settings -- Shasta R (volcanic, northernmost, lowest, wettest), Kings R (granitic, southernmost, driest, highest, poorest), and the American R (metamorphic, wealthiest). Novel methods to monitor and model ongoing and future changes in rain and snowmelt in the headwaters will be coupled with process-driven modeling and measurement of evapotranspiration, groundwater recharge, and withdrawal in the lowlands. Models will consider changes in water policy and infrastructure, and resulting impacts on energy production and consumption. Collaboration between the Campuses and Labs will build teams that include people in all career stages who study aspects of the water cycle from remote sensing of snow to water policy. Collaborators from LLNL and LBL contribute expertise in isotopic tracing of water, high-performance computer modeling of groundwater and surface water, and energy implications of water management. This proposal strengthens DOE's mission, to ensure America's security and prosperity by addressing energy, environmental, and nuclear challenges through science and technology. The alliance between UC faculty, postdoctoral fellows, and students with scientists at LLNL and LBL will improve understanding of how changing climate and water demand will affect water resources through the middle to the end of this century. Our proposal will nurture a generation of scientists in the nexus of climate, water, and energy. An advisory board of water practitioners will help target our findings to help water managers make the best decisions for California's precious water resources.



## **Securing smart campuses: a holistic multi-layer approach**

*Host Campus:* Riverside

*Lead Investigator:* Michalis Faloutsos

*Collaborative Research and Training Awards*

*Collaborating Sites:* Los Angeles, San Diego, Santa Barbara, Los Alamos

*Start Date:* 3/1/2018     *End Date:* 2/28/2021     *Amount:* \$3,530,278

***Abstract:***

The vision of this proposal is to build security for "smart campuses", that present a microcosm of smart cities and more generally of cyberphysical systems of systems (CPSS). Campuses, including academic, national labs or enterprises, will increasingly integrate sensing, computation, and communication in their physical environment to control operation and efficiently serve their communities. Campuses already consist of multiple interacting layers and systems, ranging from human mobility & crowdsourcing, to infrastructure such as building HVAC systems, to transportation, to medical and emergency services, to computing and communication infrastructure, and to monitoring infrastructure such as cameras; in the future they are expected to integrate other services including automated transportation, camera-equipped monitoring drones etc. Leveraging interactions among these layers with data-driven learning and decision loops can offer significant benefits; for instance in terms of saving energy, reducing operating and maintenance costs and enabling the increase of campus population density that can be comfortably accommodated. However, to successfully move towards increased integration and automation, we need to make safety, security and privacy a core design component. This proposal will develop a holistic framework to enhance the security, privacy and safety of campus operation, building on our team's expertise in CPS security, information & wireless security, software & hardware security and privacy-preserving machine learning. Our work will span a range of goals from establishing vigilance across many attack surfaces, improving the safety of legacy systems and establishing principles of security for emerging systems, leveraging crowdsourcing to achieve low cost sensing while preserving personal privacy, securing Internet-of-Things (IoT) firmware, addressing attacks that exploit the interaction between the cyber and physical world, and expanding the availability of emergency communication in the case of incidents. As part of the experimental validation of the proposed research, we will leverage the rich dataset collected by LANL on HVAC systems, as well as access to the LANL testbed and unclassified high-performance computing resources. Our work will help campuses provide safety guarantees and be better prepared for adversarial and accidental incidents.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### The Future of California Drought, Fire, and Forest Dieback

*Host Campus:* Los Angeles

*Lead Investigator:* Alex Hall

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Davis, Irvine, Los Alamos, Lawrence Berkeley, UC Division of Agriculture and Natural Resources

*Start Date:* 3/1/2018      *End Date:* 2/28/2021      *Amount:* \$3,681,721

**Abstract:**

From 2011 to 2015, California experienced a drought of historic severity, due to a persistent precipitation deficit and extreme warmth. The drought was bracketed by two extremely wet years in 2010 and 2016, and was accompanied by unprecedented tree mortality and wildfire in California's wildlands. Over the 21st century, climate scientists predict continued warming and an increase in swings between extremely wet and dry conditions. Since wet conditions favor vegetation regrowth and fuels buildup, and warm, dry conditions favor forest dieback and wildfire, these predictions raise questions critical for California's future: Are the extreme forest dieback and fire conditions seen during the recent drought a harbinger of even greater future changes? What do future changes mean for California's unique ecosystems, forest and fire management practices, and economy? Here we propose an effort to answer these questions through collaboration among climate scientists, satellite experts, vegetation modelers, fire scientists, and ecologists. The project will be grounded in analysis of observed relationships between fire, tree mortality, and climatic conditions during the recent drought. We will then develop computer simulations of climate, vegetation, and fire to determine the causes of recent tree mortality and fire variations. We will quantify the role of recent climate change in worsening the observed forest dieback and fire. The project's capstone will be high-resolution climate change projections to simulate the impact of warming and increases in precipitation extremes on 21st century vegetation growth, fire, and forest dieback. We will also assess how future forest and fire management might evolve to mitigate the largest impacts of climate change on California's wildlands. The first-of-their-kind climate, vegetation, and fire simulations will deepen our understanding of the complex interactions within California's wildlands, and will leave a technological legacy in the form of a modeling framework that is easily applied to other regions. The research process will train young scientists in societally relevant interdisciplinary research, the results will help stakeholders plan effective climate change adaptation and mitigation, and our outreach efforts will educate the public about climate change impacts on the treasured lands and resources they depend on.

## **Climate Impact of Manure Management from California Dairies**

*Host Campus:* Riverside

*Lead Investigator:* Francesca Hopkins

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Davis, Irvine, Los Alamos, Lawrence Berkeley

*Start Date:* 3/1/2018     *End Date:* 2/28/2021     *Amount:* \$3,839,477

*Abstract:*

Climate Impact of Manure Management from California Dairies The California dairy industry is a large contributor to greenhouse gas emissions, producing approximately 50% of methane (CH<sub>4</sub>) and 10% of nitrous oxide (N<sub>2</sub>O) emissions statewide. The majority of these emissions come from manure, where emission rates are thought to differ greatly among different manure management techniques. In order to fulfill statewide emission reduction goals for short-lived climate pollutants, the California Air Resources Board has recently targeted CH<sub>4</sub> emission sources for near-term mitigation. However, few studies of CH<sub>4</sub> emissions from dairy manure have been performed in California. Recent top-down atmospheric observations and inverse model analyses of atmospheric CH<sub>4</sub> and N<sub>2</sub>O levels in the San Joaquin Valley suggest that emissions from dairy agriculture are underestimated in the state inventory. However, the dearth of California-specific information leads to uncertainty in the state inventory that poses an obstacle to efficient, well-informed mitigation planning for emissions from this sector. In addition, the efficacy of proposed mitigation solutions, such as anaerobic digesters for manure waste, is not well quantified or tested in practice. We propose to combine top-down atmospheric methods with bottom-up process-level measurements and operational insight to improve both facility specific and regionally integrated estimates of greenhouse gas emissions from management practices at California dairies. Using a unique combination of subject area knowledge, high resolution data sets, biogeochemistry, atmospheric composition observations, and inversion modeling, we will quantify and apportion CH<sub>4</sub> and N<sub>2</sub>O emissions to their sources with the goal of improving understanding of the driving processes and their respective control techniques. By working across scales, we will provide an integrated regional emissions estimate with sufficient detail to unambiguously quantify dairy livestock emissions as distinct from other greenhouse gas sources. This study will give a thorough scientific treatment to the greenhouse gas emissions from the entire manure management cycle in ways that have been done for other CH<sub>4</sub> emitting sectors, such as natural gas, to enable complete, empirically informed mitigation decisions.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### UC-Lab Center for Electricity Distribution Cybersecurity

*Host Campus:* Riverside

*Lead Investigator:* Hamed Mohsenian-Rad

*Collaborative Research and Training Awards*

*Collaborating Sites:* Irvine, Los Angeles, Santa Barbara, Lawrence Livermore, Lawrence Berkeley

*Start Date:* 3/1/2018      *End Date:* 2/28/2021      *Amount:* \$3,748,698

*Abstract:*

This proposal will bring together a multi-disciplinary UC-Lab team of cybersecurity and electricity infrastructure experts to investigate, through both cyber and physical modeling and physics-aware cybersecurity analysis, the impact and significance of cyberattacks on electricity distribution infrastructure and develop new strategies for mitigation of vulnerabilities, detection of intrusion, and protection against detrimental system wide impact. As the deployment of distributed energy resources (DERs) such as solar panels and energy storage devices is proliferating, electricity distribution systems are becoming drastically more complex and more dynamic. There are numerous inputs and controls pushed and pulled from these emerging energy resources and other grid equipment, some of which connect the resources to the public Internet. Further, the installation of millions of smart electricity meters and recent breakthroughs in micro-synchrophasor sensors and smart inverter controls are accelerating the rate at which measurement data is generated and control commands are dispatched. However, these technological advancements in sensing, controls, and communications of electricity distribution systems have exposed this critical infrastructure to new vulnerabilities, threatening its functionality and reliability. Each of the new layers of data integration and control that are being added to electric distribution systems can create new cyberattack surfaces and privacy breaches that are yet to be identified, understood, and quantified; and this challenges the vision of a renewed and more efficient electric grid. Traditionally, the focus in cybersecurity of electricity infrastructures has been on securing large power plants and control centers. In contrast, this project will create a paradigm shift to make serious efforts also to secure DERs and electricity distribution networks, through enhanced and comprehensive cybersecurity measures, reinforced by physical measures such as electric isolation. Otherwise, attacks could compromise a number of distributed cyber and physical components, turning them into "physical botnets" against the electricity infrastructure – analogous to how computer botnets work in distributed denial-of-service attacks (DDoS) in the Internet. This project will build a new knowledge base to address both theoretical and practical challenges in electricity distribution cybersecurity. It will position the UC-Lab team early-on at the forefront of this emerging field of great national interest.

## **Political Conflict and Stability in Dynamic Networks**

*Host Campus:* Los Angeles

*Lead Investigator:* Arthur Stein

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, San Diego, Santa Barbara, Los Alamos

*Start Date:* 3/1/2018    *End Date:* 2/28/2021    *Amount:* \$3,032,554

*Abstract:*

At the heart of international politics are the cooperative and conflictual relations between states and rebel and terrorist groups. Challenges and opportunities for bilateral ties are posed by their being embedded in a larger setting. The proverb “the enemy of my enemy is my friend” captures this dynamic in which links between pairs of actors are affected by the relationships of each with others. This has huge consequences for interstate and intra-state relations and for critical security questions such as the impact of foreign intervention, or the reverberating impact of a change in international alignment. These relationships constitute a network whose instabilities and dynamics are not well understood. We propose applying to such political relationships a sociological theory (structural balance) developed for networks of interpersonal relationships. The theory requires both analytic development and empirical assessment. The theory originally dichotomized relationships into positive and negative, but we will incorporate the consequences of degrees of cooperation and conflict. The theory stipulates conditions of balance and equilibrium, but does not delineate the specific relationships that will change to bring any set of unbalanced relationships into balance. This will be an analytic extension developed in the project. The empirical assessment of the behavioral dynamics of structural balance will make use of a database of political events, that includes both states and rebel groups, and that codes cooperation and conflict. In addition, surveys and survey experiments will be used to assess the issues and attitudes that underlie structural balance in conflict and post-conflict settings. The project addresses key security concerns, among them being the foreign policy implications of regime change, the reverberating consequences of an outbreak of a civil war or conversely of a peace agreement, and the consequence of an external intervention into a domestic dispute. More broadly, the general model developed of networks of cooperative and conflictual ties will have broader implications for studying political and social relationships. The proposal brings together political scientists who have focused on international and civil conflict with sociologists and applied mathematicians who have worked to develop, assess, and apply networks.

## **Macromolecular movements by simulation and diffuse scatter**

*Host Campus:* San Francisco

*Lead Investigator:* James Fraser

*Collaborative Research and Training Awards*

*Collaborating Sites:* Irvine, Riverside, San Diego, San Francisco, Los Alamos

*Start Date:* 3/1/2017      *End Date:* 2/28/2021      *Amount:* \$1,914,700

*Abstract:*

Macromolecules, such as proteins and RNA, move between different structures to accomplish their functions in cells. Many of the major challenges that prevent biologists from engineering macromolecules to perform new functions, interpreting the mechanisms of mutations in the context of disease that abolish function, or discovering new drugs to alter function originate from an inability to resolve the motions between the different required structures. Advances in high throughput computing are now enabling us to view these motions in simulations of macromolecules of increasingly larger sizes and for increasingly longer time scales. However, to fully exploit the potential of molecular simulations we face a major challenge in improving accuracy and time scale. Comparisons with experimental data are essential for making progress in both of these areas. While most experiments report on the average structure, pioneering work by Wall (LANL) and others has shown that X-ray diffuse scattering, which can uniquely reporting on correlations between atoms, can be leveraged to dramatically improve simulations. Diffuse scattering is therefore particularly well suited to improve accuracy and to benchmark acceleration schemes to achieve longer time scales in simulations. Our cross-disciplinary collaboration will include computing (UCI, UCSD, LANL) and experimental X-ray crystallography (UCSF, UCSD, UCR). We will take advantage of the UCOP-MPRI funded beamline at LBL, which has recently been upgraded with a photon counting pixel array detector that allows extremely accurate measurement of the diffuse signal. Through collaborative research exchanges, seminars, and graduate student training, our group will use high throughput computing to accomplish three aims: 1) determine the optimal acceleration scheme to increase agreement of simulations with experimental diffuse scattering data. 2) optimize the simulation of macromolecular crystal systems. 3) apply advanced simulations and X-ray diffuse scattering to discover new conformational states of important macromolecular drug targets. Our collaboration will therefore advance the field of molecular simulations by increasing the accuracy and time scale of simulations through comparisons to a novel experimental observable. We will make progress on these fundamental issues while applying our discoveries to important biological targets.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Designer Mesoscale Quantum Dot Solids

*Host Campus:* Irvine

*Lead Investigator:* Matthew Law

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Davis, Irvine, San Diego, Los Alamos

*Start Date:* 3/1/2017    *End Date:* 2/28/2021    *Amount:* \$3,617,546

*Abstract:*

In this project, a multidisciplinary team of researchers from UC Irvine, UC Davis, UC Berkeley, UC San Diego, and Los Alamos National Laboratory will develop and study thin films of semiconductor quantum dots (QDs) that combine the size-tunable optical properties and unique photophysics of QDs with the electrical properties of bulk semiconductors, yielding high-performance, designer mesoscale materials for applications in next-generation energy conversion and photon detection. 3D QD films with unprecedented electronic coupling and spatial and energetic order will be made by self-assembly, surface passivation, and matrix engineering. Assembly of the films will be studied and optimized by in situ liquid cell transmission electron microscopy (TEM). We will use in situ atomic-scale imaging and spectroscopy by scanning probe and photoemission techniques to map surface chemistry and electronic structure during each step of film fabrication. The atomic-scale structure of the QD films will be determined by scanning TEM and electron tomography. Atomistic density functional theory and transport calculations will be performed to model the electronic structure and charge transport properties of the films, focusing particularly on the emergence of delocalized electronic states between the QDs and the impact of local structure and defects on carrier diffusion lengths. Exciton and carrier dynamics will be measured by ultrafast photocurrent and time-resolved optical spectroscopies. Spatially- and time-resolved charge transport measurements will be conducted using several different experimental approaches. UC students will perform some work at LANL facilities. This coordinated research program of fabrication, structural characterization, surface science, and transport will result in a new class of QD superlattice films in which charges move via band conduction rather than site-to-site hopping, yielding the major improvements in carrier mobility, lifetime, and diffusion length needed for advanced optoelectronic applications. In addition to excellent charge transport by control of coupling and disorder at the mesoscale, the films will show indefinite stability, tunable doping via selection of surface and matrix composition, and compatibility with various types of QD building blocks. Project results will be generalizable to other mesoscale systems, both inorganic and organic.

## UC-National Laboratory Fees Research Program

*Abstracts for Active Awards*

### Mesoscopic 2D materials: many-body interactions&applications

*Host Campus:* Los Angeles

*Lead Investigator:* Chee Wei Wong

*Collaborative Research and Training Awards*

*Collaborating Sites:* Berkeley, Los Angeles, Merced, Riverside, Santa Barbara, Lawrence Berkeley, Lawrence Livermore, Los Alamos

*Start Date:* 3/1/2017      *End Date:* 5/31/2020      *Amount:* \$3,680,510

**Abstract:**

Advances in mesoscopic materials growth and discovery have pioneered breakthroughs in device electronics and optoelectronics. Semiconductor heterostructures have led the path in today's lasers, computing electronics and optical communications. The recent discovery of stable atomic-scale two-dimensional materials, such as graphene and semiconducting transition-metal dichalcogenides, provides a fundamental route towards the understanding of charge carrier interactions, enabled by the extremely strong Coulomb interactions and light absorption in these 2D atomic crystals. Our efforts in this regard have ranged from high carrier density plasmas to many-particle neutral and charged electronic states, to single-exciton-photon interactions involving coherent fields, to heterojunction charge dynamics in next-generation device applications. In this UC-NL CRT program, our synergistic team proposes to establish UC scientific leadership in atomic-scale semiconductor optoelectronics, with five correlated Thrusts of high impact: (1) Atomic-scale 2D materials definition: growth, microscopy and defect control with atomic granularity; (2) Many-body excitonic interactions and dynamics in the 2D heterostructures; (3) Single exciton-photon interactions in the 2D heterostructures; (4) Interfaces and contacts to the 2D heterostructures; and (5) Integrated early-career scientist, postdoctoral, and student training, with diversity emphasis. Our Thrust integrates across our four core expertise areas in mesoscopic science: (A) atomic-scale materials control and physics, (B) first-principles and theoretical modeling, (C) electron and optical spectroscopy, and (D) mesoscopic device applications. Our proposed team matches world-class optical and transport spectroscopy, device physics, with ab initio computational and condensed matter theory. Our CRT effectively integrates the unique strengths and equipment of each committed campus - national lab. Extended cross-disciplinary exchanges are planned, with a co-faculty/lab mentorship (theory, materials and experiment). Career development between lab/faculty scientists are enhanced through the new scientific advances proposed, supported by symposiums on atomic-scale optoelectronics, periodic seminars and an integral focus on undergraduate research such as summer internships and lab-supervised research classes. The PIs have successful minority PhD training programs, partnering with HBCU/ minority-colleges towards this UC-NL program. Budget: \$3.75M with \$2,043,944 in lab matching.