

**Laboratory Directed Research  
and Development Program  
FY 2017**

**June 2018**

**Report on  
Ernest Orlando Lawrence  
Berkeley National Laboratory**

**Laboratory Directed  
Research and Development  
Program**

**FY 2017**



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# Introduction

The Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab or LBNL) is a multi-program national research facility operated by the University of California for the Department of Energy (DOE). As an integral element of DOE's National Laboratory System, Berkeley Lab supports DOE's missions in fundamental science, energy resources, and environmental quality. Berkeley Lab programs advance four distinct goals for DOE and the nation:

- To perform leading multidisciplinary research in the computing sciences, physical sciences, energy sciences, biosciences, earth and environmental sciences, and energy technologies in a manner that ensures employee and public safety as well as protection of the environment.
- To develop and operate unique national experimental facilities for qualified investigators.
- To educate and train future generations of scientists and engineers to promote national science and education goals.
- To transfer knowledge and technological innovations and foster productive relationships among Berkeley Lab's research programs, universities and industry in order to promote national economic competitiveness.

Berkeley Lab's research and the Laboratory Directed Research and Development (LDRD) program supports DOE Strategic Themes that are codified in DOE's 2014 Strategic Plan, with a primary focus on the theme of Scientific Discovery and Innovation. For that, the Fiscal Year (FY) 2017 LDRD projects support Goal 1 through multiple strategic objectives described in the plan. In addition, LDRD efforts support the goals of Management, Performance and Nuclear Security (unclassified fundamental research that supports stockpile safety and nonproliferation programs). The LDRD program also supports Office of Science strategic plans, including the 20-year Scientific Facilities Plan and the Office of Science Strategic Plan. Berkeley Lab's LDRD research also supports the strategic directions periodically under consideration and review by the Office of Science Program Offices, such as LDRD projects germane to new research facility concepts and new fundamental science directions.

Berkeley Lab's LDRD program also plays an important role in leveraging DOE capabilities for national needs. The fundamental scientific research and development conducted in the program advances the skills and technologies of importance to our Strategic Partnership Projects (SPP) sponsors. Among many directions, these include a broad

range of health-related science such as breast cancer studies for the National Institutes of Health, accelerator research supported by the Department of Defense, detector and engineering technologies useful to the Department of Homeland Security, and particle detection valuable to the Environmental Protection Agency. Projects in imaging, data analytics, and networking are of potential applicability for programs in the Department of Veterans Affairs.

The *Berkeley Lab Laboratory Directed Research and Development Program FY2017* report is compiled from annual reports submitted by principal investigators following the close of the fiscal year. This report describes the supported projects and summarizes their accomplishments. It constitutes a part of the LDRD program planning and documentation process that includes an annual planning cycle, project selection, implementation and review.

Berkeley Lab's LDRD program is a critical tool for directing the Laboratory's forefront scientific research capabilities toward vital and emerging scientific challenges. The program provides the resources for Berkeley Lab scientists to make rapid and significant contributions to critical national science and technology problems. The LDRD program also advances Berkeley Lab's core competencies, foundations and scientific capabilities, and permits exploration of exciting new opportunities. All projects represent work in forefront areas of science and technology. Ideas eligible for support include:

- Advanced study of hypotheses, concepts or innovative approaches to scientific or technical problems;
- Experiments and analyses directed toward "proof of principle" or early determination of the utility of new scientific ideas, technical concepts or devices; and
- Conception and preliminary technical analyses of experimental facilities or devices.

The LDRD program supports Berkeley Lab's mission in many ways. First, because LDRD funds can be allocated within a relatively short time frame, Berkeley Lab researchers can support the mission of the Department of Energy (DOE) and serve the needs of the nation by quickly responding to forefront scientific problems. Second, LDRD enables Berkeley Lab to attract and retain highly qualified scientists, and to support their efforts to carry out world-leading research. In addition, the LDRD program also supports new projects that involve graduate students and postdoctoral fellows, thus contributing to the education mission of Berkeley Lab.

Berkeley Lab has a formal process for allocating funds for the LDRD program. The process relies on individual scientific investigators and the scientific leadership of Berkeley Lab to identify opportunities that will contribute to scientific and institutional goals. The process is also designed to comply with DOE Orders, in particular DOE Order 413.2C (dated October 22, 2015). From year to year, the distribution of funds among the scientific program areas changes. This flexibility optimizes Berkeley Lab's ability to respond to opportunities.

Berkeley Lab's LDRD policy and program decisions are the responsibility of the Laboratory Director. The Director has assigned general programmatic oversight responsibility to the Deputy Laboratory Director, with administration and reporting on the LDRD program supported by that office. LDRD accounting procedures and financial management are consistent with the Laboratory's accounting principles and stipulations under the contract between the University of California and the Department of Energy, with accounting maintained through the Laboratory's Chief Financial Officer.

In FY2017, Berkeley Lab was authorized by DOE to establish a funding ceiling for the LDRD program of \$27M including General & Administrative (G&A) overhead, which equated to ~3.5% of Berkeley Lab's FY2017 projected operating and capital equipment budgets. This funding level was provided to develop new scientific ideas and opportunities, and to allow the Berkeley Lab Director an opportunity to initiate new directions. In all, about \$25.5M was expended for operating expenses.

In FY2017, scientists submitted 159 proposals, requesting about \$36.5M in funding prior to assessing laboratory overhead. Ninety projects were funded, with awards ranging from \$61K to \$766K.

## Single-shot sub-nanosecond microscopy

Principal Investigator: Daniele Filippetto

### *Project Description*

The purpose of this project is to lay the foundation for the next leap in electron instrumentation, towards ultrafast time-resolved images nano-scale dynamics in matter. The instrument we will finally allow to film structural changes in materials as they happen, separating in space and time the different modes of structure reaction resulting from initial impulsive excitation in non-reversible phenomena, such as nucleation sites and in-situ nanoparticle dynamics, as for example laser-initiated self-assembly in liquids.

We will study the feasibility of using RF technology to extend the temporal resolution of electron microscopy by six orders of magnitude, from millisecond to nanosecond. An electron microscope column will be designed based on the parameters achievable by the APEX electron gun, a unique high brightness source developed by our group at LBNL. The work will clarify the trade offs between spatial and temporal resolution and providing a guide for the development of a future microscope with sub-nm/sub-ns resolution.

We will complete the design and beam dynamics simulations of nano-focusing optics using strong permanent magnets. Such design could eventually allow performing Ultrafast STEM experiments with nanometer resolution on the present HiRES beamline with very inexpensive electron optics. A one-day workshop on ultrafast science using electron probes will be organized to discuss with future potential users of the LBNL UED experiments and desirable instrumentation features.

### *Accomplishments*

We have designed a complete electron column for the APEX source. We studied the role of aberrations from the objective lens in the spatial resolution for electron beam parameters compatible with single-shot sub-nanosecond resolution. The divergence at the sample has been optimized with to obtain 1 nm resolution. The design uses three condenser lenses to give full flexibility in terms of sample illumination and magnification, and uses parameters compatible with the construction of a real column. Indeed, the magnetic field strength used for the focusing optics is achievable with standard warm technology. The size and distance between element columns are realistic and compatible with fabrication. The sample position has been optimized as possible to the objective lens longitudinal center, to facilitate insertion and extraction of sample holders from the column.

An alternative way of focusing high beams has also been investigated: a triplet of permanent magnet quadrupoles with focusing strength has been designed and fabricated. Beam dynamics simulations showed the possibility of obtaining beam sizes at the sample as small as 50 nm RMS. The system is currently in the beamline and the first tests are underway. Initial measurements already led to spot sizes as small as 2 micrometers, the smallest ever measured with an RF source at these energies.

In April 2017 a one-day workshop on “Science with ultrafast electrons” has been organized at LBNL. Experts from all over US gathered to discuss the present results and future prospective of UED/UEM techniques. The workshop generated a large interest. The main request in terms of instrumentation development from the workshop attendees was the ability to probe nanoscopic regions of the samples without degrading the temporal resolution.

## Sub-10 fsec Synchronization for Small-scale Ultrafast Science

Principal Investigator(s): (John, Byrd and Gang, Huang)

### *Project Description*

One of the main scientific goals of the present decade is the study of the ultrafast dynamical processes down to femtosecond time scales. The primary experimental technique is the optical/x-ray/electron pump-probe where an optical laser pulses excites a molecular system and a subsequent x-ray or electron pulse probes the state of the system. The enabling technology for this pump/probe is the ability to precisely synchronize the relative arrival times of the pump and the probe and maintain this synchronization for the duration of an experiment.

The purpose of this project is to dramatically improve the synchronization between pump and probe towards sub-10 femto-second level. This will enable the dream of making “movies” of the complex dynamics in bio-science, chemical science etc.

This project is based on the Advanced Photon-injector EXperiment (APEX) platform and the High repetition Rate Electron Scattering beamline (HiRES) to develop advanced control around it to achieve stable synchronization. The advances in producing high brightness electron beams with femtosecond bunch lengths have allowed ultrafast electron diffraction (UED) to emerge as a complementary tool to x-ray FELs as a probe of ultrafast dynamics. The relatively small size of a UED facility (<10 meters) provides unique opportunities for synchronization.

We will achieve this by mitigate of the noise source and suppress the unidentified jitter by high gain feedback system including beam based feedback.

### *Accomplishments*

In the first year of this LDRD, our most significant accomplishment has been fully explore the noise from each components in the system. Realized the difference between the idealized lab condition and the operating APEX/HiRES machine and started to control the jitter and drift of the system. We analysed the stability of electron beam and the jitter and drift in different subsystems, including the laser phase stability, laser pointing stability, RF cavity field stability, RF amplifier power supply stability etc. With the measurement result, we have organized a workshop to discuss this stability issue on APEX/HiRES and concluded with system improvement plan: a) Use fiber coupled remote DAC and photodiode to eliminate noise pickup on the long cable. b) Use the up-to-date electronics hardware to minimize the channel to channel cross-talk and white noise. c) Improve the firmware and software for the cavity and laser control with easy parameter optimization. d) Implement independent beam arrival time diagnostic tools, destructive and/or non-destructive and prepare for beam based feedback.

We designed the fiber coupled remote DAC and characterizing the low noise piezo amplifier and piezo damage criteria of the new laser oscillator in APEX. We designed the LLRF system upgrade based on the LCLS-II gun/buncher low level RF system.

## Development of a compact laser-driven ion beam accelerator for Discovery Plasma Science

Principal Investigator: Qing Ji  
Co-PI(s): Sven Steinke and Stepan Bulanov

### *Project Description*

The purpose of this project is to lay the foundation of an advanced laser-driven ion acceleration system using the PW laser at the Berkeley Lab Laser Accelerator (BELLA) center, with beam transport/handling capability to achieve ion beams at various beam energies and intensities as high as  $10^{10}$ /shot. This technology can not only be used as an injector for conventional accelerators, but also has a variety of potential applications, such as radiography, biomedical research in cancer treatment, material science and warm dense matter research, and studies of fast ignition schemes etc.

We will carry out realistic 2D and 3D modeling of the interactions between PW laser pulses and materials to find the optimum scenario for the PW laser at BELLA to generate ions with kinetic high energies ( $> 250$  MeV for protons,  $> 800$  MeV for helium,  $> 1$  GeV for carbon etc.). Concepts for high repetition-rate targetry, beamlines and detectors to use the full capabilities of BELLA (1 Hz) will be developed. With the ultra-high intensity ( $> 10^{21}$  W/cm<sup>2</sup>) achieved by the unique PW laser in addition to short focal length optics, advanced nano-engineered targets, theory and simulation of ion generation, leading expertise in ion beam control and manipulation, we will develop a design for a new generation of high performance ion accelerators.

### *Accomplishments*

Based on some FY 2016 achievements, such as physics design of laser-ion acceleration experiments using the long focal length BELLA beamline, target design of high-repetition rate (1Hz) for Target Normal Sheath Acceleration (TNSA) mechanisms, and fabrication of a Thomson Parabola Ion Spectrometer, we have carried out the solid target experiments and produced high intensity of protons up to 7 MeV with a diverging angle less than 250 mrad. We also performed a series of 2D TNSA simulations of laser driven ion acceleration from a thin CH foil using WARP code. In the TNSA regime, with the CH target thickness of 1  $\mu$ m, the simulations show the production of the collimated proton beam with the maximum energy of about 10 MeV, which agrees quite well with the experimental results obtained at the BELLA laser facility ( $I \sim 7.26 \times 10^{18}$  W/cm<sup>2</sup>,  $\lambda = 800$  nm). Furthermore, the maximum proton energy dependence on different setups of the initialization, i.e., different angles of the laser incidence, different gradient scales of the pre-plasma, was explored. Simulations of transporting these laser-driven ions using an active plasma lens is also in progress. The results of both simulation and experimental studies were presented at several international conferences and published in peer-reviewed journals.

We also have engaged program managers at DOE Fusion Energy Sciences in their high energy density physics program and have received some funding ( $\sim$  \$240K) to carry out several selected collaborative experiments proposed by users from universities and national labs.

## **A New Concept for High Average Power Ultrafast Lasers**

Principal Investigator: Russell Wilcox

### *Project Description*

The purpose of this project is to demonstrate a scalable method of adding ultrafast pulse beams coherently in order to produce a high energy, single beam. This process of coherent addition is necessary when using fiber lasers as sources, because each laser is limited in output energy. While fiber lasers are attractive for their efficiency, beam quality, robustness and broad bandwidth, they suffer from small aperture size and therefore small output energy of order 10mJ. To achieve Joules of energy, hundreds of outputs must be added together, requiring a scalable technology.

We will develop a new, efficient method of adding ultrafast pulses, using only two optical elements irrespective of the number of beams to be combined, while preserving the ultrashort pulse width of the source laser. This method employs diffractive optical elements, which can be fabricated to add of order hundred beams, and which have demonstrated high efficiency and power handling capability in high power CW applications. Our approach will be demonstrated using a few beams, and supported by theory and numerical modeling to extend experimental results to high beam-count designs.

### *Accomplishments*

Our most significant accomplishment has been to demonstrate addition of eight, 120fs beams in a 2-D array, while preserving pulse width. Our source was a fiber modelocked oscillator followed by fiber amplifiers and splitters, to provide eight phase-controlled and timed beams into the combiner. The 120fs pulse was dispersed in the fiber system, then compressed after the combiner. Compressed pulses from one input beam versus those from the combiner yielded nearly identical pulse profiles. The efficiency of combination was close to that expected theoretically, given the intrinsic efficiency of the combining optics. To control the combining system, we have developed a new method of error analysis, using the rejected, higher order beams as information as to the relative phases of the input beams. This approach can scale with high beam number, in contrast to the currently used methods which slow down in proportion to the number of phase-controlled beams.

We have also succeeded in developing a theoretical basis for scaling the concept, which is supported by numerical modeling. Our method of combination cancels angular dispersion while allowing temporal and spatial dispersion. We have shown that the uncorrected dispersions do not contribute significantly to energy loss in scaled-up designs with order 100 beams, given our target pulse width regime of 30-100fs. These calculations using perturbation theory are supported by numerical simulation of interfering optical fields, with a reduced number of beams but a full account of the beam profile and pulse width.

## High-Pressure Soft X-ray Spectroscopy of Fluids

**LDRD Postdoc:** Ruimin Qiao; **ALS:** J.-H. Guo, A. MacDowell, M. Kunz, and C. Wang; **ESD:** B. Gilbert, J. Ajo-Franklin, and P. Nico; **MSD:** D. Prendergast, J. Schuck, and J. Urban

This LDRD is proposed to construct the high-pressure (HP) fluid flow cells for soft X-ray (SX) spectroscopy and scattering experiments. The HP-SX cells will enable multiple soft X-ray spectroscopy and scattering characterization tools at ALS for novel measurements with the focus on the molecular structure of fluids relevant to geological carbon sequestration (GCS) of CO<sub>2</sub> and with impact to the *in-situ* study of CO<sub>2</sub> storage in MOF materials and membrane technology in water-energy environment science. It has also potential applications of studying catalytic reactions in real-world industrial conditions.

The LDRD postdoc, Ruimin Qiao was hired in March 2016. The technical goals of the project are: 1) To create SX transparent windows stable beyond the critical point of CO<sub>2</sub> (75 bars; 31°C); and 2) To construct single-windowed HP flow cells for SX spectroscopy.

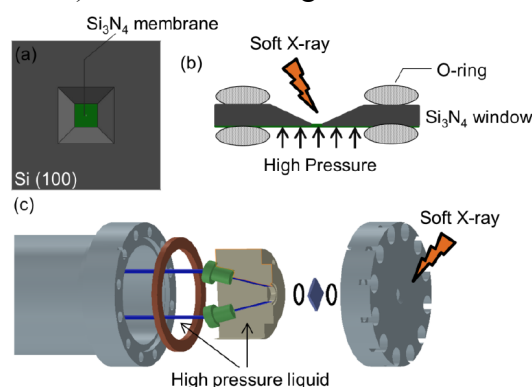


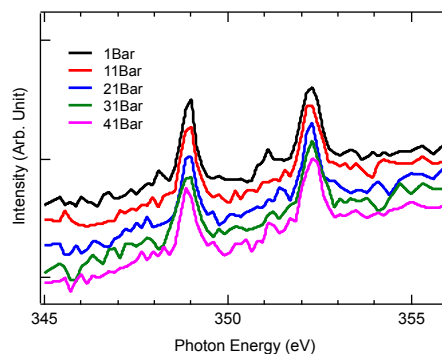
Figure 1. Si<sub>3</sub>N<sub>4</sub> membrane window and the high-pressure soft x-ray cell. (a) Front view of Si<sub>3</sub>N<sub>4</sub> window. (b) A diagram showing the principle of the high-pressure cell. (c) The assembly drawing of high-pressure soft x-ray cell.

Figure 1 shows the principle parts of the high pressure XAS cell and assembly drawing of the high pressure sXAS cell. It utilizes two identical Viton O-rings with the outer diameter of 6 mm and inner diameter (ID) of 4 mm to support the Si<sub>3</sub>N<sub>4</sub> window. The bottom O-ring also has the function to confine the high-pressure liquid, while the top O-ring seals the vacuum from the

atmosphere in the case of sXAS experiments. The commonly used SN-membrane windows (100-nm thick membrane with 1 mm x 1 mm opening on the 200 μm thick Si-wafer) shows a burst pressure at about 2.75 bar. We started the test on this kind of window and were able to achieve a pressure of above 60 bar by using 200-nm thick SN-membrane window with 65 μm x 65 μm opening and 500 μm thick Si-wafer. The experiment indicate that the known theoretical specs may not to entirely correct, thus we are refining the theoretical modeling parameters and planning further experimental tests. New membrane windows are fabricated with support from Weilun Chao, a CXRO scientists for achieving higher pressure.

Figure 2. The Ca L-edge x-ray absorption spectra (total fluorescence yield) of 5M CaCl<sub>2</sub> aqueous solutions collected at different pressure. All the spectra have been vertically offset and normalized by setting the pre-edge and the L<sub>2</sub> peak at same value.

Figure 2 To test the performance of the high pressure liquid cell for sXAS, we collected Ca L-edge XAS spectra of 5M CaCl<sub>2</sub> aqueous solution at different pressures up to 41 bar, which are shown in Fig. 6(a). For this measurement, Si<sub>3</sub>N<sub>4</sub> membrane has a square shape (75 μm x 75 μm) and 100 nm thick, and the Si frame is 6.35 mm x 6.35 mm of 500 μm thick. Ca L<sub>3,2</sub>-edge absorption edge is sensitive to the local chemical environment of Ca, and it is possible that the observed trend indicates a change in the average number of waters of hydration.





## Probing chemical kinetics in MOF materials by X-ray Photon Correlation Spectroscopy

Principal Investigator: Sujoy, Roy

### *Project Description*

The project is aiming for a better understanding of the gas adsorption dynamics in a group of micro-porous sorbents, namely Metal-Organic Frameworks (MOFs), using X-ray photon correlation spectroscopy (XPCS). The time depended nanoscale structural fluctuation probed by the experiment can help reveal the nature of the gas-MOF interaction and possible intermittent state, thus lead to better fine tuning of MOF structure for energy efficient CO<sub>2</sub> removal from post combustion flue gas.

To achieve this target, a system with *in-situ* material activation and gas delivery ability under ultra-high vacuum environment needs to be developed. And this system must grant enough photon transparency to enable time-dependent analysis of the structure fluctuation, in the meantime, it has to be capable of standing the ultra-high vacuum environment to enable soft X-ray experiment. Once the system is ready, a series of high-performance MOF materials will be investigated to extract any useful structural information about the CO<sub>2</sub>-MOF interaction. The result will be the first spatio-temporal correlation study of MOFs and the result will be fed back to our MOF-synthesis collaborator to help improve the next generation MOF sorbent.

### *Accomplishments*

Since last year, an improved version of gas-compatible *in-situ* cell has been redesigned, assembled and tested at beamline 12.0.2. The cell now consists of a titanium body, compress sealed gas input and output, two custom made silicon nitride membrane with heater and spacer implanted. The membranes are secured and sealed by two O-ring and a metal cover. The new design aim to solve the leakage caused by the flexibility of Polyether ether ketone(PEEK) in the old version. Titanium offer better rigidity and smooth surface to improve the performance under ultra-high vacuum. The electrodes are mounted on a deeper and wider slot with PEEK insert to avoid short circuit and provide better contact with the membrane. The total size is still kept approximately 0.8 inch and can be mounted on a custom made insert rod so that it can fit into the XPCS chamber at beamline 12.0.2. The system is connected to a mass flow controller with adjustable flow speed built at the beamline. MOF samples can be deposit and heated under vacuum on one of Silicon Nitride membranes which has gold heater fabricated on the surface. This heating process will drive away all the pre-adsorbed solvent, gas or any other molecules which may affect the CO<sub>2</sub> adsorption. This setup is being tested at the beamline.

We also arranged several collaboration with scientists who are interested in similar setup to carry out XPCS study of other soft materials, including nanoparticles colloids, polymers and gels. And two simplified version of the *in-situ* cells with liquid sample compatibility were also made to serve these projects. The liquid cell is a simplified version without heating ability but can be mounted on the beamline sample transfer system. A few experiments utilizing the liquid cell have been conducted with promising results. One work that has yielded result is the development of a technique where it is possible to observe nanoparticle motion in aqueous solution in real time. The technique is coherent x-ray scattering based and has possibility to be used in other systems. We are currently preparing a paper on our results at this moment.

## Soft X-ray Interferometry

Principal Investigator(s): Andreas Scholl, Sujoy Roy, Ken Goldberg

### *Project Description*

The goal of this LDRD is to develop an x-ray version of Fourier Transform Spectroscopy, x-FTS. Valence electronic states and soft excitations determine the functionality of a material, the nature of ordering and of phase transitions, the time scale of fluctuations, and the catalytic activity of surfaces. Often nanoscale information is needed and nanoprobe x-ray absorption and x-ray scattering are elemental tools that allows us to measure electronic structure and shallow excitations with element, site and symmetry selectivity.

Interferometric methods will give us access to spectroscopic phase contrast, allowing us to directly measure the real part of the complex index of refraction and thereby the electronic, chemical and magnetic properties of a material. Phase-sensitive interferometry should give exquisite sensitivity and the technique will be used for dilute systems and to measure small effects, such as spin accumulation. Using zoneplates as beamsplitters, nanoscale spatial resolution will be automatically built into the technique and we will profit from any brightness upgrade of the synchrotron source. Fourier transform methods will also enable ultra-high resolution resonant spectroscopy with sufficient resolution to measure soft excitations, for example those related to phonons, magnons or Cooper pairs, and they should surpass the energy resolution that can be achieved using dispersive optics.

### *Accomplishments*

We developed an interferometric setup at ALS beamline 12.0.2, which is based on a pair of sub-micron slits integrated into x-ray transmissive samples to create two overlapping and interfering wavefronts on an x-ray sensitive 2D detector. Registration and intensity of the fringe pattern encode the complex optical properties of the sample, the absorption and the refraction coefficient, which are thereby measured in parallel. We have extensively modeled the setup and the expected experimental data in order to a) compare simulated with experimental data, to b) project the expected sensitivity of the measurements, and to c) understand random and systematic measurement errors. This modeling showed that exquisite sensitivity can be reached but that the mechanical stability requirements are very high, requiring a very stable setup.

We developed metal deposition and FIB techniques at the LBNL Molecular Foundry to manufacture accurately shaped sub-micron slit patterns on silicon nitride membranes and conducted demonstration experiments on FeGd samples. We build a test set up at ALS beamline 12.0.2 by modifying existing equipment. We conducted experiments on magnetic FeGd multilayers as function of energy and magnetic field. Setup and sample allow us to monitor the varying x-ray optical properties of the material and determine its magnetic and electronic state via XMCD and NEXAFS. In order to analyze the data and determine the energy dependent complex index of refraction, we have developed methods based on Fourier transform and autocorrelation techniques that allow us to interpret the 2D fringe patterns. The analysis of the data is ongoing. We are continuing these experiment and are developing an advanced setup using a zone-plate nanofocus setup, which will allow us to conduct interferometric experiments at much higher spatial resolution.

## High-dimensional ptychographic imaging for studying nanoscale dynamics, chemistry and morphology at the ALS and ALS-U

Principal Investigator: David Shapiro

### *Project Description*

The Advanced Light Source (ALS) has established itself as the world leader in ptychographic imaging by achieving the highest resolution ever recorded and demonstrating spectro-microscopy with nanoscale resolution in the study of chemical phase transformations in battery electrode materials. We have developed a powerful capability which is unique in the world, however, new experimental and computational methods are needed in order to address the reality that soft x-rays have limited depth of field at high spatial resolution and thus cannot achieve high resolution when imaging three-dimensional structures using standard methods. The limited depth of field removes one of the key advantages of x-ray microscopy, long penetration depth. In order to take full advantage of optimized x-ray beamlines at the ALS and ALS-U we will develop experimental and analytical methods for ptychographic imaging of chemically heterogeneous and three-dimensional systems at high spatial resolution. These techniques will be particularly important for *in situ* microscopy of materials in an enclosed medium such as electrochemistry in functional batteries or hydration reactions. The ability to image complex structures at high resolution is an essential tool for materials science and this proposal will bring that tool to the energy sciences through the x-ray ptychographic microscopy program at the new COSMIC imaging beamline.

### *Accomplishments*

Working with the ALS detector group we have optimized our data acquisition system for high-resolution coherent x-ray diffraction measurements. Currently, our prototype ptychographic microscope is commissioning at a low brightness x-ray bend magnet beamline but will be moved to the very high coherent flux COSMIC beamline in early 2017. At the current beamline, high-resolution measurements can be achieved with very long dwell times. Such measurements are therefore possible but practically challenging. Regardless, using various nano-material systems we have experimentally verified the presence of limited depth-of-field in our ptychographic reconstructions as resolution is increased. This effect presents itself as defocus artifacts when imaging extended objects and ultimately limits the reconstructed resolution in both two and three dimensions.

Utilizing multi-slice ptychographic reconstruction algorithms, which account for sample depth effects, we have shown the ability to computationally extend the depth of field of our images and enhance the resolution of reconstructed projections. We have applied our advanced analysis to the study of self-assembled nano-porous SnO<sub>2</sub> battery anode materials. We are able to clearly resolve the complex internal morphology of four materials with different preparation protocols. The addition of a polymer during synthesis by spray pyrolysis results in different final morphologies which depend upon the polymer concentration with high concentrations leading to a highly nano-porous architecture ideal for battery anode applications. Using our ptychographic tomography methods we are able to observe the change in nano-morphology with the increase of polymer additive concentration and we are able to quantify the porosity of the ideal porous material. Other imaging methods either do not have the spatial resolution to visualize the porosity (visible light, conventional x-ray microscopy) or cannot penetrate through useful volumes of material (electron microscopy).

## INTERFACIAL CHEMICAL KINETICS VIA PATTERN-ENHANCED IN-SITU SOFT X-RAY SCATTERING

Principal Investigator(s): Cheng Wang

Co-Investigator: Isvar Cordova, Alexander Hexemer, Sujoy Roy, Jinghua Guo, Wanli Yang,  
Howard Padmore, David Prendergast, Adam Weber

### *Project Description*

This project explores the physical limits of using resonant scattering to probe nanoscale interfaces by developing model patterned electrodes to enhance the scattering signal sensitivity at a specific  $q$ -value. The goal of this enhancement is to enable *in-situ* spatiochemical probing that will provide deeper insights into interfacial chemical kinetics that are key to understanding many of the basic phenomena at the heart of chemistry, biology and materials science. Most of the strides that have been made in the latest *in-situ/in-operando* characterization techniques operate on timescales that can only probe a system at steady state; thus prohibiting the detection of the non-equilibrium transient behavior that governs its chemical kinetics. The ability to bridge this temporal gap without sacrificing nanoscale sensitivity will lead to a fundamental understanding of properties such as reactivity, stability, and strength, and allow us to define models that aid in the design of the next generation of complex energy materials and devices.

To address these challenges, we are harnessing the world's first Resonant Soft X-Ray Scattering (RSoXS) beamline. RSoXS is an appealing characterization technique because it exploits X-ray absorption transitions (*i.e.*, spectroscopy) to enhance the X-ray scattering cross section of a given material in order to produce statistically significant combined chemical and morphological information over a relatively large sample area. However, most scientific queries that call for *in-situ* characterization are interested in studying dynamics at a given interface, a region where the scattering volume is typically much smaller relative to the bulk. This makes interfacial structure very hard to probe without enhancement from an ordered superstructure (*i.e.* long-range periodicity). Since most samples of interest to the *in-situ* research community do not possess an interface with well-defined intrinsic long-range periodicity, we propose to test model systems with pre-defined geometries or patterns.

### *Accomplishments*

The key to producing RSoXS signals strong enough to monitor morphological and/or chemical changes taking place at the interface *in-situ* is in optimizing the design and nanofabrication of the patterned samples. Therefore, our first efforts were devoted to modeling the scattering patterns that we could expect for simple line grating structures in order to optimize the scattering signal from the interfacial regions. Given a high-quality line grating pattern with 50 nm linewidths and 100 nm pitch, our models predicted that we would be sensitive to sub-nm structural changes at the interface and that we could expect a dramatic change in signal intensity as we approach resonant absorption energies the chemistry of the surface/interface in such a line grating is different from that of the bulk.

Experimentally, we have successfully fabricated these line patterns and used them to detect the native oxide surfaces of various transition metal oxides with sub-nm precision and using short exposure times. Concurrently, we have also finalized the development of a specialized holder that will enable all the forthcoming *in-situ* RSoXS characterization with these patterned samples. Two manuscripts reporting these results for peer-review are currently in preparation.

## Identifying Bioactive Compounds across the Tree of Life: In Bacteria, Plants, and Human Organoids

Mina J. Bissell, Aindrila Mukhopadhyay, Ben Brown, Jennifer Mortimer

**Description:** Using existing assays (as well as some newly developed) to discover beneficial or toxic effects of compounds in JBEI and to develop platforms for bioactivities of compounds across phylogeny.

**Accomplishments:** p-coumarate, protocatechuate (lignin derived intermediate from plant biomass), Ethyl methyl Imidazolium Acetate and Cholinium Lysinate ([EMIM][OAc] and [Ch][Lys] , ionic liquids used in pretreating plant biomass) and limonene,  $\alpha$ -pinene (a final product of biomass bioconversion) were tested across microbial, plant and human platforms for specific bioactivities. Results as follows.

**Bacteria:** Sixteen strains of *Arabidopsis thaliana* root microbial community were measured for growth response and morphology upon treatment with the compounds. Tests were performed at 4-5 different concentrations in biological triplicate and technical replicates. We identified a set of microbes where significant growth effect was observed. Pilot studies were performed to identify microbial pairs that had beneficial or inhibitory interaction. An agar plate-based assay was also developed to examine the synthetic lethal phenotypes. Key strains were isolated and cultured for resequencing, and future research.

**Plants:** A synthetic ecosystem of *A. thaliana* (a model dicot system), and a subset of its rhizobiome was developed to screen the selected chemicals. *A. thaliana* was treated individually, and in co-culture with individual rhizobiome members. Assays were conducted in biological replicates of  $n \sim 30$ , as is required in plant assays. The effects of treatment with multiple concentrations of each chemical were characterized as well as co-inoculation with soil bacteria to examine toxicity of a given chemical e.g. ionic liquids. A microbial strain was identified that can ameliorate the effects of such detrimental chemicals in *A. thaliana* seedlings. The compound/microbe regimes were also performed with *Sorghum bicolor*, a monocot system.

**Human:** Compounds were tested in cell culture assays in both conventional 2D substrata and in a physiologically relevant 3D 'reversion assay' and 'therapeutic assay', which faithfully models a multicellular tumor *in vivo*. This therapeutic assay was developed further for testing normal and malignant breast cells in 3D to see if compounds could have beneficial or toxic effects by either eliminating or 'reverting' cancer cells. Although R-Limonene and  $\alpha$ -Pinene belong to the same category, they exhibited differential effects in the therapeutic assay; R-Limonene showed notable killing activity of cancer cells whereas  $\alpha$ -Pinene did not. We found also that  $\epsilon$ -Caprolactam caused cytostatic/cytotoxic effect in cancer cells, suggesting it is a promising candidate for breast cancer therapy and that ionic liquids, [EMIM][OAc] and [Ch][Lys] caused a pro-apoptotic effect in normal and cancer cells, suggesting they may cause harmful effects. A patent disclosure on this sensitive assay is being prepared, as it can serve as a novel high throughput-screening platform for efficacy validation of bioactive compounds.

**Computational Analysis:** 16S targeted sequencing data was used to confirm microbial strain identity. Interestingly, several strains did not correspond to their expected identities. A nonparametric testing framework was developed to identify chemical perturbations that resulted in significant changes in growth profiles of microbes. Preliminary Nanopore sequencing and assemblies for 15 isolates are available, including 3 high-priority strains exhibiting mitigation of toxicant effects on plant root growth. A semi-manual root analysis pipeline was implemented for plants. A multi-feature image segmentation platform for the analysis of human culture data was implemented that reproducibly identifies shifts in cell-community morphology. A pipeline for co-assembling long-read Nanopore whole genome sequencing data with Illumina MiSeq data was implemented. These high-quality assemblies will be single contig for core microbial genomes and include assemblies of plasmid/phage DNA and epigenetic modifications. These resources will support future RNA-Seq analysis.

## Impact of gut microbiome on genetic susceptibility to chemically induced colon cancer

Principal Investigator(s): Jian-Hua Mao and Antoine M Snijders

### *Project Description*

The gut microbiome (GM) is known to play important roles in host physiology, health and disease. The significance of common variations in GM composition for disease susceptibility is still poorly understood. However, human studies are challenging because it is impractical to control the subject's environment for long periods of time and hence difficult to test the effect of GM on disease susceptibility. Mouse models offer many advantages because of our ability to control both the genetic and environmental components of risk. Therefore, the long term goal of this project is to exploit the power of mouse genetics, together with Omics analyses to determine the influence of individual variations in gut microbiome on disease susceptibility.

We will use genetically diverse Collaborative Cross (CC) mouse models to investigate the impact of GM on Azoxymethane (AOM)-induced colon tumor susceptibility. A large cohort of 480 CC mice generated from 30 CC strains (16 mice per strain) will receive an intraperitoneal injection of AOM (10 mg per kg body weight) at 8-weeks old once a week for 6 weeks for tumor induction. The gut microbial composition will be measured during the course of the cancer study using 16S microbial profiling of fecal samples. We will determine whether abundance of GM can be correlated with different cancer phenotypes, such as tumor number, metastasis, tumor pathology, etc. Then germ-free mice will be inoculated with specific microbial isolates to determine the effect of specific microbes on AOM induced CRC development using an established gnotobiotic resource at LBNL. Global transcriptome analysis of colon tumors will be carried out to identify pathways and gene interaction networks affected by GM.

### *Accomplishments*

406 mice from 20 strains have been treated with AOM (5 mg per kg body weight) and are currently being assessed for tumor development. 168 mice from remaining 10 strains are underway for treatment of AOM and will be monitored for tumor development.

We have discovered that **1) CC strain dependent acute toxicity after standard AOM regimen:** 5 of 14 CC strains exhibited toxicity to AOM treatment at standard dose (10 mg per kg body weight). We have identified three genetic loci that control such AOM toxicity. No toxicity was observed in any of the 20 CC strains when the dose was reduced to 5mg/kg.

**2) impact of gut microbiome on memory and anxiety:** All mice have been individually tested for anxiety (open field assay) and memory (passive avoidance assay) prior to AOM treatment. We have found that the abundances of Lactobacillaceae and RF36 are significantly positively correlated with memory. In addition, using gnotobiotic mice, we have confirmed that probiotic treatment of germ-free mice with different species of lactobacillus significantly improved memory. **A related patent has been filed.**

**3) AOM induced change in composition of microbiome is strain dependent:** Freshly produced fecal samples were collected prior to the first injection and 24 hrs after the last injection. The gut microbial composition was measured using 16S microbial profiling. We observed relative abundance shifts and alterations in phylotype composition of the dominant bacterial orders *Clostridiales* and *Bacteroidales*. *Clostridiales* decreased and *Bacteroidales* increased.

**Biosurfactant Production by Engineering Microbial One Carbon Conversion**

Principal Investigator(s): Steven Singer

*Project Description*

Direct microbial conversion of gaseous one carbon feedstocks ( $\text{CH}_4$ ,  $\text{CO}/\text{CO}_2 + \text{H}_2$ ) is an attractive approach to generating biofuels and bioproducts. Petroleum production often generates large amounts of associated natural gas containing large amounts of  $\text{CH}_4$  that is flared. This waste natural gas could be converted into biosurfactants, which are currently used to enhance oil recovery in mature petroleum reservoirs. Rhamnolipids, have been shown to be particularly effective biosurfactants in applications from petroleum recovery to crop protection and soil treatment and have been discussed as a replacement for currently produced synthetic surfactants. However, rhamnolipids are produced from organic substrates and are too costly to be employed. The overall goal of this proposal is to produce rhamnolipids from  $\text{CH}_4$  and develop the capability at LBNL to grow bacteria on gas substrates to generate biofuels and bioproducts.

*Accomplishments*

We obtained *Methylobacterium alcaliphilum* 20Z and demonstrated growth on plates and in liquid culture using methanol. Robust methanol growth enabled rapid genetic manipulation in the lab and the construction of vectors for rhamnolipid producing strains. We established a set-up to grow the strains of *M. alcaliphilum* on methane in collaboration with LBNL ES and H. We have established LC-MS conditions for detecting the production of rhamnolipids and transformed *E. coli* strains with the rhamnolipid biosynthesis genes that we will use to produce standards for detecting the products. We have established a collaboration with San Diego State University to accelerate both methanotroph strain engineering and develop techniques for methane cultivation.

We were able to obtain two grants from the Energy Biosciences Institute sponsored by Shell Oil related to this LDRD. Both of these grants rely on data and background produced during the first year of this LDRD.

## **URBan Integrated System (URBIS)**

Principal Investigator(s): Tianzhen Hong, Michael Wetter

### *Project Description*

More than two-thirds of people in the U.S. live in urban areas, where most buildings and infrastructures are aging. Cities are facing growing challenges of retrofit and expansion to increase operational efficiency to reduce resource use and GHG emissions, and to meet sustainability goals and improve resiliency to combat nature extreme events. We propose to design and develop a data and computing platform to support urban systems research and development. The platform enables city stakeholders to make holistic and quantitative decisions considering complexity and opportunity of urban systems.

We will build the foundation of data and workflow automation, and integrate existing urban data models, energy modeling and optimization tools into the platform using open standards, i.e., Modelica for district energy simulation, Functional Mockup Interface (FMI) for co-simulation and CityGML for 3D city models. We will also explore the concept of emergent behavior, how a group of buildings together can have potentially much lower energy use than the simple sum of individual building performance. We will demonstrate the usability of the URBIS platform through: (1) retrofit analysis of buildings in a city block that reduces their energy use by up to 40%, and (2) an optimal design and operation of low-exergy district energy systems that targets energy savings of up to 40%.

### *Accomplishments*

Our most significant accomplishments include: (1) development of the City Building Energy Saver (CityBES) which builds upon CityGML and open city data that can model every building in cities and visualize their performance. CityBES is used for retrofit analysis of 940 commercial buildings in Downtown San Francisco that achieve 30-50% energy savings; (2) CityGML datasets breakdown in 15 planning districts for City of San Francisco covering its entire building stock; (3) development of agent-based distributed control for bidirectional district energy systems that reduce energy cost by 13% to 40% compared to the same district energy systems with conventional control, and that allow modular extension of district energy system, (4) quantification of exergetic efficiency of bi-directional district energy systems vs. conventional systems as a function of load diversity and system size.

We assessed for what load diversity and system size bi-directional district energy systems are exergetically favorable to individual heating and cooling at each building, and compared this metric to load diversity of different mixed-use districts. We participated in and co-led the Global City Teams Challenge Energy SuperCluster, and contributed several studies to the development of the white paper on city energy.

We also launched a journal club to read and discuss research articles on urban sciences. A direct follow-on funding has been achieved through the DOE exascale computing project, multiscale coupled urban systems (ramping up in FY18).



## **Advancing Clean Energy Innovation Decision Science**

Principal Investigator: Margaret Taylor

### *Project Description*

Technological change is driven by private sector actions such as research, development, design, and marketing, in the pressure of economic competition. It is also shaped by public policies and programs, particularly when the technologies in question support public goals like a clean environment or national security. This project uses scientific methods to better understand how private and public actions affect the way that “clean” energy-related technologies are invented, incorporated into commercial designs, and adopted by consumers and businesses. As this understanding is of particular interest to decision-makers interested in facilitating innovation, we coin the phrase “clean energy innovation decision science” (CEIDS) to represent the body of knowledge that this research contributes to.

This project focuses on two main activities that advance CEIDS theory and empirics. The first activity is the development of an empirical platform designed to enhance the research of the broader community of CEIDS scholars by reducing the transaction costs associated with theory creation and empirical testing. The second activity is the development of new theory on when regulation might enhance versus constrain innovation with outcomes of relevance to a product’s cost and quality.

### *Accomplishments*

For the first activity, the project team has assembled data that are pertinent to the three most prominent market failures that economic theory considers to be relevant to public action in the distinct domains of clean energy and innovation: the negative externality of pollution; the positive externality of knowledge spillovers; and the complicating influence of market concentration. The team has designed an organizational structure through which that data will be accessible through a simple online information system focused on the value chains of technologies that compete with each other to supply U.S. power markets. These focal technologies are natural gas power plants, onshore wind turbines, and utility-scale photovoltaic systems. The information provided in the online platform include data on each value chain step’s strategic conditions, performance and cost trends, and approaches to capturing the returns to knowledge creation.

For the second activity, the project team conducted a systematic assessment of cases of regulation and innovation on which to build theory and has begun the process of economic theory-building and empirical theory-testing. The case assessment took two forms: a review of the academic literature on cases in which *ex ante* regulatory cost and/or performance projections differed from *ex post* outcomes; and an analysis of OMB compilations of “economically significant” regulations dating back over twenty years. In its assessments, the project team focused on cases in which both non-regulated quality improvements arose after regulation and in which there was variation with respect to the scalability of the technical compliance options involved. For the first phase of theory-building and empirical theory-testing, the team selected domestic appliances that are subject to minimum efficiency performance standards. We are now in the process of establishing the most promising mathematical models to build from and in cleaning relevant cost and quality data.

The team has also secured funding for a complementary vein of CEIDS research which involves a novel application of discrete choice analysis in order to enhance the diffusion of a public administration innovation – streamlined permitting for clean energy technologies.

## In Situ Multi-modal Probing of Chemical Reactions via Windowless Micro-reactors

Selim Alayoglu, Stefan Minasian, Don Tilley, John Hartwig, Musahid Ahmed

### *Project Description*

Earth-abundant first-row transition metals have the potential to replace toxic and expensive precious metals in many energy-related applications for homogenous catalysis. However, incompatibilities with conventional experimental methods have thwarted mechanistic studies, and have prohibited rational development of catalysts with improved activity, selectivity and versatility. For monitoring homogeneous catalytic transformations in the liquid phase, we proposed deployment of micro-droplet reactors coupled to spectral methods using X-ray synchrotron radiation, mass spectrometry and optical-laser based spectroscopies. The novel windowless reactor design enables simultaneous application of mass spectrometry as well as IR, UV/Vis, and X-ray absorption spectroscopy (XAS). The entirely windowless configuration is particularly advantageous for detection of intermediates or other low concentration species using soft X-ray radiation, where use of windows could render spectroscopic detection difficult. The proposed reactor scheme generates micro-droplets that are 100-500  $\mu\text{m}$  in size at the tip of capillary tubes under controllable gas atmospheres (non-polarizable light gases such as He and  $\text{H}_2$ ). This micro-droplet reactor scheme will be employed to probe low-Z elements at the K-edge as well as core level transitions of the first-row transition metals. By such a multi-modal probing of catalytic transformations in micro-reactor environments, a refined mechanistic picture of catalytic chemistry could be determined, and used for experimentally-led rational design of next generation catalysts and catalytic networks.

### *Accomplishments*

The synergistic effort has encompassed organic and inorganic synthesis, synchrotron instrumentation, and spectroscopy. We initially designed and built a microdroplet reactor which serves as an experimental chamber to generate flowing micro-droplets and to measure XAS spectra from liquid solutions. Preliminary results were obtained at O and Mg K absorption edges from aqueous solutions of  $\text{Mg}(\text{NO}_3)_2$  using continuously flowing micro-droplets at the ALS. For tender X-rays, Pd  $L_3$ , Cl K and Co K absorption edges were successfully monitored.

We have explored aryl silanes ( $\text{Ph}_n\text{SiH}_{4-n}$ ;  $n = 0-4$ ), which are involved in a wide range of organic transformations including as substrates in the catalytic hydrosilation of unsaturated carbon-carbon and carbon-heteroatom bonds. Our approach utilized a scanning transmission X-ray microscope (STXM) and employed microfluidic solution cells with ultra-thin windows to overcome challenges in the measurement of  $\text{Ph}_2\text{SiH}_2$  and  $\text{PhSiH}_3$ , which are non-conducting organic compounds and liquids at room temperature. Spectral assignments were confirmed using time-dependent DFT calculations, which allowed for comparison of transitions into directly comparable excited states for each of the silanes. The experimental and theory results provided unique insight into periodic trends in electronic structure and orbital mixing for a series of aryl silanes, and demonstrate a spectroscopic approach that may be useful for studying hydrosilation catalysts, intermediates, and substrates. Accordingly, preliminary work has begun to measure the Si K-edge spectra of compounds with reactive silylene functionalities ( $\text{M}=\text{Si}$  double bonds) that have been implicated in hydrosilylation catalysis. Si K-edge XAS was used to characterize the silylene functionalities, which revealed a low energy Si  $1s \rightarrow \pi^*$  transition in the Si K-edge XAS that may be a signature of the  $\text{M}=\text{Si}$  bonds.

## Gas-Phase Ion Chemistry of Late Actinide and Early Transactinide Elements

Principal Investigators: John Gibson, Kenneth Gregorich, Jacklyn Gates, David Shuh

### Project Description

The chemistry of an element is characterized by its propensity to form bonds with other elements, which underlies the organization of the periodic table. For metals (M), chemistry is dominated by compounds with light atoms (X) such as oxygen, nitrogen and halogens. Bond dissociation energies (BDEs) to cleave M-X bonds provide fundamental chemical insights. Dominant metal oxidation states are determined by their ionization energies (IEs), which indicate the ease of electron removal. The chemistry of the 3d/4d/5d transition metals and 4f lanthanides are generally well-established and fit within the known framework of the periodic table. For the late 5f actinide (AN) elements, Fm<sub>100</sub> to Lr<sub>103</sub>, and the transactinide (TAN) 6d elements, Rf<sub>104</sub> to Cn<sub>112</sub>, there are no known BDEs and only one measured IE. The very low first IE of Lr was determined as 4.96 eV; no other IEs have been reported. Experimental constraints have limited studies of the chemistry of the late AN and TAN elements to elementary solution behavior, and the synthesis/volatility of a few elements and compounds. No<sup>2+</sup> in aqueous solution, identified at LBNL in 1968, indicated divalent character of No. Theoretical efforts have focused on understanding limited experimental properties, such as the volatility of RfCl<sub>4</sub>. Other than the first IE of Lr, there have been no measurements of BDEs or IEs for late AN and TAN compounds and atoms. The utility of computations is constrained by the absence of experimental evaluations.

The goal is to employ a unique capability at LBNL to study gas-phase reactivity of short-lived AN and TAN isotopes, produced and studied *in situ* on an atom-at-a-time basis. Reactivity results will reveal new chemistry, and provide key physical (IE) and chemical (BDE) properties.

### Accomplishments

The apparatus was commissioned and its overall performance confirmed. Effective recoil ion transmission and mass resolution was demonstrated for <sup>200</sup>At<sup>+</sup> and <sup>201</sup>At<sup>+</sup> produced by bombarding a <sup>165</sup>Ho target with <sup>40</sup>Ar, resulting in the release of 5 or 4 neutrons, respectively, i.e., <sup>165</sup>Ho(<sup>40</sup>Ar,4/5n)<sup>201/200</sup>At. A key chemistry accomplishment was demonstration of the overall feasibility of the proposed atom-at-a-time ion-molecule reaction approach with the reaction of Ho<sup>+</sup> with O<sub>2</sub>. Online production of <sup>151</sup>Ho<sup>+</sup> at the 88 inch cyclotron was from the nuclear reaction <sup>115</sup>In(<sup>40</sup>Ar,4n)<sup>151</sup>Ho. It is known from conventional studies with stable Ho isotopes that the following chemical reaction is exothermic and occurs spontaneously under the near-thermal conditions in a quadrupole ion trap: Ho<sup>+</sup> + O<sub>2</sub> → HoO<sup>+</sup> + O. This reaction, specifically the HoO<sup>+</sup> product, was observed by FIONA after introduction into the ion trap of O<sub>2</sub> along with Ho<sup>+</sup>. The known absolute rate constant for this pseudo-first order reaction provided a reagent pressure calibration from the HoO<sup>+</sup> product yield as a function of the O<sub>2</sub> flow rate and the reaction time.

Having demonstrated the utility of the methodology and performed calibration of the apparatus, the first new heavy ion-molecule reaction was studied: No<sup>+</sup> + O<sub>2</sub>. This reaction did not result in NoO<sup>+</sup>, this in contrast to the reactivity behavior of most of the homologous 4f lanthanide elements such as Ho<sup>+</sup>. The demonstrated low stability of NoO<sup>+</sup>, in which the oxidation state would be No(III), validates the characterization of No as a divalent element. This is the first direct study of the reactivity of No or any AN beyond Es, and will lead to reactivity studies of other heavy AN and TAN elements with O<sub>2</sub> and other reagents. The initial results with No furthermore suggest that No<sup>2+</sup> does not abstract an electron from O<sub>2</sub>, paving the way for the first determinations of second IEs of late AN and TAN elements.

## Spotlighting Catalysis: *In situ* and *Operando* Characterization of Photoelectrochemical Assemblies

Principal Investigators: Francesca M. Toma, Ian D. Sharp, Mary K. Gilles, Shaul Aloni, Ethan Crumlin

### *Project Description*

This project aims at coupling light into *in situ* and *operando* electrochemical measurement systems, which comprise i) photoelectrochemical atomic force microscopy (PEC-AFM), ii) scanning transmission X-ray microscopy (STXM), and iii) ambient pressure X-ray photoelectron spectroscopy (AP-XPS). We leverage recent advances in *operando* electrochemical characterization to extend these approaches to photodriven chemical transformations and study heterogeneous photocatalytic reactions at the nanoscale. The combination of these methods will enable unprecedented access to catalytic mechanisms, dynamic chemical and morphological transformations, and photocorrosion processes at the nano and mesoscale level, ultimately enabling mechanistic insights that will guide materials design and improve performance.

### *Accomplishments*

To accomplish our goal, we have demonstrated a multimodal approach involving PEC-AFM, AP-XPS, and STXM. Specifically, we have mapped the correlation between morphological and functional heterogeneity in bismuth vanadate ( $\text{BiVO}_4$ ), the most promising metal oxide photoanode for photoelectrochemical water splitting, by photoconductive atomic force microscopy. We have demonstrated that the image contrast in conductive mapping depends on the Schottky barrier, trap-related effects, and the geometric field enhancement at the interface between the probe and the photoanode. We have found that the transport mechanism can be attributed to space-charge-limited current with the presence of trap states, and that this material is highly defect tolerant with no additional recombination sites at grain boundaries.<sup>1</sup> In addition, we have studied independently the effect of humidity, oxygen level, and illumination wavelength on photo-carrier transport and trapping/de-trapping of defect states on  $\text{BiVO}_4$  photoanodes,<sup>2</sup> thus providing unprecedented control over experimental parameters that determine functionality. Our analysis demonstrates that unraveling charge transport mechanism at the nanoscale is necessary for the rational design of novel energy conversion systems.

With a combined electrochemical AFM/AP-XPS multimodal approach, we have studied a polycrystalline platinum surface at the electrified solid/liquid interface under oxygen evolution conditions. With this unique approach, we have elucidated previously inaccessible aspects of the surface chemistry and structure as a function of the applied potential, allowing us to propose a reaction mechanism for oxygen evolution on a platinum electrode in alkaline solutions.<sup>3</sup>

Finally, we have characterized chemical heterogeneity *ex-situ* in  $\text{BiVO}_4$  by monitoring V L-edge and O K-edge on pristine samples and as a function of the corrosion process by STXM and photoemission electron microscopy to gain bulk and surface information.<sup>4</sup>

## PROBING REACTIVE INTERMEDIATES IN MICROENVIRONMENTS

Principal Investigator(s): Kevin R. Wilson and Frances A. Houle

*Project Description*

Chemistry confined in micron-sized compartments is of central importance for biology (cells), geochemistry (mineral pores), atmospheric chemistry (aerosols), and potentially for the development of new catalytic methods. There is compelling evidence that when reducing the reaction vessel to micron dimensions, bimolecular reactions speed up by several orders of magnitude. The molecular origin of this acceleration is unclear, thus providing a compelling basic science need to understanding how compartment features (surface vs. bulk) control chemistry in microenvironments.

This work seeks to understand why bimolecular reactions are accelerated in microenvironments by:

1. Developing a high velocity droplet collision reactor, with sub-microsecond inertial mixing times, to directly observe transient intermediates, which will clarify how confinement perturbs bimolecular reaction in liquid microenvironments.
2. Combining experimental measurements of kinetics, products and reactive intermediates with spatially and temporally resolved stochastic kinetic simulations to understand how surface and bulk reaction sites, diffusion, and surface charge state control reaction mechanisms in droplet microenvironments.

*Accomplishments*

Our most significant accomplishment has been to develop two experimental platforms that allow bimolecular liquid phase reactions to be initiated by a binary droplet collision. The first system is based upon a novel branched quadrupole electrodynamic balance. In this trap the droplets are oppositely charged to ensure a collision. The resulting fused droplet can then be re-trapped (by its excess charge) and held for a fixed reaction time after which it can be ejected into a mass spectrometer. We are currently using this setup to measure how mixing times depend upon droplet size and velocity. This is done by initiating a rapid pH jump as the droplets collide, which quenches the fluorescence of a Rhodamine 610 dye. We have observed mixing times in the range of 60-70  $\mu$ s, which is much faster than can be achieved using a conventional stopped flow apparatus (~0.5-1 ms).

A second droplet reactor with much faster inertial mixing times is currently being tested. The design for this second reactor draws heavily on F. Houle's modeling results and her detailed analysis of previous designs. In this reactor high velocity droplet collisions in free space allow rapid and reproducible mixing for the study of a number of test reactions. We used this reactor to demonstrate that we could quantitatively measure the reaction of OH radicals with a fluorescence dye. Efforts are currently underway to measure mixing times in this setup and to construct a suitable mass spectrometer interface to examine short lived reactive intermediates.

## HARNESSING THE SOIL MICROBIOME FOR FOOD AND FUEL SECURITY

Principal Investigator(s): Eoin Brodie, Peter Nico

### *Project Description*

Current crop yields need to be nearly doubled on a global scale to meet growing population demands; including increased utilization of marginal lands and better management of fertilizer inputs (Vance et al., 2003; Cordell et al., 2009). Phosphorus (P) is one of the most limiting plant nutrients, with yields on 30-40% of the world's arable land limited by P availability (Runge-Metzer, 1995). P deficiency is largely due to poor mobility of inorganic P in soil solutions, making it largely inaccessible to plants (Hinsinger, 2001). During soil formation and aging (pedogenesis) P transitions from a mineral form to a labile form that is available for plant uptake. However much of the labile P can be sorbed onto the surfaces of soil particles, immobilized into soil organic matter, or incorporated into recalcitrant inorganic forms. These processes result in eventual depletion of mineral P and labile P with an accumulation of the occluded and organic forms of P that are not accessible to plants (Izquierdo et al., 2013).

The soil microbiome has evolved the capacity to mine critical nutrients for its own benefit and potentially that of other system inhabitants, such as plants. This project aims to gain an understanding of the microbial mechanisms of soil phosphorus (P) solubilization and how those mechanisms can be harnessed and developed into robust plant-soil-microbe associations that deliver P to bioenergy crop plants growing on marginal lands.

### *Accomplishments*

Previously at the nutrient limitation observatory at the Ecological Staircase in Mendocino Co. we identified phytic acid as the primary organic form and that its availability was regulated by complexation with iron. This overlooked mechanism may be a key constraint on terrestrial productivity in much the same way as iron-carbon complexes regulate carbon stabilization in soils. We have proven in the laboratory that iron complexed phytic acid is not accessible to phosphorus hydrolyzing enzymes but that the addition of common organic acids (oxalate, citrate, malate) as well as microbial iron chelating compounds (siderophores) release the phytic acid allowing enzyme activity to proceed (a manuscript is currently in preparation). We have characterized these mechanisms in 24 of the most effective P solubilizing bacteria that we isolated and have sequenced their genomes and identified many of the pathways involved (a manuscript is currently in preparation). A new collaboration with scientists at EMSL was established to search for the siderophores in soils across the Ecological Staircase. We developed an assay to determine the amount of P that could be released by these mechanisms in soils and have tested it at the Ecological Staircase. This assay is now being adapted to other soils with a view to a new soil testing product. Our hyperspectral method for detecting P limitation/status in plants has been tested successfully on switchgrass crops in lab, greenhouse and field tests and a manuscript is in preparation.

With new knowledge of metal-organic P forms we are designing new consortia of microbes that first dissolve iron and then hydrolyze phytic acid for plant uptake, combined with complementary microbes that solubilize P from aluminum minerals. These consortia will be tested at the greenhouse scale using bioenergy feedstocks (Switchgrass and Sorghum) and a food crop with a high P demand (Soy).

## **The Soil Metazoan Microbiome: A compartment of importance to soil nutrient cycling**

Principal Investigator(s): Javier A. Ceja-Navarro

### *Project Description*

In soil ecosystems, different bacterial, archaeal, and eukaryotic organisms interact and mediate the inputs of organic matter and the availability of key substrates, including phosphorous and nitrogen, thereby controlling biogeochemical cycles. Although bacteria and fungi are numerically the most abundant organisms, they represent only a fraction of the soil's total biomass that also includes protists, nematodes, and arthropods together with their associated microbiomes. These "other" eukaryotic populations represent important biological compartments that are both diverse and numerically significant, and collaborate above and below the soil surface. They facilitate nutrient and energy transfer, which in turn impacts the composition and activity of the soil microbiome and the productivity of vegetation.

The main goal of this project is to study of metazoan-associated microorganisms and the "other" components of the soil food web, with the application of a multi-scale approach that will enable the characterization of the contribution of soil metazoans, and their microbiomes to nutrient cycling, and a better understanding of the conditions in which the associated microbiomes are active.

We have studied the diversity of arthropods in the soils of the Ecological Staircase in Mendocino, CA and the composition of their associated microbial communities. For this, developed a strategy for the isolation of DNA from single arthropod specimens (100 microns and higher) in high-throughput mode that allows the extraction of 90 specimens at once. As part of our survey, we also worked on the isolation of plant polymer degrading and nitrogen fixing microbes from selected groups of arthropods that will later by use to test for the association between host and symbiont. This study has also moved towards the characterization of nematode and protist populations of the analyzed soils to get a better characterization of the different trophic levels of each environment.

### *Accomplishments*

After optimizing the protocols for DNA extraction in high-throughput we managed characterize the microbiome of 400 isolated arthropod specimens, an accomplishment that represents the largest survey of host-associated microbial communities. The most abundant groups included Collembolans, Mites, Diplurans, Millipedes, Centipedes, and Termites. We succeeded in identifying their associated Bacterial and Archaeal populations by sequencing the 16S rRNA using the Illumina Miseq platform. We have gathered a collection of 200 bacterial isolates from 13 different bacterial species. These bacterial isolates have the metabolic machinery to either or degrade cellulose, lignin, fix nitrogen, solubilize phosphorus. We have also developed approaches to extract nematode and protist from soil and successfully identified their populations in our different studied soils. This work has been presented at the ASIMOLAR meeting of microbial physiologist and allowed me to mentor 2 students from UC-Berkeley and the University of Puerto Rico. Developed approaches by this LDRD have been adapted for the study of other ecosystems of relevance to DOE.

## Ultra High Resolution Climate Projections to Support Climate Readiness in the San Francisco Bay Area

Principal Investigator: Andrew Jones

### *Project Description*

The purpose of this project is to develop the scientific basis for understanding and predicting climate at decision-relevant scales in urban environments. While we have initially used the San Francisco Bay Area as a testbed, we have now extended the approach to three additional major metropolitan areas. The project aim is to conduct ultra-high resolution climate simulations that examine interactions among existing microclimates, modifications to the built environment, energy and water use, and global climate change. The initial simulations using the Weather Research and Forecasting (WRF) model are designed to determine how climate change will affect the risk of extreme heat events and how modifications to the built environment and landscape irrigation could ameliorate or enhance such risks at the neighborhood and regional scales. Urban modifications examined include the widespread adoption of white roofs and diminished water use for landscape irrigation. More broadly, this project will enhance basic scientific understanding of land-atmosphere interactions in urban environments and develop a standing capacity for addressing a range of climate-related urban risks such as flooding due to extreme precipitation, changes in energy and water demands, and changes in air quality.

### *Accomplishments*

Using satellite observations of land cover, albedo, green vegetation fraction, and sea-surface temperatures, we have successfully adapted our urban climate modeling system to the four largest metropolitan regions in California including the San Francisco Bay Area, Sacramento, Los Angeles, and San Diego. We are able to reproduce major features of the present-day urban climates including temporal variations in temperature and evapotranspiration, as well as microclimatic variation across multiple neighborhoods and counties. We have assembled a spatially and temporally dense database of meteorological observations that we are using to further evaluate the model's representation of fog, sea breeze, the effects of topography, and other local-scale features, which are essential for understanding how microclimates will change in response to global climate change and changes to the built environment.

Mesoscale atmospheric processes such as fog and sea breeze represent important processes that drive the characteristics of urban microclimates in coastal zones. To further validate and refine our modeling framework with respect to these phenomena, we have assembled diverse fog observation data sets derived from satellite observations and ground-based observations. Preliminary analysis indicates that the model overestimates fog prevalence in the coastal cities examined. This lays the foundation for further model evaluation and improvement, as well as an analysis of how fog and sea breeze dynamics might shift with large scale future climate change.

Finally, we have deployed the modeling framework to understand climatic controls on the demand for irrigation water in urban environments. Expanding upon our initial analysis of the San Francisco Bay Area, we have shown for the first time that heat mitigation strategies, such as reflective roof coatings known as “cool roofs”, can substantially impact irrigation water demand. We showed that summertime irrigation demand could have been up to 10% lower with widespread adoption of cool roofs over a 15 year period that includes the recent drought of 2012-2014 across the urbanized counties of CA. Conversely, we find that direct reductions in irrigation can enhance the urban heat island.



## PREDICTING THE MAXIMUM RATE OF CARBOXYLATION BASED ON OPTIMAL LEAF RESOURCE ALLOCATION

Principal Investigator: Trevor F. Keenan

### *Project Description*

The purpose of this project is to dramatically increase our ability to understand, from first-principles, the governing drivers of global photosynthesis, and how plants adapt photosynthetic capacity under a changing climate. Photosynthetic traits such as the velocity of carboxylation are known to vary with changes in climate and soil properties. These observed relationships have been included in land surface models through empirical equations. A fundamental mechanistic understanding remains lacking, however, making spatial and temporal extrapolation difficult at best. In addition, the current approach gives little, flawed (through empirical extrapolation), or no consideration for the known acclimation of photosynthesis to changes in growth conditions and climate. Recent advances in the theory of optimal resource allocation, along with technical advances that greatly increase the amount of data available, now provide a path through which to test hypotheses regarding the primary governing controls.

In this project, we propose to use recent theoretical developments to generate testable hypotheses as to the mechanisms governing biotic adaptation of photosynthesis. Ultimately, the project will provide a mechanistic predictive capacity for photosynthesis suitable for incorporation in the next generation of land surface models. This research will thus advance key tools used to quantify and predict long-term ecosystem changes.

### *Accomplishments*

In this second year of the project, our efforts have been focused on further developing and testing the theory from year 1. In 2016, we published a novel database necessary to test the predictions generated from first-principles theory. In developing the plant trait database, we used advanced methods to account for light-dependent trait plasticity through plant canopies, which revealed previously unaccounted-for plant trait relationships. The results, published in *Nature Plants*, represent a significant advancement in the field. In FY17, the new post-doc on the project, Nick Smith, has augmented this database to be the largest database of global measurements of plant photosynthetic capacity.

We have also succeeded in developing a theoretical prediction of photosynthetic capacity at global scales. Importantly, this theoretical prediction relies purely on optimal plant resource use, and does not rely on nutrient availability. It thus overturns a decades-long assumption that nutrient availability determines photosynthetic capacity. The resulting manuscript, led by Nick Smith, is currently in review in a high-impact journal.

In addition to the above we have established significant collaborations with leading researchers both in the US and internationally. These efforts are reflected in the publications listed below. We also have attended both the Ecological Society of America (ESA) and American Geophysical Union (AGU) annual meetings, and convened a session on plant canopies at AGU.

## **Assessing Microbial Functions at Terrestrial-Aquatic Interfaces by Metagenome-Based Metabolic Flux Analysis**

Principal Investigator: Tas Baas, Neslihan

### *Project Description*

This project aims to determine dynamics in microbial populations and functions that control soil carbon and nutrients turnover at terrestrial to aquatic interfaces. Streams receive substantial terrestrial deliveries of organic carbon (tOC). 47-55% of the soil carbon from tropical, arctic or temperate ecosystems is transported into the rivers. tOC was assumed to be recalcitrant to aquatic microbial degradation, however this assumption is now being re-evaluated. Recently, aquatic microorganisms in streams were found to degrade terrestrial carbon and result in a significant CO<sub>2</sub> input to the atmosphere. Discretization of the microbial responses resulting in this feedback fills a big gap in our knowledge. Deciphering microbial responses requires differentiating amongst carbon and nutrient use and fluxes through microbial metabolism which cannot be measured directly and comprehensively. In order to address this bottleneck this project implements a novel metagenome-based metabolic flux analysis (MFA) approach. While via sequencing of community DNA metagenomics enables access to genes and functions, genomes assembled from metagenomes can be used for genome-scale models of cellular metabolism from which metabolic fluxes can be calculated. This project integrates metagenome data to genome-scale MFA in order to generate a next generation analysis approach and provides new avenues for data integration to larger scale modeling efforts.

### *Accomplishments*

Our accomplishments are in multiple folds. We established collaborations in Rocky Mountain Biological Laboratory, CO (RMBL) and set-up sampling locations along East River that were monitored for two consecutive years. Through 2016-2017, we collected river water and hyporheic zone samples to observe changes in microbial community composition and functions via metagenomics. We focused on high to low flow and carbon input periods and flash flood events (i.e. summer monsoon) and developed methods and collaborations to measure tOC inputs. Via HPLC, excitation-emission matrix (EEM) fluorescence spectroscopy (with Colorado School of Mines) and <sup>13</sup>C-NMR (with UC Merced, ongoing) changes in tOC - namely humic acids, sugars and proteins- were identified. In East River, seasonal variations, driven by changes in river discharge rates and tOC concentrations, were major drivers of microbial populations. Microbial communities attached to particulate matter were spatial variable, whereas benthic communities showed strong temporal changes. We are currently in preparation of a manuscript to describing environmental gradients and tOC inputs that shaping microbial communities.

We set up lab-scale incubation experiments with river water fed with <sup>13</sup>C-carbon and humic/fluvic acids. We tracked CO<sub>2</sub> production to calculate the changes in microbial carbon use efficiency (CUE) and DNA synthesis -via thymidine analogue bromodeoxyuridine- within the microbial communities to distinguish between actively replicating and latent/dormant populations. Our analysis showed that CUE differs seasonally where early season tOC input results in CO<sub>2</sub>-fluxes. Our initial 2017 budget request was substantially reduced so to complete planned work we developed a JGI-CSP proposal in which metagenomes and metabolites from these incubations will be analyzed. In parallel to this LDRD, Garcia Martin group published a tool kit named jQMM (Birkel et al., BMC Bioinformatics 2017) that will facilitate MFA analysis. Through the JGI-CSP we will generate <sup>13</sup>C-metabolite and sequencing data for developing genome-scale models from microbial metagenomes and constraining fluxes in MFA.

## REMOTE MONITORING OF SOIL - PLANT RESPONSES TO WATER AND METAL STRESS

Principal Investigator: Yuxin Wu

### *Project Description*

The soil - plant biome is perhaps the most critical entity of both natural and managed ecosystems, which mediate a range of processes important for life and life quality. In spite of its importance, integrated and robust methods to monitor interactions between the soil and plant compartments are limited. Our objective is to develop new sensing methods and joint interpretation approaches to quantify agricultural soil-plant biome responses to water and metal stresses. A better understanding of the soil - plant biome response to water stress and fertilizer soil metal content is critical to the development of future agricultural practice adaptation strategies.

Specifically, we will develop new electrical geophysical and remote sensing methods to sense and quantify key soil and plant traits with a focus on electrical methods and hyperspectral imaging. The key traits of interests include plant root properties, soil metal concentrations and plant canopy properties. In addition to developing the new sensing methods, we will integrate the diverse datasets from multiple methods to identify co-variabilities between the above and below ground traits and explore potential remote diagnostic signatures that indicate the soil-plant biome is approaching a critical threshold in terms of stress response.

### *Accomplishments*

We focused our effort on understanding the electrical signals of corn roots in order to explore a quantitative link between electrical resistance and induced polarization signals and the key plant root traits, such as total root volume, using plant-in-box experiments in both hydroponic and soil settings. A characteristic spectral electrical signal from corn roots was revealed which showed a peak charge relaxation frequency at  $> 1000$  Hz and a large signal magnitude, both of which are much higher than those typically observed for soils. This suggested a relatively simple method to separate the signals between the roots and soils for better root quantification.

In addition to the below ground plant root sensing, hyperspectral imaging of the corn leaves were conducted in parallel to explore leaf nutrient characteristics and the correlation between the root and the hyperspectral measurements. Hyperspectral imaging based quantification of relative concentration of leaf nutrients, including C, N and P, revealed changes of leaf nutrient status during the life cycle of the plants, specifically, the relocation of leaf nitrogen during senescence, which was not observed for phosphorous.

We conducted joint analysis of the electrical signals and the hyperspectral measurements to evaluate their correlation with root traits and their predictability. The results show that while the electrical signals is a good predictor of root properties, adding the hyperspectral measurements improves the results.

These initial results have showed the potential of the new root measurement technology and the joint use of above and below ground plant characterization methods for a better understanding of the behavior of the plant-soil biome. These results will be further developed and used to guide field-based studies in the next phases.

## **Automated Translation of Applications to Large-Scale Programming Systems**

Principal Investigator: Scott B. Baden

### *Project Description*

The purpose of this project is to develop translation strategies to automate the process of reformulating MPI applications to reduce communication overheads and wait times. Due to technological factors, communication costs are increasing with time. Since MPI is the predominant development infrastructure for HPC applications on distributed memory supercomputers, the tools developed in this project could have a broad impact by facilitating code modernization of legacy applications.

The project comprises two tasks. The first task will be to make improvements to an existing translator (Toucan) that reformulates MPI source as a data driven program that overlaps communication with computation automatically. The second task is a new translator to convert MPI source into a PGAS (partitioned global address space) program. This translator will reduce communication overheads for finer grained and irregular communication patterns that are often present in adaptive algorithms. The second translator will rely on developments with the first: it will use some of Toucan's software components and rely on Toucan to establish a performance baseline. Establishing a performance baseline via Toucan is important because it is not practical to manually restructure legacy applications to meet the goals of either translator.

### *Accomplishments*

Toucan's runtime system and translator logic were improved to enable it to tackle a large production code: the Cart3D aerospace design simulator developed for NASA. Communication wait times were reduced between 33% and 55%. Since this code has a large user community (aircraft design at NASA), Toucan now is an enabling technology for modernizing production MPI software.

Subsequent to this work, hierarchical decomposition strategies were developed that enabled Toucan's run time system to support higher levels of overdecomposition to improve pipelining of communication and computation in stencil methods. Overdecomposition subdivides the workload into more tasks than processing cores, but adds communication in the form of memory-to-memory copying of ghost cells. Though this copying occurs within a shared address space, we found that a diminishing point of returns was soon reached, where improved pipelining via increased overdecomposition factors was offset by higher data motion overheads, due to more numerous ghost cells. To reduce ghost cell overheads, we developed a hierarchical partitioning strategy that splits overdecomposed tasks across shared memory, maintaining a low surface to volume ratio of communication to computation. The outcome was a significant improvement in communication hiding (83%), due to the ability to utilize higher levels of overdecomposition (8 times more tasks). We are now developing a strategy for Cart3D, which uses an unstructured mesh.

A postdoc joined the PIs group on 11 September, and has begun developing compact applications both in MPI and in UPC++, a PGAS library under development by the PI's Pagoda ECP Project. The next step is to design the translation algorithm required to restructure the MPI source into a PGAS program and following that, the implement the translator using ROSE.

## **DEVELOPING A SCALABLE SIMULATION AND ANALYSIS FRAMEWORK FOR CMB-S4 ON XEON PHI BASED SUPERCOMPUTERS**

Principal Investigator: Julian Borrill

### *Project Description*

The purpose of this project is to provide critical support to the design and execution of the proposed CMB-S4 Cosmic Microwave Background (CMB) experiment, which will use the fluctuations in the CMB polarization on various angular scales to address a number of questions in fundamental physics ranging from the energy scale of inflation to the number of neutrino species and their mass. In order to achieve the unprecedented sensitivity required to detect these signals CMB-S4 will need both to gather a data set orders of magnitude larger than any previous experiment and to control its instrumental and environmental systematics to exquisite precision.

Building on the tools developed for the Planck satellite mission, we will deploy the massively parallel data synthesis and reduction capabilities needed for the design of the CMB-S4 experiment, the validation and verification of its analysis pipeline, and the uncertainty quantification and debiasing of its final science results. This will include tools to model all significant systematic effects, including both instrumental effects such as beam asymmetry, bandpass mismatch, and auto- and cross-correlated noise, and environmental effects such as galactic and extragalactic foreground contamination, atmosphere, and ground pickup. We will then optimize this framework for the current generation of Xeon Phi based supercomputers currently being deployed at DOE High Performance Computing (HPC) centers including the National Energy Research Scientific Computing (NERSC) Center, in particular focusing on the threading and vectorization challenges posed by its large numbers of low power cores.

### *Accomplishments*

Our most significant accomplishment has been to use 600,000 cores of NERSC's *Cori-2* system to synthesize and reduce the data – including the sky signal, atmosphere, and instrument noise – from an experiment with 50,000 detectors over 7 frequencies observing 25% of the sky for 1 year. This dataset was about 30 times larger than the entire Planck mission data; the full CMB-S4 data will be another 30 times larger still.

This heroic computation required significant new code development, in particular to be able to generate thousands of realistic realizations of the wind-driven atmospheric water vapor respecting the full 2- and 3-D Kolmogorov spectra, and then to observe the sky through them. Each realization corresponded to a single 20-minute constant elevation scan by the telescope, with its own precipitable water vapor level and wind velocity parameters.

It also required a major optimization effort, in particular to transition the code base from tens to hundreds of threads per core while preserving its computational efficiency, and to launch a python-wrapped framework on such a large number of cores, deploying a container-based approach built on the Docker/Shifter paradigm.

We are now extending these capabilities to support realistic observations from any location on Earth using historical weather data, and in particular to generate simultaneous observations from the South Pole and the Atacama Desert, as anticipated for CMB-S4. We are further adding the ability to incorporate beam- and bandpass-mismatch on telescopes with tens of thousands of detectors.

## Exploring the Limits of Low-Energy, Real-Time, Streaming Data Processing with Neuromorphic Computing

Principal Investigator(s): Paolo Calafiura

### *Project Description*

Neuromorphic computing is a low-power, alternative computing framework suitable for certain problems. Kalman filters are powerful mathematical tools used in a wide array of automation and tracking problems. **Our specific goal is to implement Kalman filters in neuromorphic computing platforms for high-throughput, low-power, high-performance computing with continuous outputs.** In year 1, we developed implementations of Kalman filters (KF) in spiking neural networks, achieved state-of-the-art decoding of human brain signals using DNNs, and uncovered critical bottlenecks in mapping software networks to IBM TrueNorth (TN) chip. In year 2, we leveraged recent advances in deep learning to overcome the discovered bottlenecks, and evaluated both software and hardware implementations of neural networks on two domains: charged particle tracking for high-energy physics (HEP), and prediction of movement from neural signals for brain-machine interfaces (BMI).

### *Accomplishments*

In year 1 our most significant accomplishment has been to implement for the first time a multi-dimensional steady-state Kalman filter algorithm in IBM's TrueNorth neuromorphic architecture. The TrueNorth chip encodes data using spikes, and we implemented both a rate-encoded, serial version of the algorithm and a rate-and-spatial encoded, parallel version to reduce latency. The algorithm has been successfully applied to track the time evolution of simple simulated physical systems and the performance of the algorithm has been compared to a traditional numeric Kalman filter, whilst varying a number of parameters, including rate encoding, spatial encoding, sample rate, and the relative ratio of measurement errors and process noise. This allowed us to evaluate the pros and cons of the TrueNorth architecture and its potential in the two science domains we have investigated. We have published our first-year results in Nov 2017. Building in part upon this work, we started a new project aimed at prototyping the applications of deep neural networks to charged particle tracking in HEP. The HEP.TrkX project involves scientists from LBNL, FNAL, and Caltech. Each institution received approximately \$175K of funding in FY17 from DOE ASCR and Comp HEP.

In year 2 we continued developing our TrueNorth Kalman filter algorithm. In terms of science applications, our efforts were focused on BMIs in collaboration with UCSF. Specifically in FY17: 1) we developed a procedure to perform precise numerical linear algebra in spiking neural networks; 2) we identified challenges performing streaming subtraction that are fundamental to a strictly positive code; 3) we derived analytic expressions relating the error in the network to the size of the problem and the amount of space (i.e., energy) on the chip; 4) we successfully applied the TrueNorth Kalman filter to neural data from monkey arm reaching and human pitch production.

We will present our year 2 work at the CoSyNe 18 workshop. We are applying for follow up funding based on this work with the NSF.

## Enabling Extreme-Scale Many-Query Computational Physics

Principal Investigator: Matthew J. Zahr

### *Project Description*

Many-query analyses - from optimization to uncertainty quantification to optimization under uncertainty - quickly become computationally intractable if the underlying simulation requires weeks of computing time on a supercomputer. We focus on the development of fast numerical methods to enable many-query analyses of extreme-scale computational physics problems. The immense potential economic and societal impact of many-query multiphysics applications - such as optimal design of next-generation combustion engines - make these an exciting, rewarding, and challenging class of problems.

The proposed research program aims to contribute numerical methods, and an associated codebase, that will prove useful in solving extreme-scale, many-query multiphysics problems. The research program is split into three modular components: (1) an adaptive, data-driven discretization for faster queries, (2) an improved solver for faster processing of individual queries, and (3) a class of algorithms to recover high-order convergence in the presence of discontinuities where efficient, low-order methods currently dominate. This constitutes a three-pronged approach to reducing the computation burden of many-query multiphysics problems.

### *Accomplishments*

As a result of the LDRD funding for FY17, substantial research output was produced, most notably being publications, code development, and research collaborations. With collaborators at Stanford University and the Army Research Laboratory, I published a journal article that introduces a method to dramatically accelerate multiscale simulations. I also published a book chapter and a conference paper on a numerical framework for using high-order methods to optimize time-dependent partial differential equations. Additionally, we published a conference paper and submitted a journal article on a new method for resolving discontinuous solutions of PDEs, e.g., shock waves, using very coarse high-order discretizations.

In addition to our quantitative research output, the LDRD funding has lead to the formation of a number of collaborations. A MRI research group in Sweden approached us about using our optimization methods to super-resolve MRI via data assimilation. Initial experiments are promising and will result in publications later this year and we will apply for follow-up funding. Additionally, the LDRD funds have lead to collaborations with a number of graduate students and their advisors.

The LDRD funds for FY17 also resulted in two significant pieces of software. *cplib* is a C++ code that integrates arbitrary computational physics applications into a single fully discrete framework. The main functionality includes high-order primal, sensitivity, and adjoint timestepping and supports time-dependent PDE-constrained optimization. *femlib* is a fully differentiated,  $n$ -dimensional finite element library written in C++. It is equipped with a number of single- and multi-physics applications and includes support for a number of multiscale methods as well as shape and topology optimization.

## **ExaGrid: Large-Scale, Asynchronous Co-Simulation of Advanced Electric Grid Systems**

Principal Investigator: Cy Chan

### *Project Description*

Energy researchers require fast, efficient co-simulation platforms to study the interactions of the complex large-scale, distributed systems integrated in future smart grids. Current simulation tools focus on different aspects of smart grids without capturing the global picture. Our project examines the feasibility and techniques required to extend this capability to model areas as large as California and even the USA. To simulate such areas, there are thousands of nodes for the power system simulation, and millions of component controllers interconnected through communication systems. Current tools were not designed to achieve the scale of simulation that researchers will require to study the dynamic behaviors and advanced control strategies of the future electric grid.

We have designed and prototyped a parallel simulation platform to evaluate hypothetical scenarios on large, integrated smart power grids, including advanced controllers, demand response, and high penetration of distributed generation resources. We have explored simulation algorithms and system design to determine requirements for achieving scalability of the platform on current and future HPC systems. ExaGrid has built upon the Virtual Grid Integration Laboratory (VirGIL), a non-HPC modular co-simulation platform, to explore how using high performance computing systems and methods can accelerate the simulation and run experiments for much larger electrical systems.

### *Accomplishments*

In the second year of this project, we focused on developing and improving the parallel power flow solvers that are an integral part of electrical grid simulations. For example, in quasi-steady-state simulations, a power flow solution may be required to calculate the state of the grid at every time step. Often, the power flow solver can take a large percentage of execution time depending on the simulation being performed. We explored three different power flow solver approaches to handle various electrical grid scenarios. First, we implemented a forward backward sweep algorithm that works efficiently for radial distribution systems without loops. Second, we implemented a parallel Newton-Krylov solver that utilizes the bi-conjugate gradient stabilized iterative algorithm to solve the inner Jacobian system and demonstrate a 5x speedup in the Krylov solver compared to serial execution for a 48,000 bus single-phase transmission network.

Finally, we implemented a three-phase, unbalanced distribution system solver using the Newton-Raphson algorithm leveraging the SuperLU sparse linear solver for the inner Jacobian system during each Newton iteration. This solver utilizes the current injection method and both speeds up execution time (more than 10x) and enables much larger systems to be solved compared to an existing non-parallel method (Z-Bus) due to efficiencies in both computation and memory usage. Furthermore, we explored how to efficiently permute the sparse Jacobian systems to reduce fill-in during the linear solve and to localize the cache access pattern during the sparse matrix vector multiplication in the Krylov solver. A paper describing our work will appear in the IEEE Conference on Innovative Smart Grid Technology in February 2018.



## Exploiting Physics-Based Concurrency in Time-Dependent Extreme-Scale Multiphysics Simulations

Principal Investigator: Marcus Day

### *Project Description*

Extreme-scale time-dependent multiphysics simulations of PDE-based systems will need to exploit an unprecedented level of algorithmic and computational concurrency in order to make effective use of leading-edge high-performance computing hardware with a million or more cores. In this work, we investigated a numerical time-stepping strategy that intertwines the concurrent evaluation of constituent processes, each evaluated on subsets of the available compute cores, as one approach to obviate the need to scale the evaluation of all processes over the entire machine. We are interested specifically in cases where the constituent processes require implicit coupling in order to ensure that the time-stepping algorithm perform robustly.

### *Accomplishments*

We explored two key research directions in order to evaluate whether our proposed time-stepping strategy would be viable for practical multiphysics simulation applications:

1. ***Concurrent Implicit Spectral Deferred Corrections (CISDC)***: We developed CISDC as a modification to a multi-implicit variant of spectral deferred corrections (SDC). The key concept in SDC methods is to construct an iteratively corrected approximation to a high-accuracy time step that is based on low order updates. The CISDC variant applies to coupled problems and stages the updates in way that removes direct coupling between the iterations, thus allowing for concurrent evaluation of the component processes.
2. ***Bulk asynchronous evaluation***: Within the AMReX software library, we extended the data structures and algorithms that are used to numerically evolve a wide variety of multiphysics flow problems. The extensions support relatively minor changes to a bulk-synchronous code in order to support a "fork-join" parallel execution model where component processes can be evaluated concurrently using subsets of the available compute cores.

As a prototype application of our CISDC algorithm we sought to replace the time-stepping strategy in the CCSE code, LMC. LMC evolves  $N$  (typically  $N=10-100$ ) species, including advection, diffusion and reaction chemistry processes. Each time step in LMC begins with the computation of an advection velocity. Advection based on this velocity proceeds via standard time-explicit stencil-based operations. Diffusion and reactions in LMC are stiff relative to advection, are tightly coupled, *and* contribute to source terms that affect the velocity field. A time-implicit diffusion step, independent over each of the  $N$  species, is followed by a time-implicit integration of stiff ODEs representing reaction chemistry, which is independent over all cells in the computational domain. In each of these processes, the others appear as iteratively lagged source terms, and all represent potential sources of concurrency in the context of CISDC.

In the submitted manuscript (listed below), we present the proposed CISDC algorithm in a general multi-process setting, as well as specifically in the context of the LMC equations. This algorithm, along with the extended AMReX tools, represents a complete and relatively general approach and toolset for concurrent evolution of multiphysics applications. The next steps involve testing and validation of the approach for specific applications. We have already made considerable progress down this road for extreme-scale combustion simulations. But because the tools were developed in a general context, we believe we are well positioned to explore the potential of our approach on a wide range of complex, coupled multiphysics applications.

## Modeling the Earth's Hydrological Cycle from Watershed to Global Scales

Principal Investigator(s): Hans Johansen

### *Project Description*

This project built a state-of-the-art prototype model of land-atmosphere hydrological cycle at ultra-high resolutions. Our hypothesis is that current models cannot accurately predict water resource availability, due to under-resolved simulation of precipitation events (such as cloud systems) interacting with orography (terrain), and leading to under-resolved hydrological predictions for precipitation and snowpack. A National Academy report [A National Strategy for Advancing Climate Modeling, 2012, p. 89-91] has called for this capability, which is needed by government agencies for science-driven policy and infrastructure decisions.

Our approach was to: (1) integrate climate and hydrological simulation capabilities that capture the effects of high-resolution precipitation events; (2) generate ensembles of ultra-high resolution simulations using NERSC systems; and (3) establish bounds on model uncertainties when compared with observational data. Typical regional atmosphere models under-resolve orography, so we will leverage our high-resolution simulations to create watershed-level hydrological modeling capabilities.

### *Accomplishments*

Our most significant accomplishment is that we identified a combination of climate and hydrology mechanisms that underlies significant errors in water resource predictions in global climate models (GCMs). We used highly accurate short-term simulations [1,2] of the hydrological system, driven from both global and regional climate scales, and validated against high-resolution data sets and regional observations. First, we identified issues with orographic representation in GCMs that can be alleviated with variable-resolution (VR) capabilities, ranging from typical 55 km and 28 km GCM resolutions down to 15, 7, and even 3.5 km, using the large-scale simulation capabilities of the NERSC Cori supercomputer. We found that, despite this being too expensive for most GCM simulations, resolved regional topography was required for correct large-scale atmosphere-ocean-land drivers in California and Nevada hydroclimatology.

Second, we identified issues with precipitation transport in mountainous regions, where windward and leeward ratios were resolution-dependent and did not match observations well. We determined that it was imperative to use a transport-aware microphysics schemes ([Morrison and Gettelman, 2015]) instead of a previous microphysics scheme [Morrison and Gettelman, 2008] which differ in rainfall/snowfall parameterizations, leading to significant errors. At horizontal resolutions < 20 km, the importance of orographic uplift in cooling impinging storm systems was needed to improve the windward/leeward distribution of precipitation and snowpack, which has significant implications for water resources in the California Sierra Nevada.

The third source of error was a systemic cold-bias that worsens with increasing horizontal refinement, especially at higher elevations in mountainous regions. Our comparison with VR-CESM, as well as the WRF-Noah and WRF-CLM models, in the Central Valley, Sierra Nevada, and Great Basin, indicated hydrology responses and energy balances have a cold-bias from atmosphere-land emissivity feedbacks. This affects snow accumulation and melt; we studied this in a snowmelt-controlled watershed (Upper San Joaquin), to look at the hydrologic and land surface processes using a watershed-scale modeling toolset called PAWS.

These results contributed to a thesis and were presented at the Fall 2017 AGU meeting [3,4].

## High Performance Computing for Large-scale Mobility Modeling

Principal Investigator(s): Xiaoye Sherry Li

### *Project Description*

The arrival of electric cars, shared-ride services and self-driving automobiles are changing the existing transportation systems and revolutionize the mobility modes of the country. The purpose of this project is to establish the critical computing expertise needed for modeling and forecasting the changing demand of energy, transportation infrastructure and policy. We will focus on computing tasks needed for modeling highway and arterial traffic.

This work will collaborate closely with the SMART Mobility effort led by Alex Bayen and Anand Gopal at ETA. We will develop new parallel algorithms using HPC resources to help analyze and model urban transportation systems, including mobility patterns (demand), changes in the road networks or public transportation, fueling infrastructure, parking and more. Specific tasks include: convex optimization solution to the dynamic traffic assignment (DTA) problem for behavior analysis, a new distributed memory multi-scale traffic simulation platform, an accurate and robust ensemble consensus method for traffic flow demand prediction, and co-simulation of transportation and power systems based on the DTA model. We will implement all these algorithms using the MPI standard library to achieve inter-node parallelism and the OpenMP library to achieve intra-node parallelism. For development, we will mainly use the parallel systems at NERSC, but our codes will be portable to many other parallel machines. Ultimately, the new parallel codes could be integrated together and fed into a holistic energy policy model for a metropolitan area, a state or the whole country.

### *Accomplishments*

Our most significant accomplishment has been to develop a new parallel implementation for traffic assignment (TA) problem to model drivers' behavior and traffic equilibria. The Frank-Wolfe algorithm is widely used in such computation. It is an iterative descent method in which repeatedly computing the shortest paths between all Origin-Destination (OD) pairs accounts for more than 90% of the total execution time. The sequential algorithms may take minutes to hours (depending on demands) for simple medium size problems. We parallelized FW algorithm with concurrent shortest-path calculations using Python and MPI. Our parallelization strategy was to use multiple nodes of Edison to run multiple shortest path algorithms. We tested the LA Network taken from OpenStreetMap (14,617 nodes, 28,376 links, 99,097 OD pairs). When using 5 computing nodes (120 cores) of Edison machine at NERSC, the Frank-Wolfe computation time reduced by a factor of 32 on average.

We developed an automated framework to solve the traffic prediction problem. Instead of selecting a single method, we combine predictions from multiple methods to generate a consensus traffic flow prediction. Our new ensemble learning model exploits the temporal characteristics of the data, and balances the accuracy of individual models and their mutual dependence through a covariance-regularizer. We apply our proposed model to multi-step-ahead arterial roadway flow prediction. In tests, our method consistently outperforms recently published ensemble prediction methods based on Ridge Regression and Lasso. Our method also produces steady results even when the standalone models and other ensemble methods make wildly exaggerated predictions.

## Fast numerical methods for Green's function in mesoscale simulation

Principal Investigator(s): Lin Lin

*Project Description*

The purpose of this project is to develop a general methodology for coupling quantum physics and classical physics for multiscale systems, without introducing system dependent parameters, in the framework of Kohn-Sham density functional theory. We obtain various physical quantities such as energy, electron density and forces, by setting up an appropriate boundary condition at the quantum-classical interface. Our goal is to develop new numerical methods that can be used to treat large scale *ab initio* calculations for open systems with non-trivial boundary conditions, such as dislocations in materials, and further for systems at the mesoscopic level.

We develop Dirichlet-to-Neumann (DtN) map type techniques for formulating the boundary condition of Kohn-Sham density functional theory for an open system. The DtN map avoids the ill-defined problem of finding boundary conditions for individual eigenpairs of an eigenvalue problem, and consistently provide boundary conditions for the density matrix via a number of Green's functions. We can further capitalize the pole expansion and the selected inversion (PEXSI) method for efficiently solving the discrete linear systems with the non-Hermitian boundary conditions due to the DtN map.

*Accomplishments*

We have successfully developed the PEXSI-Sigma formulation for quantum-classical interface fully at the numerical linear algebra level. We demonstrate that consistent boundary conditions can be formulated using an auxiliary Green's function corresponding to a physical configuration. This formulation is particularly attractive for 2D and 3D systems, and can reduce the computational complexity to at most quadratic, thanks to its interface with the pole expansion and selected inversion method (PEXSI). Our preliminary result implemented in DFTB+ package has demonstrated promising results for systems such as dislocation dipoles in graphene sheets. **Based on this work supported by LDRD, I have obtained the 2017 DOE Early Career award for further development along this direction.**

Phonon calculations based on first principle electronic structure theory, such as the Kohn-Sham density functional theory, have wide applications in physics, chemistry, and material science. The computational cost of first principle phonon calculations typically scales quadratically with respect to the system size and is very expensive. We developed a new method for reducing the computational complexity of computing the full dynamical matrix, and hence the phonon spectrum, to cubic scaling. The key concept for achieving this is to compress the polarizability operator adaptively with respect to the perturbation of the potential due to the change of the atomic configuration. Such an adaptively compressed polarizability operator allows accurate computation of the phonon spectrum. The reduction of complexity only weakly depends on the size of the band gap, and our method is applicable to insulators as well as semiconductors with small band gaps.

## Unconstrained Functionals for Massively Parallel Scaling of Conjugate Gradient Eigensolvers

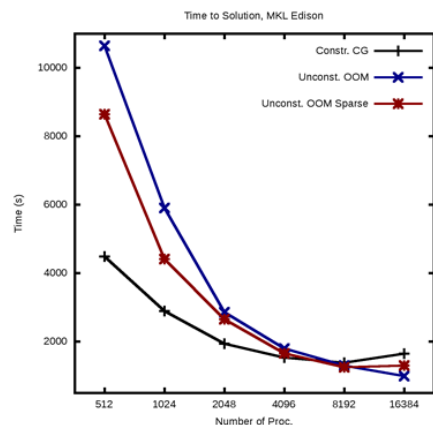
PIs: Osni Marques (CRD) and Andrew Canning (CRD)

### Project Description:

A large number of scientific applications require the solution of eigenvalue problems. In many cases, only a small percentage of the eigenpairs are required, rather than the full spectrum, which favors the usage of iterative eigensolvers. However, the scaling of iterative eigensolvers is limited by a reorthogonalization step that needs to be applied to the iterate vectors, through the diagonalization of a certain subspace matrix (or, alternatively, through the Cholesky or QR decomposition). This subspace matrix is typically much smaller than the original matrix for which eigensolutions are sought, thus limiting the parallel scaling. This project investigated eigensolvers based on an unconstrained functional approach, which eliminates the reorthogonalization step that is typically required in standard iterative eigensolvers. We focused on solvers based on the Conjugate Gradient (CG) method, which is widely used due to its stability and its ability to accurately obtain eigenpair degeneracies. The main goal of this project was therefore to develop a highly parallel scaling method, based on an unconstrained functional approach, which completely eliminates the reorthogonalization step. This allows the scientific community to better exploit existing massively parallel multicore computers as well as future exascale machines. In particular this work greatly benefits the materials science and chemistry community, the majority of whose codes and computer runs use iterative eigensolvers.

### Accomplishments:

Unconstrained energy functionals have been used in the past for eigenfunction problems in electronic structure calculations for sparse method approaches. Such functionals lead to a different cost/energy function, which has a minimum corresponding to the solution of the desired eigenfunction problem without the need for an explicit reorthogonalization after the CG steps. We revisited the unconstrained functional approach to CG eigensolvers in current codes for electronic structure calculations, in the context of the present and future massively parallel multicore computers, and large scale physical systems that can be studied today with iterative solvers. Our goal was to examine how much the unconstrained methods can improve parallel scaling over the conventional methods, and also to compare their convergence properties. The unconstrained method was implemented in the PARATEC, Quantum Espresso and CP2K materials codes. The main issue with the implementation in the CP2K code was that the preconditioner used in the



code for the more standard methods already implemented in the code did not work well for the new unconstrained functional. Part of the recent work has consisted in developing a new preconditioner for the CP2K implementation. To show the potential gains offered by unconstrained functionals based CG, the figure shows the parallel speed up to 16384 cores on NERSC's Edison (Cray XC30) for a 4x4x4 GaAs Crystal (512 atoms): the convergence of unconstrained OMM (Orbital Minimization Method, blue and red curves) can be slower than traditional CG (black curve), but the runtime is reduced for a larger number of cores due the improved parallel scaling.

## Design of Quantum Chemistry Simulations for Superconducting Circuits

Principal Investigator(s): Jarrod, McClean

### *Project Description*

The purpose of this project is to design and demonstrate quantum simulations of quantum chemistry problems using superconducting circuit simulation systems developed at Berkeley. Quantum simulations on quantum computers have the potential to revolutionize the field of computational chemistry and physics.

One of our main objectives is to design quantum simulations to compute the energy spectrum for small molecules, and to extend the formalism to compute excited states in addition to ground states, and to explore algorithm-specific error correction.

This project has maintained a close partnership with the integrated experiment/theory team encompassing the groups of Siddiqi and Whaley from the Materials Science Division/UC Berkeley who have been focusing on building, controlling and analyzing the capabilities of the superconducting qubit circuit technology. This partnership has the potential to establish LBNL at the forefront of quantum computing from hardware to simulation.

### *Accomplishments*

During 2017 the project has made great progress on both the theoretical development efforts and collaborating with experimental sides of quantum computing efforts to develop software and algorithms for quantum chemistry on superconducting qubits.

Our new theoretical method, formulated last year to extend the capabilities of hybrid quantum-classical variational methods to excited state energies and properties, was implemented on a 2-qubit prototype quantum simulator in collaboration with the Siddiqi group in the Materials Science Division/UC Berkeley. This yielded the first scalable demonstration of the computation of molecular excited states. As predicted, our method was also found to correct decoherence based errors in the testbed without the use of formal error correction, which could represent a novel error suppression method for more general computations.

Another aspect of the work was to explore alternatives to atom-centered Gaussian basis sets for chemistry simulations with a framework of quantum simulation to lower the costs of the classical portion of quantum simulations. We reported progress in the use of a planewave basis in place of Gaussians.

An open-source Python based fermion simulation package, FermiLib, was completed in collaboration with Ryan Babbush at Google and Damian Steiger at ETH Zurich of the ProjectQ Team. The goal of this package was to eliminate the need for expert domain knowledge to engage in quantum algorithms research in chemistry and related fields. This package was released under an open source license, and interoperates with the ProjectQ software framework.

## CONTINUING DIGITAL COMPUTING PERFORMANCE SCALING POST MOORE'S LAW

George Michelogiannakis, Dilip Vasudevan, David Donofrio, Jeff Bokor, John Shalf,  
Ramamoorthy Ramesh

### *Project Description*

The purpose of this project is to investigate a variety of emerging technologies that are becoming ready to be deployed at scale and promise to preserve digital computing performance scaling. As the predicted slow down and eventual stop of performance scaling of traditional CMOS transistors approaches, researchers are actively developing novel devices, memories, 3D integration technologies, and accelerators including fixed-function hardware. However, these technologies tend to be evaluated at isolation and little work exists to evaluate such technologies at the architectural level. This is useful for technology developers so they can quantify their technology's high-level impact, for architects so they can better understand which technologies should be part of a future strategy for digital computing, but also for programmers to know early what new machines will feature.

In this project, we will develop a comprehensive modeling tool flow called PARADISE and use it so evaluate a collection of emerging technologies towards their future potential for HPC. PARADISE is composed of four levels, with the lowest being physical modeling of individual devices (transistors) and the highest being chip-level architectural power and performance modeling. Low levels train high levels such that new technologies can be given as inputs at the physical level, with PARADISE constructing power and performance models for higher levels. Using PARADISE, we will evaluate the impact that three devices, fixed-function accelerators, non-volatile memory, and 3D integration have to climate modeling and density functional theory.

### *Accomplishments*

We have successfully developed all four levels of PARADISE: We incorporated models for tunnel FETs, carbon nanotube FETs, and negative capacitance FETs, as well as fixed-function hardware for FFT, matrix-matrix multiply, AES, and other smaller important computational kernels for HPC. To keep PARADISE open source, we extended an open-source RTL logic simulator with power models we generated, such that we can perform power estimation based on behavioral or synthesized RTL. In addition, we verified the accuracy of our results based on two published designs, one using tunnel FETs and another using carbon nanotube FETs. Also, we have created automation scripts to make the transition from lower to higher levels effortless, such that new technologies can be entered into PARADISE at the lowest level and rapidly be modeled at any other level with performance and power models generated at a level being used to train the next higher level.

We are currently working to include resistive RAM and 3D integration models into PARADISE. In addition, we are working to verify the correctness of PARADISE by comparing against other published designs, as well as by comparing against the output of our various open-source tools against well-established commercial tools. In parallel, we are developing a design optimization methodology using heuristic solvers which will choose among all emerging technologies available in PARADISE that were previously mentioned and will generate an architecture that improves on a given metric (such as performance over power) for a given application. This methodology will then be used to choose among available technologies and thus formulate a strategy for continued performance scaling of our two HPC applications.

## **Acceleration of Temporal Integration for Real Time - Time Dependent Density Functional Theory**

Principal Investigator(s): Michael Minion, Bert de Jong

### *Project Description*

Many important renewable technologies including photovoltaics and thermoelectric generators, are driven by the time-dependent electronic response to external fields. Real-time time-dependent density functional theory (RT-TDDFT) provides a way to directly model the time evolution of the underlying physical processes; however, state-of-the-art numerical methods for RT-TDDFT are currently too costly to model realistically-sized molecules and time-scales long enough to couple electron dynamics with nuclear motion. We propose to develop and analyze a novel parallel-in-time RT-TDDFT algorithm that will harness petascale and future exascale architectures to simulate electron dynamics for molecular size and time scales beyond the reach of the state-of-the-art. The new methods will be implemented in the NWChem computational chemistry package for use by the wider research community.

### *Accomplishments*

During the first year of the project, the focus of our research has been on the development, implementation, analysis, and testing of new higher-order parallel in time methods for the general problem of nonlinear isospectral flow differential equations. The equations for RT-TDDFT are of this form, and the current method implemented in the NWChem package for RT-TDDFT is a second-order Magnus type method. We first developed higher-order Magnus integrators based on an iterative Picard method for handling the nonlinearities. The Picard form allows for parallelization across the Fock matrix builds across quadrature nodes and the matrix exponentials that comprise the bulk of the computational effort. Methods with up to sixth-order accuracy have been analyzed, yielding the ability to take time steps that are an order of magnitude larger than conventional methods. We then tested a second dimension of parallelism by pipelining the Picard iterations over many time steps using libpfasst, a library for the parallel full approximation scheme in space and time (PFASST) developed at LBNL. Although this approach appears promising, we also developed new integrators based on implicit Munthe-Kaas Runge-Kutta methods. This second approach allows for even higher-orders of accuracy and is readily extended to the multi-level structure used in PFASST. We have begun the process of implementing the implicit M-K R-K schemes in the NWChem project and will be concentrating on this effort for the second year of the project.



Solving Problems in Materials Theory via Quantum Networks  
Principal Investigator(s): Joel Moore

*Project Description*

This project concentrates on theoretical analysis of problems in quantum dynamics that are motivated by experiments on solid-state materials and atomic systems. Another goal of the project is to connect real-world problems to simulation by quantum networks of a few qubits, as created with superconducting devices, or by analog quantum emulators made from atoms. Specific examples to be studied were quantum dynamical processes ranging from transport of charge and energy in one spatial dimension, through non-abelian Berry phases in superconducting qubits, to optically generated dynamics in solids.

*Accomplishments*

A major accomplishment in the final year of the LDRD was an example of quantized energy pumping in a non-equilibrium system. This work was led by the LDRD-funded postdoc (Michael Kolodrubetz) and is currently under review at Physical Review Letters. Another paper, already published in Physical Review Letters, concerns the time evolution of a quantum system when energy is injected by a periodic perturbation at the boundary. It turns out that subtle features of the quantum state, including entanglement, can be captured using sophisticated field-theory methods, and consideration of injected energy in this system helped lead to the quantized energy preprint as well. The LDRD-supported postdoc, Michael Kolodrubetz, completed two review articles related to his pre-Berkeley work.

The work carried out in this LDRD led to the PI's joining the Ultrafast program as co-PI in order to provide theoretical modeling of quantum dynamics in solids. The PI recently chaired a DOE roundtable on applications of quantum information science to theoretical material and chemical sciences (the report is currently being completed). It is hoped that there will be additional DOE funding in this area, either through the EFRC channel or through a future FOA on quantum information science.

# Scaling Interactive Science for Data-Intensive Discovery

Fernando Pérez and Shreyas Cholia

Data Science and Technology Department, Computational Research Division

## *Project Description*

The goal of the proposed research is to enable scalable interactive science for data-intensive workflows on HPC systems. Today's large-scale experiments and simulations produce large amounts of data that need to be analyzed, often in a regime that far exceeds the capacity of local clusters and desktops. While HPC systems and the supporting workflow tools have long supported remote execution of jobs, these solutions largely focus on asynchronous, batch execution. However, scientific insight frequently requires interactive, iterative exploration and analysis. We will address key research questions that will enable fluid integration of workflow technologies used to manage large-scale computations in data-intensive science, with the notebook systems that are widely used in computational research.

## *Accomplishments*

Our work is based on the Jupyter<sup>1</sup> platform that provides rich interactive notebooks that can combine natural language narrative, live code and interactive widgets. Our primary goal for this effort has been the development of a system that enables Jupyter notebooks to drive interactive workflows in large-scale computing. Our software toolkit, called "Kale" (source available via Github<sup>2</sup>), serves as a reference implementation for this work. Kale is being designed and developed against real-world requirements gathered during user interviews we conducted with science teams that have interactive HPC workflow needs. Kale enables task management and interactivity in HPC workflows. This includes interactive "IPywidgets" on the front-end that enable a graphical interface in the Jupyter notebook for interacting with the workflow, and a backend service component that interfaces directly with the HPC tasks. Our initial prototype has included a fully functional set of Docker containers so that this can be downloaded and run in a standalone environment.

This work was published and presented as a demo for the Gateways 2017 conference, and as a poster at Jupytercon 2017. Our demo included a live interactive workflow that runs the LAMMPS molecular dynamics simulation code.

We have integrated our work with the Fireworks workflow management system, in order to demonstrate feasibility of running this system with existing workflow tools. To ensure flexibility beyond Fireworks, we are extending support for other workflow tools and libraries.

We are currently exploring and developing various features in Kale including:

- More fine grained "human-in-the-loop" workflow control for managing live running workflows.
- Improved user interfaces for visualizing and interacting with complex workflows.
- Extensible support for multiple workflow systems.
- Running notebooks as subtasks within a workflow.
- Expanding the use cases to address workflows in multiple domains including High Energy Physics, Astronomy and Materials Science.
- Integration with the NERSC Cori system, and the production Jupyter deployment.

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<sup>1</sup> <https://jupyter.org>

<sup>2</sup> <https://github.com/Jupyter-Kale/kale>

## Open Framework for High-Performance Streaming Analytics

Principal Investigator(s): John Wu

### *Project Description*

To realize the grand visions such as Smart Grid, Smart City, Smart Building and so on, we have to gather and analyze massive amounts of information, identify key signals in the data, and automatically respond to them appropriately. In this process, a large number of sensors produce constant streams of data that need to be integrated and organized before sophisticated pattern detection and discovery algorithms could be applied. This LDRD project is to develop a few key techniques for integrating these streams. The initial task will be focused on data reduction and local feature extraction. Ultimately, we foresee this project to establish a core set of techniques for a high-performance stream analysis engine that would ingest streaming sensor data from a variety of sensors, fuse data streams to form coherent sources of information, identify important events specified by users, and deliver the resulting signals according to common industrial standards. We plan to demonstrate the effectiveness of these algorithms on a set of microPMU data collected from LBNL's own electric power supply lines. This would serve as the basis of additional applications on Smart Grid, Smart City, Smart Building, and other environments that require real-time data analysis and control.

### *Accomplishments*

Our work on streaming analytics proceeds in two broad themes: statistical feature extract through IDEALEM[1, 2] and incremental machine learning on streaming data[3, 4].

Bulk of the streaming data from scientific simulations and experiments consists of numerical values, and these values often change in unpredictable ways over a short time horizon. Such data values are known to be hard to compress, however, much of the random fluctuation is not essential to the scientific application and could therefore be removed without adverse impact. We have developed a compression technique based on statistical similarity that could reduce the storage requirement by over 100-fold while preserve prominent features in the data stream. We achieve these impressive compression ratios because most data blocks have similar probability distribution and could be reproduced from a small block. The core concept behind this work is the exchangeability in statistics. To create a practical compression algorithm, we choose to work with fixed size blocks and use Kolmogorov-Smirnov test to measure similarity. The resulting technique could be regarded as a dictionary-based compression scheme. In this paper, we describe the method and explore its effectiveness on two sets of application data. Our recent work extends the technique to work with data that are not stationary, but have long term trends that need to be captured explicitly [1]. In addition, we have also conducted a number of studies to validate the technique under different application scenarios. For example, in one case, we study the Fourier components of the reconstructed data and show that in addition to preserving unique features in data it is also faithfully preserving the Fourier components whose periods extend more than a few blocks.

On machine learning over streaming data, we have two publications in the last year [3, 4], both of which are related to electricity. In one case, we apply machine learning to predict electricity usage in the future and in the other case, we apply machine learning to classify the type of insulation failures in power transformers.

## Neuromorphic Image Analysis and Pattern Recognition

Principal Investigator(s): Chao Yang (CRD)

Other investigators: Karen Davies (MBIB), Alex Hexemer (ALS), Thorsten Kurth (NERSC), Peter Nugent (CRD, NERSC), Dilworth Parkinson (ALS), Nicholas Sauter (MBIB), Daniela Ushizima (CRD, NERSC, BIDS)

### *Project Description*

The purpose of this project is to reformulate a number of image analysis and pattern recognition problems arising in DOE science applications as neuromorphic computing problems. In particular, we propose to use properly trained convolutional neural networks (CNNs) to solve a number image classification and feature extraction problems in the areas of structural biology, materials science and cosmology. We investigate the construction and architecture optimization of these CNNs and the feasibility of deploying these CNNs on new energy efficient computer architectures that are designed specifically to mimic this type of neural network. An example of such new computer architecture is the IBM's TrueNorth neurosynaptic system. We examine the effect of different depths for CNN architectures as well as the TrueNorth's low precision arithmetic on the reliability of a CNN.

### *Accomplishments*

We investigated the possibility of using pretrained CNNs as a screening tool to veto certain diffraction events (such as those images that contain no Bragg spots) in a serial X-ray crystallography experiment, so that data with little value can be quickly pruned and discarded instead of being stored for further examination and analysis. We showed that with a modest set of carefully annotated images collected from previous experiments, a CNN can be trained to successfully distinguish Hits from Misses in most cases. Compared to automatic spotfinding tools implemented the *DIALS* software toolbox, which still require manual parameter tuning, the CNNs trained here have a slightly lower success rates (but still above 90%) in identifying images that are considered to be Misses by a human expert. However, they have much higher success rates in identifying images that are considered to be Hits. We found that the accuracy of CNN classification depends largely on the quality of the annotated data used to train the network. Because images produced by serial X-ray crystallography often contain additional features that reflect the type of detector used and the way the samples are prepared and delivered, which are not part of the annotation used for training, a CNN trained on one dataset cannot necessarily be applied to images collected with differing experimental methods (*e.g.* detector type and sample delivery system). Although it is desirable to train a universal CNN that can be used to screen images from all experiments, our results suggest that training such a CNN may be difficult, or may require larger datasets than what we have used.

We also investigated the possibility of using CNN for picking particle images from micrographs collected from cryo-electron microscopy experiments. We used manually annotated images to train the CNN, and deployed the CNN on Ristretto, which is a modified version of the CAFFE CNN software that allows low precision arithmetic in various CNN calculations. Our results show that the CNN based particle picking is more reliable than existing automated particle picking tools.

## TRANSPORTATION SYSTEM SCIENCE FOR ENERGY SAVINGS

Principal Investigator(s): Anand R. Gopal

### *Project Description*

Globally, there is significant excitement that trends toward increased use of mobility-on-demand (MOD), falling prices of electric vehicles (EVs) and, greater vehicle automation could radically reshape passenger transportation. The importance and pace of each of these megatrends vary in key regions of the world. Mobility-on-demand (MOD), provided primarily by transportation network companies (TNCs) like Uber, Lyft, Ola and DiDi, is growing rapidly everywhere in the world but their growth rates are particularly fast in China and India. As a result, the share of annual miles traveled by TNC vehicles is rapidly increasing, exceeding 10% in China today and likely to exceed 15% of total passenger car vehicle miles traveled (VMT) in both China and India in 2018. A promising pathway to deep decarbonization of transport, is to begin with electrification of the vehicles used in TNC service around the world. This project assesses the case for TNC electrification and the subsequent impact on the electrification of the rest of the passenger vehicle fleet in China, the US and India.

Specifically, the project addresses the following research questions:

1. How does the economic payback period for a TNC electric vehicle compare with a private electric vehicle in each region?
2. What is the breakdown of operating costs for TNC vehicles in each region by fuel, labor, capital, maintenance etc?
3. How much will TNC electrification contribute to lower battery costs induced through learning rates?
4. By how much will increased demand for MOD inhibit future private vehicle miles traveled in each region?

### *Accomplishments*

The comparative economic payback period analysis shows that electric TNC vehicles have lowered payback periods of 12 years in China, 9 years in India and 7 years in the US when compared to private EVs. These results show that the incentives for a TNC owner or operator to choose an electric vehicle is very strong since they stand to save a large amount in fuel costs over the life of the vehicle. However, the initial purchase price of the electric vehicle is higher which requires innovative financing solutions to overcome.

In the US, the operating costs of a TNC vehicle is dominated by labor, which accounts for approximately 80% of the total costs, while in China and India, labor costs are less than 35% of the total costs, while fuel accounts for more than 35%. Hence, TNC businesses in the US stand to gain substantially more from vehicle automation than from electrification, while the reverse is true in China and India.

Given the rate of increases in demand for TNC services, there is a corresponding surge in demand for TNC vehicles. If these vehicles are all electric, the project analysis finds that these sales alone can reduce battery costs by as much as 16% from learning. Since batteries are the major cost component of any EV, TNC electrification by itself can substantially lower the capital costs of EVs worldwide.

The large-scale electrification of TNCs is promising and economically compelling. Key barriers to overcome are financing and the deployment of charging infrastructure.

## Dark Fiber and Distributed Acoustic Sensing : Opportunities for Critical Infrastructure and Environmental Monitoring

PI: Jonathan Ajo-Franklin, Co-I: Barry Freifeld, Tom Daley, Inder Monga, Xiaoye Li

### *Project Description*

The goal of this project is to pioneer the utilization of distributed acoustic sensing (DAS) and unused telecom fiber (“dark fiber”) to provide seismic sensing capabilities at an unprecedented combination of resolution (1-10 m) and spatial scale (10s of km); we seek to test the resulting datasets for applications in classical seismology (EQ detection/location), geotechnical characterization, and environmental sensing. Key properties we hope to estimate in support of this goal include soil shear modulus, a time and depth variable property crucial to understanding coupling of ground motion to infrastructure as well as stability, and water content, a parameter of importance in both agriculture and aquifer management. While a variety of approaches exist for point measurement of such properties, no existing networks combine lateral extent (10s of km), high spatial resolution (m), and high temporal resolution (hours) to assist in infrastructure and water system management. Estimates of near-surface mechanical properties, variations in soil moisture, and spatially extensive estimates of ground acceleration could be used as a starting point to develop the next generation of critical infrastructure components including both surface and subsurface water management systems as well as adaptive linear and vertical infrastructure. As a secondary goal, we hope to leverage the same system to make direct measurements of local, regional, and teleseismic earthquake (EQ) ground motion, thus providing a large scale dataset for EQ detection, location, and analysis.

### *Accomplishments*

Our most significant accomplishment to date has been the acquisition of an unprecedented 200 TB passive seismic dataset using a section of ESnet’s Dark Fiber testbed. This dataset, which includes 12500 channels recorded at 500 Hz over 7 months, covers a 22 km profile between West Sacramento, CA and Woodland, CA. The dataset was of surprisingly high quality, particularly over a central section traversing agricultural land. Preliminary analysis has demonstrated detection of local, regional, and teleseismic earthquakes using the array as well as continuous ambient noise recording. The ambient noise data, largely surface waves generated by local rail activity and traffic, was processed and inverted to generate a 7 km profile of near-surface soil properties. The surface wave profile successfully identified both the surficial aquifer boundary as well deeper variations in the soil profile; both interfaces were confirmed through comparison to drilling logs obtained from local wells. On-going analysis is exploring the utility of the same inversion approach for groundwater monitoring, a study which requires longer acquisition times over seasonal precipitation cycles. As of November, broadband inertial sensors were also deployed on the profile to allow quantitative comparison of DAS response.

A second accomplishment in 2017 was completion of a study exploring earthquake recording using prior DAS array deployments. The work included (a) a quantitative comparison of DAS EQ recording for trenched fibers to a precisely calibrated broadband sensor, (b) evaluation of beamforming using DAS arrays, and (c) collection of a catalog of seismic events recorded on DAS. While not using the ESnet array described above, this preliminary study provided insight into the utility of large trenched DAS arrays for earthquake seismology and was well-received by the community.

## Multi-Scale Modeling of Geochemical Impacts on Fracture Evolution

Principal Investigator(s): Bhavna Arora and Sergi Molins

### Project Description

Understanding fracture evolution is essential for many subsurface energy applications, including shale gas, CO<sub>2</sub> sequestration, or geothermal energy extraction. The purpose of this project was to develop a multi-scale model for the simulation of geochemical impacts on fracture evolution. While a *Darcy-scale representation* –i.e. treating the porous medium as a continuum– may oversimplify the processes within complex fracture geometries, a *pore-scale description* – i.e. with explicit consideration of the pore space geometry– requires a model resolution that makes it extremely expensive computationally. The model developed combines a pore-scale description and a Darcy-scale representation within a single adaptive simulation framework.

The resulting simulation capability enables us to improve our understanding of geochemical behavior of fractures. Further, the model can be used more generally as a framework to combine subdomains at different scales or even to combine sub-models implemented in different codes.

### Accomplishments

1. Development of the computational framework that implements our conceptual model including the sequential iterative solver for the multiscale problem that couples the pore-scale and Darcy-scale sub-problems.
2. Implementation of a novel coupling approach that uses the embedded-boundary method to provide the connection between the pore-scale and Darcy-scale subdomains via flux matching and boundary condition swapping at their interface.
3. Debugging and validation of the approach against CrunchFlow results for simple geometries and moderately complex geochemical problems.
4. Application of adaptive mesh refinement to the multiscale problem to improve the computational efficiency, whereby the domain is only finely resolved where needed based on the geometry of the interface and/or the concentration gradients.
5. Description of the model in a draft manuscript, currently being finalized for submission.

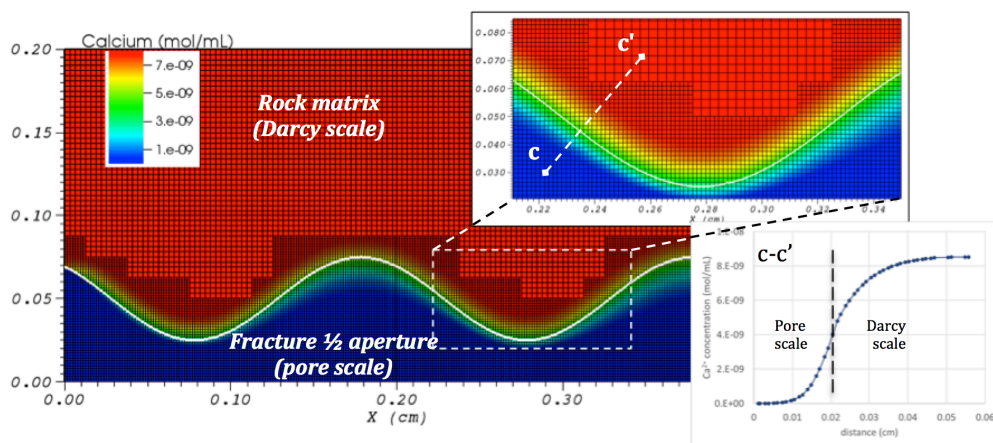


Figure: Calcium concentrations in a fractured domain where calcite is dissolving in the rock matrix. The embedded boundary (in white) defines a sinusoidal surface fracture. The mesh is adaptively refined within the fracture aperture and in the rock matrix near the fracture surface. Continuity of fluxes and concentrations is enforced at the interface between subdomains.

**Project Title** (IDENTIFYING THE SOURCE AND MAGNITUDE OF REDOX RELATED METAL ISOTOPE FRACTIONATION: AN ESSENTIAL TOOL FOR EARTH SYSTEM SCIENCE)

Principal Investigator(s): (John Christensen)

*Project Description*

The purpose of this project is to identify and quantify the mechanisms of metal isotope fractionation during reduction-oxidation reactions using carefully planned laboratory experiments. The existence of isotope fractionation during these reactions has been widely observed in laboratory and geologic environments for more than 25 years, however the understanding of why there is isotope fractionation and what mechanisms are most important in producing isotope fractionation at environmental conditions is still minimal. The data from the study will provide some of the first experimental observations of uranium and iron isotopic fractionation during reduction-oxidation transformations. The data will also allow us to create computational models that will be used to interpret the rates and efficiencies of reduction-oxidation reactions relevant to field scale environmental questions such as transport of organic carbon in soils and radionuclide contaminant transport.

We will develop a new protocol for quantifying metal redox reactions at aqueous fluid-mineral surface interfaces and we will directly probe the role of metal speciation in solution as a control on redox transformations. A recent study by Stylo and coworkers (2015) and 2 earlier studies (Rademacher et al., 2006; Stirling et al., 2007) suggest that uranium isotope fractionation only occurs due to microbially mediated redox transformations and that inorganic transformations result in no fractionation. This result is interesting because it is in conflict with underlying theory that uranium isotope fractionation is an equilibrium process and that most microbially mediated redox reactions are thought to be irreversible kinetic reduction reactions. Our new experiments are designed to test whether there is truly a difference between microbial and inorganic reduction or if the earlier works misinterpreted the meaning of their experimental results.

Our hypothesis is that degree of uranium isotopic fractionation during reduction is controlled by the relative flux of uranium atoms to and from the reductant surface. In the case where the lifetime of an U(VI) atom at the reductant surface is short there is a relatively low probability that any specific atom will be reduced. This, in turn, gives rise to the possibility of isotopic discrimination in the reduction reaction. In contrast when the lifetime of U(VI) at the reductant surface is long there is less isotopic discrimination in the reduction reaction.

*Accomplishments*

Our most significant accomplishment was to execute the planned experiments and demonstrate that abiotic uranium reduction induces isotope fractionation similar to that of microbially mediated reduction. We further demonstrated that the magnitude of fractionation was related to the exact distribution of uranium species in the  $\text{UO}_2\text{-CO}_3\text{-CaCl}_2$  system. Our findings have been presented at 2 international meetings and are described in a publication that will be submitted to the Proceedings of the National Academy of Sciences in the coming weeks.

Our results have lead to a new collaboration with DOE BES funded researchers at UC Davis and a project with a graduate student who received a DOE SCGSR award to test some of the resulting hypotheses about the exchange kinetics of aqueous U species and the application of U isotopes to field scale questions. We expect these follow up projects to be partially supported by continued funding as part of the isotope geochemistry BES project.



## **Advanced In-Situ Experiments for Understanding Induced Seismicity**

Principal Investigator: Yves Guglielmi

### *Project Description*

The topic of induced seismicity has been hotly debated in recent years, as subsurface energy activities involving injection of large volumes of fluids have increasingly led to the reactivation of existing faults (NAS, 2012). Despite concern about induced seismicity, the role of fluids in seismic nucleation remains poorly understood, in part because there is a lack of designated field experiments with controlled injection into faults and real-time monitoring of fault slip behavior. The scientific goal of this project is to develop new instruments and methods to evaluate the critical coupling between injected fluids, effective stresses, evolving fault properties and seismicity via intermediate-scale fault reactivation experiments conducted in underground mines and deep boreholes. The project positions LBNL as a premier research organization for induced seismicity research: (1) It provided partial support for the strategic hire of Dr. Yves Guglielmi of University of Aix-Marseille, a world-renowned expert on fault hydrogeomechanics, and (2) it supports further development, testing and application of Dr. Guglielmi's new high-resolution borehole packer-system for in-situ characterization of hydromechanical properties (deformation, seismicity, permeability) from semi-controlled fault activation.

### *Accomplishments*

In 2017, Dr. Yves Guglielmi first continued publishing his results about the field experiment of fault reactivation that he conducted during the 2016 year of his LDRD project. His most recent results are to show that fault leakage does not only depend on stress, in low permeable rocks such as reservoir cap rocks and host rocks for nuclear repository sites. There is also a strong effect of fault displacement rate on its permeability, and the instrument developments done by Y.Guglielmi within the frame of this LDRD allowed to highlight and monitor these for the first time in situ. Second, Y.Guglielmi has been building the complete process to develop a new borehole instrument for "Straddle Intelligent Monitoring of Fracture Pressure" (SIMFIP) in LBNL. These developments include (i) the plans of the sensor, the machining done at the GeoSciences Measurement Facility (by Paul Cook, principal scientific engineering associate at the EESA), the development of a new calibration bench dedicated to this type of probe (installed in Building 64), and finally the definition and analyses of the different calibration tests. Three SIMFIP probes are currently being built. They will be used to monitor fractures dynamic shear and permeability variations within the frame of the experiment of the Enhanced Geothermal Systems (EGS) Collab (Stimulation Investigations for Geothermal Modeling Analysis and Validation (SIGMA-V)) project which is designed to comprehensively monitor a series of hydraulic fracture stimulations and subsequent flow tests. This project is funded by the United States Department of Energy, Geothermal Technologies Office (GTO). The SIMFIP probes constitute key elements of these experiments. The LDRD funds thus allowed all the conditions for the EESA and Y.Guglielmi to build this new type of borehole instrument entirely on the LBNL site.

## DEVELOPING SCIENCE BASED SCALABLE APPROACHES TO GROUNDWATER BANKING

Principal Investigator(s): Peter Nico, Will Stringfellow, Greg Newman, James Rector, Yuxin Wu, Don Vasco, Christine Doughty, Yingqi Zhang, Nic Spycher, Mark Conrad, Nigel Quinn, Larry Dale

### *Project Description*

The purpose of this project is to advance LBL scientific expertise in subsurface science while addressing a key societal challenge, namely a resilient water supply. We are addressing four key challenges in the area of groundwater management. The first key challenge is developing a sufficiently well resolved understanding of the subsurface heterogeneity that controls the physical and chemical fate of the water once introduced into the subsurface. The critical parameters and processes required for the monitoring of groundwater banking include the subsurface soil properties, vadose zone moisture content and dynamics, water infiltration rate, and groundwater dynamics. We are monitoring these processes and parameters with two integrated geophysical methods, seismic surface wave tomography (SWT) and electrical resistivity tomography (ERT). The second key challenge is to predict how much of the applied water is actually transported into the subsurface and where it will go. To address this we are developing coupled groundwater-soil-plant-atmosphere modeling capabilities informed by the geophysical imaging and isotopic analyses. The third key challenge is predicting the water quality of both the applied water and the existing groundwater. We are addressing this challenge by coupling the developed hydrologic model with a reactive transport model that can predict chemical reactions during transport in the subsurface and be tested against sediment core and well water samples. The fourth key challenge is upscaling these approaches to the domain size necessary for large scale application. We are addressing this challenge through 1) coupling satellite based imaging (InSAR) to the other geophysical imaging approaches described above, and 2) using existing large scale models (CVHM) to conduct representativeness and data worth analysis.

### *Accomplishments*

We have made significant progress on all of our challenges and have accomplishments to report for each one. For the first challenge we have conducted ERT monitoring of two groundwater recharge sites during the last water year. Most importantly we have also collected and analyzed the first ever full waveform seismic imaging data. This is a scientific first and has utilized LBL's deep geophysical expertise as well as DOE computing resources at NERSC. For the second challenge, we have conducted isotope, D<sub>2</sub>O, tracer experiments during groundwater recharge and used those along with the geophysical data to develop 2D hydrologic models of our recharge sites. For our third challenge, we have a preliminary reactive transport model representing the dynamics of nitrate movement and reactivity within the sediments at our sites, and the impact the recharge activities have on nitrate movement. For the fourth challenge, we have successfully completed preliminary inversion of InSAR data around the Tulare Irrigation District region to assess large scale groundwater recharge resulting from the historically wet 2016/2017 water year. Preliminary results correlate well with less sophisticated estimates of water recharge and have generated significant interest from water managers.

**Project Title: Characterizing the Environmental Impact of Chemical Compounds Used in O&G Development**

Principal Investigator(s): William Stringfellow

*Project Description*

Oil and gas (O&G) development in the USA has expanded rapidly over the last decade and there is growing public concern about the environmental impacts of oil-field chemical additives and on-field produced water management practices. Rapid growth has alarmed the public in part because O&G chemical additives have not been sufficiently characterized to allow for an analysis of their environmental impacts. For this LDRD study, we conducted a systematic investigation of the environmental profiles of O&G chemicals, including properties related to contaminant mobility, recalcitrance, and toxicity. We developed a better understanding of the properties of O&G chemicals that allows the selection of chemicals with improved environmental profiles, that are more acceptable to the public, and can improve the sustainability of O&G development. We characterized the fate and transport properties for many chemicals which allows the application of predictive models in the context of local and regional groundwater investigations. We identified O&G chemicals that had not been previously investigated and conducted studies of the physical, chemical, and biological properties of these chemicals. The results of this LDRD were of interest to California, a major O&G producing state, which is providing further funding to continue this research. This research is foundational to development of better water management practices on O&G fields, that ensure the quality and availability of water for O&G production.

*Accomplishments*

Major accomplishments of this LDRD include an evaluation of the types, frequency of application, and quantities of chemicals used in O&G development. It was shown that chemical additives used in hydraulic fracturing, which is a tightly regulated O&G field activity, are also widely used for other O&G development activities, suggesting that green chemical alternatives are available for all O&G field activities, not just hydraulic fracturing (Stringfellow *et al.* 2017a). Papers were published that for the first time evaluated the environmental management of chemicals use for acid fracturing and matrix acidizing (Stringfellow *et al.* 2017a, 2017b). Using data science approaches, it was determined from fundamental physical and chemical properties which O&G additives could be treated using existing water-treatment technology and which could not (Camarillo *et al.* 2016). It was demonstrated that a class of commonly used biocides called quaternary ammonium compounds (QACs) were poorly characterized (Camarillo *et al.* 2016) and research was conducted under this LDRD to measure QACs in environmental media and develop treatment technology for produced water. The California Department of Oil Gas & Geothermal Resources and the State Water Resources Control Board is funding further scientific research in follow-up to the research started under this LDRD project.

Data Driven Approach for Monitoring and Control of Distribution System Assets  
Principal Investigator(s): Jhi-Young Joo (formerly Emma Stewart and Michael Stadler)

### *Project Description*

This project aims to address key technical challenges in modernization of the national electric grid, by combining multidisciplinary expertise in Grid Integration, Buildings Technology, data analytics and cyber security. This will enable creation of the database archives and distributed analytics necessary to exploit and monetize streaming data from sensor networks. The key problems that we plan to address are identifying flexible micro-grid architectures, leveraging ubiquitous sensing and associated data analytics, and developing appropriate distributed control algorithms for high renewable penetration.

Specifically, in the second year of this project, we propose a two-layered approach to the grid initiative project development, overarching project development and integration of team control projects in the other focus areas of inverter control and electric vehicles.

In 2016, GIG will be integrating their Hardware-in-the-Loop system (HIL with Opal-RT), with the FLEXLAB PV+storage test site. HIL allows the team to test complex embedded systems, novel inverter control, electric vehicle integration, and demand response, without needing a live electrical grid infrastructure, which can often be limiting to the scope of demonstration projects. The second prong of this approach will include the addition of the grid teams' projects to the HIL platform. The Grid Initiative, in addition to demonstrating the 100% PV case in the HIL grid integration platform, propose to add additional contributing projects proposed by staff in ETA.

### *Accomplishments*

Our most significant accomplishments have been 1) to set up a HIL system in FLEXLAB, called FLEXGRID, and 2) to develop and publish novel distributed control algorithms that detect anomalies of distribution assets. FLEXGRID has been set up with the Opal RT real-time digital simulator connected to the PV panels, inverters, microsynchrophasors ( $\mu$ PMUs), and batteries installed at FLEXLAB, as shown in Figure 1. It is currently being used for three supporting projects funded by DOE, and has been shown to DOE managers and collaborators. Data streams from  $\mu$ PMUs and inverters have been successfully connected and demonstrated. FLEXGRID provides tremendous opportunities in verifying control strategies with new data streams and control devices such as inverters in a real-world environment that can be difficult to replicate at a power distribution system. We anticipate more projects and proposals to utilize FLEXGRID for demonstration purposes that strengthen the projects.

We have also developed, demonstrated, and published distributed control algorithms for high renewable penetration using data analytics and flexible microgrid architectures, as shown in the publications list.

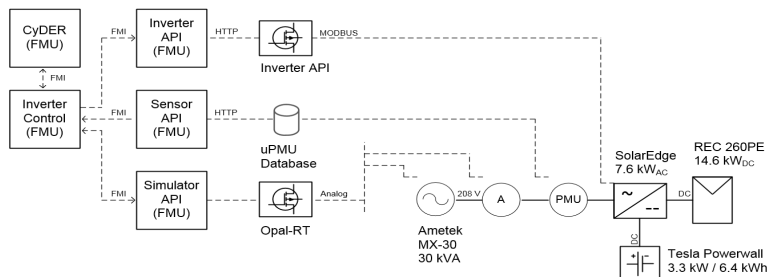


Figure 1. FLEXGRID hardware-in-the-loop test setting

## Enhanced Seawater Desalination from Materials Architectures Derived from Porous Aromatic Frameworks

Jeffrey R. Long, Jeffrey J. Urban, and Robert Kostecki

### Project Description

The goal of this project is to design polymers, specifically porous aromatic frameworks (PAFs), for seawater desalination by the capture of NaCl ions from aqueous solution. Due to their high porosity, synthetic tunability, and chemical and thermal stability, PAFs are a promising class of materials for this application. We approached this goal by designing and synthesizing PAFs that are densely functionalized with oxygen-containing moieties, whose pore architectures mimic sodium binding groups such as crown ethers and spherands. Sodium cations will diffuse into the polymer and be chelated by multiple oxygen atoms, and  $\text{Cl}^-$  ions will accompany the  $\text{Na}^+$  ions into the polymer in order to maintain electroneutrality. With optimization of functionality and pore size, our proposed materials can potentially desalinate seawater (35 g NaCl/L) with as little as 60 g of polymer per liter. We note that this ultimate target, if achieved, would propel these materials immediately into consideration for use in emergency relief situations for one-time use in desalinating brackish water.

After extensive synthesis and screening, the leading materials identified for NaCl uptake have been studied for system regeneration using solar-thermal means. The goal is to effect regeneration of the PAF by removing the bound NaCl using minimal energy and solvent inputs. We anticipate that the small amount of current needed to regenerate the polymer could be supplied by a battery integrated with a photovoltaic panel. This system would allow PAF regeneration with a minimal energetic footprint.

### Accomplishments

We have synthesized 18 functionalized PAFs via diverse synthetic routes. The synthesized polymers contain sodium-binding groups, including carboxylic acids, phenols, alcohols, and ether chains of varying lengths.

These materials were characterized by elemental analysis, infrared spectroscopy, solid-state NMR spectroscopy and gas adsorption analysis, and were subsequently tested for desalination performance using a salinity meter (based upon conductivity) and in some cases inductively coupled plasma mass spectrometry (ICP-MS). Results ranging from no effect to a 14% decrease in salinity were observed, using 20 mg polymer in 7 mL of 3.5 g NaCl/L aqueous solution.

The leading material, which caused the 14% decrease in salinity, is a PAF-1 derivative. Upon scaling up the current leading material for further study, its desalination performance was not fully reproduced, and efforts to effectively reproduce the synthesis of this compound and to verify its NaCl capacity were unsuccessful after many trials. In light of this and other experimental obstacles, the goal of this project was redirected from NaCl capture towards the capture of trace contaminants in seawater such as boron and cesium.

## Water in Confined Spaces to enable Desalination and Separations

Robert Kostecki and Musahid Ahmed

### *Project Description*

Without water there is no life. Access to clean water for drinking, agriculture and energy generation is an engineering and scientific grand challenge in the 21<sup>st</sup> century. Traditional desalination processes are cost-prohibitive; a new way of thinking is required to make this process economically viable. Experimental data and theory models seem to indicate that water confined by solid walls to spaces smaller than a few tens of nanometers can give rise to anomalous properties which could be harnessed for desalination. It is our purpose to probe and tune these properties at the molecular level, to enable a device design that will shape a new paradigm in desalination and separation. We propose to explore the physical and chemical properties of nano-confined water via a unique blend of inorganic synthesis, and spectroscopy coupled to novel micro-droplet and aerosol methods. We will synthesize inorganic micelles (mesoporous silica nanoparticles) and carbon nanotubes with hollow cores of several nanometers in diameter. Ionic salt solutions will be introduced into these cores, and the changes in properties will be followed with X-ray, Raman, terahertz, and infrared (IR) spectroscopy. Different synthetic routes will also be explored to change the properties of the confining walls and vary the interface of the inner wall of the pore. By probing the changes that occur upon confinement in novel chemical environments, we will enable material scientists to conceptualize and design new systems for water desalination.

### *Accomplishments*

A synthetic strategy to prepare hollow core shells has been perfected, and water uptake in these systems has been demonstrated with Fourier Transform Infrared Spectroscopy. This will be extended to probing single nanoparticle water uptake using synchrotron based IR microscopy, preliminary results of which have already been acquired. A new technique for probing aqueous nanoparticles with X-ray photoelectron spectroscopy has been reported in a paper recently in the *Journal of Chemical Physics*. In the coming year, this technique will be applied to synthesized nanoparticles. Both laser (IR & Raman), and synchrotron (X-Ray, IR and Terahertz spectroscopy) methods will be applied to probe water solutions in confined spaces. The technique we are employing to study nano confined water is a type of absorption spectroscopy called attenuated total reflection (ATR) spectroscopy.

## VOLUMETRIC ABSORPTION OF SOLAR RADIATION IN LIQUIDS AND GASES BY TUNING THE EMISSIVITY OF SURFACES

Principal Investigator: Ravi S. Prasher

### *Project Description*

Solar-to-thermal energy conversion is important for many renewable energy applications, such as concentrated solar electricity production, water desalination, thermochemical reactions, water heating, and thermal storage. All of these applications involve the heating of liquids and gases. Currently, solar heating of the heat transfer fluid in all these applications is achieved through surface-based methods, where the heat is transferred via convection using heat exchangers to the fluid. This results in a solar-to-thermal energy conversion efficiency between 40–60% depending on the temperature. One potential way to significantly increase the solar-to-thermal energy conversion is to volumetrically absorb solar radiation directly into the fluid. Various researchers have tried to solve this problem by seeding heat transfer fluids with nanoparticles, thereby making the fluid black, leading to volumetric absorption of solar. This approach has not been successful in spite of ~30 years of research because the nanoparticle-laden fluid affects the performance and reliability of the pumps that pump the heat transfer fluids.

### *Accomplishments*

The main accomplishment in this year is that we have developed a thin film based selective solar absorber (SSA) that is stable at much higher temperatures compared to the state-of-the-art SSAs in ambient conditions. High temperature thermal energy plays a vital role in **electricity, industrial, chemical processing and fuel sectors**. Converting solar energy into thermal energy has been limited to temperatures of less than 900K due to the lack of stable high temperature SSA. Resolving this limitation is considered to be one of the biggest challenges for converting solar energy into high temperature thermal energy. Figure 1 shows the experimental results on the high temperature testing which shows negligible degradation.

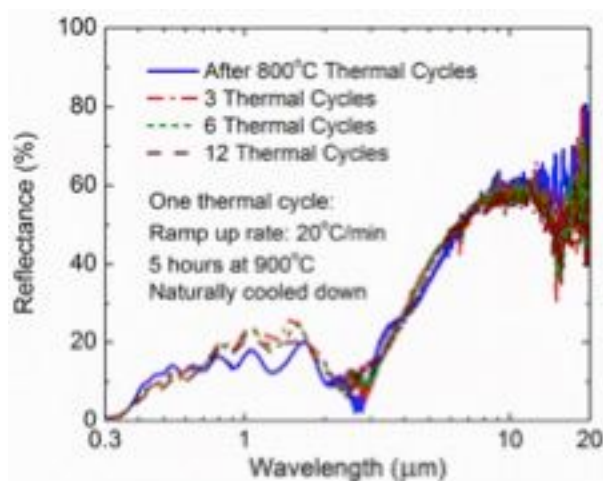


Figure 1: Reflectance of high temperature SSA

## SCIENCE OF SCALE UP

Gerd Ceder, Ravi Prasher, Vivek Subramanian

### *Project Description*

The overarching goal of this project has been to advance the science of scale up, with an initial focus on fabrication of energy storage devices. Electrochemical batteries typically consist of dried porous slurry coatings on metal foil current collectors. This project has specifically focused on the understanding the slurry rheology, the cathode materials synthesis and additive manufacturing of batteries. This project is developing competency in three areas: 1) Synthesis Science 2) Processing Science 3) Manufacturing Science

### *Accomplishments*

Synthesis Science: The synthesis of cathode materials is being studied with a machine learning and text mining approach. Using Natural Language Processing (NLP) methods synthesis procedures for lithium battery cathode materials are extracted from the large body of scientific literature. These recipes are then analyzed to better understand the synthesis of cathode materials. Agreements have been negotiated with publishers to download full text (html, xml, and pdf format) of 3 million research papers. A software tool to download the papers has been built and is fully operational. After download, papers undergo conversion to plain text so that NLP tools can be used on them. In the initial stage we have prioritized HTML and XML to text conversion and abandoned pdf to text conversion due to its complexity. To start the extraction of recipes, we successfully developed machine learning algorithms to identify the targets of reactions and their precursors with  $\approx 85\%$  precision. This precision will have to be improved to extract full recipes accurately. We are currently exploring various novel approaches with the target of  $> 95\%$  precision while maintaining  $> 50\%$  recall.

Processing Science: Understanding of the rheological properties of electrode slurry in batteries is highly desirable for optimizing and increasing the performance of batteries made from roll to roll process. Therefore it is very important to measure rheological properties with great accuracy so that rheological models can be developed. A high accuracy rheometer was bought to understand the rheology of highly dense slurry where colloidal interactions are very important. We have started to collect fundamental rheology data. Data is currently showing that size of the particle and the molecular weight of the polymer plays a very significant role in the rheology of the slurry.

Manufacturing Science: We are particularly focusing on two battery technologies herein – chip-scale batteries for emerging applications in IoT, and flow batteries. Both suffer from poor development cycles in the current state of the art. Our biggest accomplishment has been the realization of an additively fabricated chip-scale (i.e., mm-size thin film) battery delivering unprecedented energy and power density, integrated within a chip package. The performance of this cell far exceeds any other reported thin film cell, particularly at this size scale. This is an important result for emerging applications in IoT, wearables, etc. The battery is based on a thin film chemistry that we have developed. We have integrated the cell within an additively fabricated chip package to power a sensor chip.



## **Advancement of a High-Impact Desalination Technology**

Principal Investigator(s): Chinmayee, Subban

### *Project Description*

Charge-based salt separation is more energy-efficient than membrane-based methods (reverse osmosis) for desalination of widely available, low-intermediate salinity, brackish water sources. However, existing charge-based salt separation technologies (capacitive deionization, electrodialysis) rely on the use of ion-specific membranes which are expensive and need regular maintenance. The use of membranes adds considerably to the capital and operating costs of these technologies, and has limited their adoption and widespread use today. There is hence a need for new electrode materials that are inexpensive and membrane-free.

The purpose of this project is to develop novel electrodes that are based on inexpensive ion-exchange resins (IER). The use of IER in charge-based salt separation requires making good electrical contact to the insulating resins. Hence we will explore various methods to induce the necessary electrical conductivity to build a functional IER-based electrode suitable for brackish water treatment. Given the limited temperature stability of IER, this will require exploring various methods including but not limited to use of conductive additives and chemical- and plasma-based processes for surface conductive coatings. The end application of the novel electrodes will be need to be tested in-device, for which we will develop processing methods to convert the conductive IER into functional electrodes, design a prototype unit, and test the electrode robustness and salt removal capabilities in the prototype.

### *Accomplishments*

A major accomplishment has been the development of methods to reliably make electrical contact with insulating IER. A second accomplishment has been the development of processing techniques to uniformly transfer the electrode mixture as a thin-film on to a metal current collector substrate.

Another notable accomplishment has been the design and assembly of an automated testing setup along with custom software to conduct continuous cycling and performance testing of the composite electrodes in a prototype device. Preliminary results show comparable salt removal by IER-composite electrodes and electrodes used in commercial capacitive deionization units.

A key accomplishment has been identifying unique operational capabilities that result from use of IER—desalination without an applied voltage and regeneration with an applied voltage. This mode of operation is different from all existing charge-based salt separation techniques and is unique to our IER-composite electrodes. We refer to this new approach as “Electrically Regenerated Ion-exchange (ERI) technology”.

We are currently optimizing the electrode composition, and prototype operating conditions to achieve higher salt removal performance and longer electrode lifetime. Although the preliminary results are promising, extensive characterization and testing remain in order to gain mechanistic understanding of ERI technology operation.

## **Revealing Dynamics of the Functional Connectome**

Principal Investigator(s): Peter Denes, Kris Bouchard, Stefano Cabrini, Bruce Cohen

### *Project Description*

Our goal is to apply tools we have previously developed in model systems in order to demonstrate an ability for high channel count, multi-modal stimulation and recording from the brain. Large area electrical recording will capture information over a variety of spatiotemporal scales, and at high speed. Optical stimulation, including techniques for delivering light deeper than currently possible, will enable precise manipulation of neuronal activity. Lastly, employing NERSC to deal with the large data volume and analysis, together with needed computation and theory developments, will elucidate brain function, and show that we are able to provide an integrated computing solution.

### *Accomplishments*

We have: 1) built software tools to understand how characteristics of neural data acquisition effect subsequent analysis to optimize hardware for end use of the signal; 2) applied deep learning algorithms to extract complex structure from brain recordings; 3) successfully scaled our statical data analysis algorithms to run on NERSC HPC systems and applied these methods to neural data collected from UCSF and here at LBNL (see below).

We have set-up a state-of-the-art neurophysiology experimental system for in vivo acquisition of multi-modal neural data. Using this apparatus, we have: 1) performed tests of the LBNL developed E-Chip electrophysiology integrated circuit; 2) conducted basic neuroscience experiments with standard recording devices to reveal basic features of neural signals across multiple spatiotemporal scales; 3) conducted a first-of-its-kind experiment combining electrocorticography and laminar polytrodes with optical imaging and manipulation of neurons.

Our approach to very high channel count recordings has been modified from direct contact of the E-Chip to the brain, to one in which the E-Chip is bump-bonded onto a flexible electrode array. We have also produced interfaces which allow the E-Chip to be used with conventional laminar polytrodes.

For deep-tissue optical measurement of neural activity, we have paired fluorescent organic biosensors for detecting critical ions and metabolites with upconverting nanoparticles (UCNPs), which absorb tissue-penetrating near infrared (NIR) light and are able to excite surface-conjugated biosensors. We have optimized this upconverted energy transfer (UET) to greater than 95% and shown that probe photostability is increased up to 100-fold. For sensor targeting, we have developed methodology for the controlled covalent attachment of biomolecules to UCNP surfaces. UCNPs optimized for efficient UET of fluorescent pH, Na<sup>+</sup>, and K<sup>+</sup> sensors have been developed and are being deployed to monitor the ion flux underpinning neural activity.

We developed laminar polytrodes that are able to perform electrical readout (electrophysiology) and optical stimulation (optogenetics) plus control the location and shape of output light by means of optical interference. The dimensions of these devices are less invasive than many commercial neural probes and have demonstrated sufficient light output for channelrhodopsin activation within close proximity of the shank (10 – 20  $\mu$ m). We expect these results to help move brain science towards a more precise manipulation of light inside deep brain tissue for single cell optical manipulation in in-vivo neuroscience experiments.

## Nanometer CMOS for Custom Computing and Future Detectors

### Principal Investigator(s): Carl Grace

#### *Project Description*

Advances in microelectronics are key to developing better detecting tools. For many years, increases in achievable transistor density have driven improvements in detectors. Recently however, progress has slowed in part due to emerging bottlenecks in data transport. The power density of modern integrated circuits is reaching its limit and data transport is a primary drive in on-chip power dissipation.

The most straight-forward way to address the problem of too much data is not to send it in the first place. To reduce the volume of data we can process it locally, on the detector. By not sending as much data, detector speed and functionality can increase. By extracting salient features of the data and sending those out for further analysis the detector takes on an enhanced role in the system.

Single-purpose hardware can be effective, but programmable hardware is more flexible and enables processing that is matched to the experiment, even after the detector is built. In addition, custom instructions that match the hardware to the algorithm can increase performance or reduce power dissipation by over an order-of-magnitude compared to current practice. To enable custom processor development, we are leveraging emerging open-source tools, such as RISC-V, Chisel, and OpenSoC Architect.

RISC-V is an open-source Instruction Set Architecture that is extensible and can be implemented without licensing cost. To automate the development of customized RISC-V processors, we use Chisel (Creating Hardware in a Scala Embedded Language) which enables development of hardware at a much higher level of abstraction than typical practice, enhancing designer productivity. OpenSoC Architect is an open-source tool developed at Berkeley lab that enables assembly of a complex chip from components described in Chisel.

#### *Accomplishments*

We have developed a custom multi-core microprocessor based on RISC-V using Chisel. We have validated it by implementing the on a Field-Programmable Gate Array (FPGA) and running representative algorithms. We have developed a custom digital design flow in both 65 nm and 180 nm CMOS technologies and have implemented the physical design of the RISC-V processor in 65 nm. We have also succeeding in developing an implementation flow for embedded cache memories needed by the processor.

We are in the process of verifying the physical implementation and preparing it for fabrication. We will also define and implement representative custom instructions that will quantify both the performance and power dissipation improvements compared to current practice.

## MICROBIOME ADAPTATION IN RESPONSE TO ENVIRONMENTAL CHALLENGES

Principal Investigator(s): (Susan Celniker)

### *Project Description*

The purpose of this project is to characterize the role of the microbiome in adaptation to environmental challenges. The microbiome has been linked to brain health, liver function, bowel disease, and many other physiological and behavioral phenotypes in a growing number of studies. However, the response of the microbiome to chemical perturbations is poorly understood. Accidental human and animal herbicide exposures to agricultural chemicals remain a serious problem in the United States, which accounts for 32% of the total global pesticide market. Here, we will characterize the role of the microbiome in adaptation to chronic pesticide exposures at environmentally relevant doses. By using both invertebrate and mammalian models, we will elucidate the impact of the gut microbiome on host health and generate an atlas of microbiome chemical interactions.

We plan to measure the immediate and long-term responses of the gut microbiome to the top most utilized herbicides in the United States using the model organism *Drosophila melanogaster*. By utilizing both gnotobiotic and wild-type flies in our perturbations, we will isolate effects specifically due to the microbiome. In the mouse, we will study two compounds, informed by our fly model, in pre-adolescent exposure scenarios and long-term effects. As in the fly, we will use genomic and metabolomics techniques. Detailed, life course assays throughout a 12-week span will provide an extensive map of the dynamic composition of mammalian gut microbiomes. Utilizing the collaborative cross mice and also specified microbial compositions will enable the identification of microbiome chemical and genetic interactions.

We will be able to correlate pesticide-induced changes in behavior with changes in the microbiome, while controlling for genetic background. Importantly, we propose to establish a mammalian gnotobiotic resource facility at LBNL, an expertise that remains in short supply in the US and which is a critical component of the 'Microbes to Biomes' initiative necessary to make the transition from correlative science to causal proof.

### *Accomplishments*

Using PacBio technology we sequenced eight species and for six (*A. tropicalis*, *L. brevis*, *B. kochii*, *E. durans*, *L. plantarum*, *A. pomorum*), we identified a large core circular genome in a single gapless contig assembly and published five of the genomes (see the publication list below). Two others (*P. taichungensis*, *B. flexus*) are in three contigs. In the case of the well-studied *Acetobacter tropicalis* this greatly improved assembly (the previous assembly was in hundreds of small contigs and revealed >1000 new genes and fundamentally new metabolic potentials. It has long been suspected that fruit flies receive folate (vitamin B12) from their microbiomes, since feeding antibiotics strongly reduces growth and survival on folate-free media. We found that the genome of *Acetobacter tropicalis*, one of the most abundant species in the fly gut, includes a complete folate synthesis pathway. Further, in all eight species sequenced, we identified complete plasmid and viral sequences that expand the metabolic potential of these microorganisms.

In *Acetobacter tropicalis*, we found a set of enzymes required for atrazine metabolism on a single plasmid. This led us to hypothesize that gnotobiotic flies lacking this pathway should be significantly more susceptible to toxicity from atrazine than our wildtype strain. We generated axenic adult flies and recapitulated exposures. As expected, germ free (GF) flies exposed to atrazine died earlier than control flies with wild-type microbiomes. Further, we were able to fully rescue GF flies and restore wildtype survival curves by feeding flies *A. tropicalis* culture prior to atrazine exposure. We attempted similar rescue experiments with other microbes, none of which rescued, as expected. We illustrate that the GF condition does not make flies uniformly more susceptible to toxic compounds, as the wildtype microbiome offers no protection against paraquat toxicity. These studies were presented for an invited talk at the Society of Environmental Toxicology and Chemistry (SETAC) meeting in Orlando Florida (Nov 7, 2016).

## **Identification, Biomanufacturing and Characterization of Cyclic DiPeptides (CDPs), a Diverse Family of Chemicals Involved in Mediating Microbial Interactions**

Samuel Deutsch

### *Project Description*

This project seeks to improve our ability to identify new microbial secondary metabolites, such as cyclic dipeptides or other non-ribosomal peptides using a combination of synthetic biology, and OMICs platforms such as RNA-seq and LC-MS based metabolomics that can be integrated in new ways to drive and accelerate novel molecule discovery. Microbial secondary metabolites are rich sources of industrially relevant chemical compounds, since they have been linked to a number of important biological functions including plant growth promotion, mediation of microbe-microbe interactions, antimicrobial/antifungal activities and the activation/repression of a number of protein ligands including transcription factors, proteases and transporters. Next generation DNA-sequencing technologies continuously provide new microbial and fungal genomes that contain large numbers of pathways involved the biosynthesis of natural products. These sequencing and bioinformatics efforts greatly outpace the discovery and characterization rate of their products, due to bottlenecks in cell culture methods, and a lack of understanding on how to effectively activate the production of such compounds under laboratory conditions.

For this project we devised a co-culture scheme previously shown to result in the activation of secondary metabolites and applied a workflow involving DNA and RNA sequencing, metabolomics (LC-MS), DNA synthesis and advanced computational methods to discover and characterize new molecules. Although these methods have been applied at a pilot-scale level, the ultimate goal is to develop scalable workflows that can be used to discover 1000s of novel molecules.

### *Accomplishments*

As part of this study we analyzed the genomes of >100 actinobacteria recently sequenced at the JGI to identify genetic pathways that have a high likelihood of encoding secondary metabolites. These pathways are commonly referred to as Biosynthetic Gene Clusters or BGCs. By performing computational analysis on the newly sequenced genomes we were able to identify over 1400 BGCs. To select a subset of the sequenced species and prioritize BGCs for further characterization we selected 5 species based on phylogenetic diversity, the number of potential BGCs that they encode and their novelty based on a comparison to a database of previously characterized compounds. We set-up all the co-culture experiments according to our experimental design and collected samples over a time-course for RNA sequencing and metabolomics analysis. Samples were extracted and submitted for analysis and the resulting data were analyzed and integrated using a novel statistical workflow.

To date, we have identified 34 new compounds that were further classified into 15 biosynthetic groups based on their MS/MS spectra. None of these compounds matches known molecules in chemical databases. Through the RNA sequencing data we have identified at least 1 genomic cluster that can be linked to a novel NRPS molecule, although we are pursuing several other candidate clusters with additional RNA-seq experiments. Characterization of structures of these novel compounds through purification and NMR analysis is on-going.

## Deconvoluting Tissue Heterogeneity Through Single-Cell Transcriptomics

Principal Investigator: Diane Dickel

### *Project Description*

To measure organismal responses to changing environmental conditions, a strategic focus of the LBNL Biosciences Area, improved technologies are needed to deconvolute heterogeneous cell populations. Recent advances in microfluidic and sequencing technologies allow for the capture and sequence profiling of individual cells within a sample. Through sequencing the RNA present in single cells, this nascent technology has been used to profile the heterogeneity present in mammalian tissue samples. Although theoretically applicable to organisms across the tree of life, high-throughput single-cell RNA sequencing methods have not yet been applied broadly to non-mammalian organisms. The goal of this LDRD is to import and further develop Drop-seq, a nascent single cell genomics technology, at LBNL for the purposes of characterizing tissue heterogeneity in a variety of mammalian tissues, plant protoplasts, and multinucleated cell types. We will establish robust single-cell RNA sequencing protocols and analysis pipelines for each of these tissue types.

### *Accomplishments*

Over the first year of this funding, we successfully established an end-to-end single-cell RNA sequencing pipeline based on micro-fluidic and DNA barcoding technologies. After optimizing the protocol using cultured cells, we have used it to profile the gene expression of a variety of different types of mammalian tissue samples. As part of this work, we demonstrated that this technique can be used to capture the expression of a fluorescent reporter gene, in addition to native gene expression. This important advance opened up multiple avenues for using single-cell RNA-seq to study the cell types that are genetically labeled with such reporter genes. This work was included in a manuscript that has been accepted to the journal *Cell* and will be published in early 2018.

A second aim of this grant is to apply this technology to profiling organisms related to environmental and bioenergy applications. To this end, we have established protocols for performing single-cell RNA-seq on tissue protoplasts from a commonly used plant model organism. We have now performed the highest-throughput single-cell profiling of any plant tissue to date. A manuscript describing this work is in preparation.

A third aim of this grant is to apply this technology to profiling gene expression from nuclei, rather than whole cells. To date, we have performed a proof-of-principle on nuclei from mammalian tissue using our now standard pipeline. Efforts to scale up, further optimize, and apply this protocol to other organisms are ongoing.

## A Systems Biology Approach to Dissecting Regulatory and Metabolic Networks of Filamentous Fungi involved in Carbon Cycling

Principle Investigator: N. Louise Glass

### *Project Description*

Filamentous fungi have the ability to cooperate or compete for nutrient sources in nature, such as plant biomass. The mycelial network of filamentous is essential in the exploitation of ecological niches, transport and utilization of nutrients and organellar transport. We use the *Neurospora crassa* to integrate cellular pathways required for cooperation, competition and nutrient signaling by construction of regulatory hierarchies using a systems biology approach. An understanding the mechanisms of cooperation is important for understanding ecosystem function and for plant and animal pathogenesis. Filamentous fungi also compete in nature, which triggers a mutual killing response. We identified a regulatory pathways associated with cell death that, based on both functional and computational approaches, is similar to animal pyroptosis, a cell killing process associate with inflammation and innate immunity. These data will be integrated into models on how competition affects nutrient exploitation using model laboratory systems that will inform ecosystem function.

We will use genomic, biochemical and genetic tools to define the mechanisms of action of pyroptosis and innate immunity in filamentous fungi, including structural information on proteins involved in allorecognition to decipher the molecular mechanism of nonself recognition. Using population genomics approaches, we will derive laboratory experimental data, followed by computation and modeling, to extend these analyses to understand cooperative and competitive interactions of filamentous fungi in nature, using *N. crassa* as a model saprophytic fungus, who primary function in nature is to deconstruct plant biomass. We will further hypotheses on sensing, communication, competition and plant biomass utilization/carbon cycling to identify new components using both forward and reverse genetic approaches.

### *Accomplishments*

Our recent work has shown that filamentous fungi have an innate immunity system that has evolved independent from animal and plant immunity systems, but is regulated by proteins with similar structure, so called NOD-like receptors or NLRs. In filamentous fungi, these proteins regulate allorecognition and cell death of incompatible colonies following cell fusion. Genetic differences at the NLR-like loci regulate the capacity of filamentous fungal colonies to either cooperate or compete when utilizing resources, such as dead plant biomass, which in the natural habitat of *N. crassa*. Our data is the first to indicate that fungal NLR-like proteins biochemically function similarly to NLR immune receptors in plants and animals, showing that NLRs are major contributors to innate immunity in plants and animals and for allorecognition in fungi.

## **Eco-FAB: discovering the genetic basis of a beneficial microbiome to improve crop productivity**

**Research team:** PI: Trent Northen; Amélie Gaudin, Adam Deutschbauer, John Vogel, Dominique Loque, Yasuo Yoshikuni, Romy Chakraborty

### *Project Description*

This project will develop the Eco-FAB (Ecosystem Fabricator) that enables control, measurement and manipulation of the plant-microbiome and to discover beneficial plant-microbiome interactions to sustainably increase agricultural yields. A focus of this project is to discover key traits lost in current maize cultivars for attracting and maintaining beneficial microbiomes in marginal, conventional, and organic soils.

### *Accomplishments*

Experiments were conducted with 12 maize cultivars representing 4 historical groups: teosinte (wild relative), landrace (early domestication), inbred (parents of modern hybrids), and modern hybrids. All cultivars were grown in a UC Davis greenhouse with three soil types (marginal, conventional, organic). Rhizosphere soil samples were collected for bacterial isolation and microbial community analysis. Microbial community analysis of rhizosphere soil samples was conducted with 16S-V4 and ITS2 amplicon sequencing. Community composition differed between soil types and between historical groups of cultivars. Within samples from marginal soil, 3.6% of community members were significantly differentially abundant between cultivar groups, and 0.8 % were identified as indicator species for particular cultivar groups. We have isolated nearly 500 isolates from these marginal rhizosphere samples. Initial taxonomic assignment of isolates indicates that those obtained from one teosinte (PI 566704) were distinct from the other cultivars. A subset of these isolates (88), representing at least one species from each genera isolated, were chosen for plant growth promoting (PGP) traits assays (phosphate and zinc solubilization, indole acetic acid (IAA) production, siderophore production, ACC deaminase activity, HCN production, potassium solubilization and nitrogen fixation). Eighty-one among 88 isolates possess one or more PGP traits, and interestingly, genus *Paraburkholderia* showed the highest number of PGP traits followed by *Brevundimonas* and *Bacillus*, from these 40 isolates are being sequenced.

The root exudate composition of the 12 maize cultivars has been investigated. Plants were grown in newly-designed hydroponic reactors under non-sterile and sterile conditions. Root exudate samples were collected at several time points and analyzed for metabolite profiling using both GC-MS and LC-MS-MS. Under sterile conditions, diurnal and nocturnal samples were collected and are currently being analyzed to investigate the evolution of maize root exudation controlled by circadian clocks. Interestingly, the levels of organic carbon released by maize roots were found to be similar for diurnal and nocturnal samples. UV-vis spectra and fluorescence fingerprints were distinct between diurnal and nocturnal samples, and differential among various cultivars. GC-MS and LC-MS-MS data are currently being interpreted by targeted and untargeted analysis to unravel root exudate compositions. The response of a subset (4) of maize cultivars to varying phosphate availability was also studied. Preliminary experiments identified changes in root exudate composition, with 4 metabolites being detected only from phosphate stressed plants. Microbial community analysis and metabolomic analysis of root exudates are underway.



**PLANT GROWTH PROMOTING MICROBES: SIGNALING AND MECHANISMS**

Principal Investigator(s): Vogel, John

*Project Description*

Plant growth promoting microbes hold tremendous potential to greatly increase crop yields by stimulating plant growth and preventing disease. Despite their enormous potential, beneficial microbes are not widely deployed in large-scale agriculture because of their unpredictable performance. Thus, fundamental systems level knowledge about all aspects of the interaction between plants, beneficial microbes and the microbiome is needed to harness the benefits of the microbiome. The extreme complexity of the soil microbiome is a major impediment to acquiring this knowledge. This project seeks to establish a simplified experimental system to rigorously study the interaction between a model plant and a defined root microbiome and then use this system to identify plant genes required for beneficial plant-microbe interactions and/or microbial colonization of roots. We will use a forward genetic screen to identify plant mutants that affect microbiome composition or function and we will use transcriptional profiling to identify candidate plant genes involved in the interaction. Mutants and candidate genes will be characterized using the large amount of experimental tools that have been assembled in the lab over the past 14 years (e.g. sequenced mutant collections, sequenced natural accessions, efficient transformation and CRISPR, etc.)

*Accomplishments*

Based on 16s sequencing of the root microbiomes of 192 *B. distachyon* mutants that were inoculated with our defined microbiome we identified one line with a dramatically different microbiome. We are re-testing that line now to see if it is a bona fide mutant. We made several improvements to our inoculation method to improve reproducibility and throughput. Using this revised method we inoculated 384 mutants and submitted DNA samples for 16s sequencing. The mutant screen is continuing.

We hosted the collaborator who selected the improved microbiome that was the sources of many of the isolates in our defined microbiome. During his visit we analyzed 16S data from the root microbiomes at each generation of microbiome selection from replicated trials of microbiomes that were selected to confer tolerance to two different salts. We detected reproducible changes in microbiome composition suggesting that the selected microbiomes employ a reproducible mechanism to benefit plants. Interestingly, the microbiomes selected to confer tolerance to one salt did not confer tolerance to the other salt and had different microbial compositions.

## Design of High-Energy Density Alkali-Ion Systems

Principal Investigator(s): Gerbrand Ceder

### *Project Description*

Li-ion batteries provide the highest energy density of any rechargeable battery system, and as such have become the technology of choice for everything from portable electronics to electrical vehicles. To further improve energy density, we are pursuing several novel directions for energy storage technology: Solid-state batteries have the potential for increased safety as they contain a non-flammable solid state conductor, in contrast to the highly flammable organic solvents used in traditional Li-ion batteries. We have developed the capability to make fully solid-state devices without any flammable liquid electrolyte. Using a thio-phosphate solid-state conductor as separator and as additive to the cathode, pellet based cells have shown very good initial performance. However, obtaining a stable interface between these electrolytes and electrodes is difficult. Without simple yet powerful tools, these compatibility issues cannot be systematically investigated, thus hindering the generalization of design rules for the integration of solid-state battery components.

We have also been exploring non Li-ion technologies to escape the cost and resource constraints posed by Li-ion systems. Specifically, K-ion batteries have emerged as a possible energy storage in recent years, because of the abundance of K resources in the Earth's crust and oceans. K has a lower standard redox potential than Na and even Li in non-aqueous electrolytes, which can be translated into a potentially higher cell voltage compared with those of Na or Li systems. More importantly, the capability of graphite storing K ions, unlike Na system, attracts much attention. In our work we developed layered structured  $\text{K}_{0.6}\text{CoO}_2$  and  $\text{K}_{0.5}\text{MnO}_2$  cathodes for K ion batteries. They show a moderate specific capacity of  $\sim 80\text{--}100$  mAh/g by a reversible topotatic K de/intercalation reaction. Our works also demonstrate the feasibility of rocking-chair K ion batteries that uses layered  $\text{K}_{0.6}\text{CoO}_2$  cathode and graphite anode with non-aqueous carbonate electrolytes for the first time. However, for practical full cell application, they require prepotassiation process because of their K deficient composition. In addition, their low working voltage of  $< 3.0$  V limits their practical application. Therefore, further study is required to design high energy cathode materials for K ion batteries and we are currently working on it.

### *Accomplishments*

We have achieved a novel strategy of combining high-valent cations, partial oxygen to fluorine substitution, and a disordered rock-salt structure, to incorporate the  $\text{Mn}^{2+}/\text{Mn}^{4+}$  double redox couple in Li-excess cathode materials that achieve ultrahigh capacity ( $> 300$  mAh/g) and energy density ( $\sim 1000$  Wh/kg).

As for solid-state batteries, we have already developed a method combining density functional theory calculations and simple experimental techniques which can efficiently screen the compatibility of numerous electrode/electrolyte pairs. With the interface issue further understood, solid-state batteries with higher capacity and better retention will be designed.

## **Differentiation Within Order: Designing and Probing Bio-Inspired Optical Networks for Patterning Assemblies of Nanoparticles**

Principal Investigators: P. James Schuck and Emory Chan

### *Project Description*

The objective of this research is to develop methods for patterning assemblies of nanoparticles with 1-100 nm resolution. To differentiate function without independently addressing each nanoparticle in a two-dimensional lattice of inorganic nanocrystals, we aim to design nanoparticles with energy transfer interactions modeled after the reaction-diffusion networks that pattern natural organisms. Our approach is to translate the essential reaction and diffusion operations in biological pattern formation into the analogous photophysical processes in lanthanide-doped nanoparticles. Optimized networks of these energy transfer processes will produce dynamic reaction-diffusion features with nanometer resolution. This dynamic patterning could ultimately be used to produce complex mesostructures with emergent material function over millimeter length scales.

Our biologically inspired approach harnesses energy transfer between the excited states of lanthanide ions doped in colloidal nanocrystals, where the excited states of lanthanide ions exhibit the three elementary processes found in biological patterning networks: amplification, inhibition, and diffusion. We will use Kinetic Monte Carlo modeling to design a library of structures that direct these three elementary processes. We will synthesize variations of the most promising heterostructures in parallel using nanocrystal synthesis robots. Finally, we will assemble nanoparticles into superlattices that, under wide-field illumination, spontaneously produce two-dimensional patterns of light emission known as Turing patterns.

### *Accomplishments*

Our first accomplishment was to develop a Kinetic Monte Carlo suite that models energy transfer and other photophysical processes in nanoparticles with arbitrarily complex dopant compositions. These simulations were demonstrated to capture the three essential processes of patterning networks, including the amplification of the lanthanide excited state populations, as well as the diffusion of these states across nanoparticles. This KMC tool will enable the pre-screening of thousands of possible compositions for those that exhibit spatially heterogeneous light emission.

Our major experimental accomplishment has been to develop a library of nanoscale energy transfer motifs that amplify lanthanide excited states. We previously developed nanoparticles that amplify the 800-nm emission of  $\text{Tm}^{3+}$  using a process known as energy looping. To characterize whether this amplification is sufficient to sustain patterning, we used confocal microscopy to measure the stimulated emission of energy-looping nanoparticles (ELNPs) in microsphere cavities across a range of excitation powers. The amplification of  $\text{Tm}^{3+}$  excited state populations in these “whispering gallery” microcavities exhibits such high efficiency that we were able to observe continuous-wave upconverted lasing action at blue and infrared wavelengths. The low thresholds, robust lasing, and high population inversion in ELNPs strongly suggest that  $\text{Tm}^{3+}$ -doped domains can generate the non-linear amplification of excited states that is necessary to induce patterning. These early accomplishments form a solid foundation that will enable us to achieve our goal of patterning nanoscale light dynamically and far from equilibrium.

## Exploring Strong Visible Light-Matter Interactions in Correlated Oxide Materials

Principal Investigator(s): Lane W. Martin

### *Project Description*

The research program sought advances in the mesoscale science of light absorption, charge transport, and other aspects of electronic and energy materials. We aimed to discover, observe, characterize, understand, and ultimately control light absorption and charge transport in multi-component systems at the mesoscale. Building from Year 1 work, the objectives of this research program were to *explore the formation of self-assembled nanostructured metamaterials, the nature of light-matter interactions in these nanostructures, and the temperature and field-driven changes in optical response in these systems*. The program applied advanced thin-film synthesis, structural and chemical analyses, and probes of optical, electrical, and (light and dark) transport properties and will leverage existing collaborations to provide supporting first principles calculations, phase field models, ultrafast studies of dynamics, etc. in these systems. In the end, the program provided an in-depth understanding of the structural and chemical nature of self-assembled nanostructures which include correlated electron systems with strong field/temperature-dependent properties. Ultimately we will explore how these structures impact the performance of optical applications and emergent optical phenomena.

### *Accomplishments*

During this program, we have accomplished a number of important outcomes. First, we continued to work to explore the optical properties of a self-assembled metamaterial based on the innate spinodal decomposition of the  $\text{VO}_2\text{--TiO}_2$  system wherein the metal-to-insulator transition in  $\text{VO}_2$ , and thin-film epitaxy enable the production of self-organized nanostructures with coherent interfaces and a structural unit cell down to 15 nm (tunable between horizontally and vertically aligned lamellae) wherein the iso-frequency surface is temperature-tunable from elliptic to hyperbolic dispersion producing metamaterial behavior. We developed routes to control the nanostructure of these materials, thereby tuning the structure and properties of the system using growth rates, temperatures, etc. These results provide an efficient route for the fabrication of nanostructured metamaterials and other nanocomposites for desired functionalities. We are currently working on a publication to summarize this work.

Second, we probed emergent phenomena at polar-nonpolar oxide interfaces, namely the disentanglement of the critical thicknesses for electron reconstruction and the emergence of ferromagnetism in polar-mismatched  $\text{LaMnO}_3/\text{SrTiO}_3$  (001) heterostructures. Using a combination of element-specific x-ray absorption spectroscopy and dichroism, and first-principles calculations, interfacial electron accumulation, and ferromagnetism have been observed within the polar, antiferromagnetic insulator  $\text{LaMnO}_3$ . Our results show that the critical thickness for the onset of electron accumulation is as thin as 2 unit cells (UC), significantly thinner than the observed critical thickness for ferromagnetism of 5 UC. The absence of ferromagnetism below 5 UC is likely induced by electron over accumulation. In turn, by controlling the doping of the  $\text{LaMnO}_3$ , we are able to neutralize the excessive electrons from the polar mismatch in ultrathin  $\text{LaMnO}_3$  films and thus enable ferromagnetism in films as thin as 3 UC, extending the limits of our ability to synthesize and tailor emergent phenomena at interfaces and demonstrating manipulation of the electronic and magnetic structures of materials at the shortest length scales. This work heavily utilized the Advanced Light Source.

Finally, we worked with other LDRD programs (J. Neaton) to study antiferroelectric  $\text{PbZrO}_3$  thin films and exotic properties under non-stoichiometry.

## **Ultrafast Electron Microscopy: Femtosecond Nanodiffraction and Picosecond Imaging**

Principal Investigator(s): Andrew Minor, Daniele Filippetto.

### **Project Description**

We proposed a pilot project to investigate the ability of producing nanometer-sized probe with sub-picosecond relativistic electron beam to probe matter. The proposal takes advantage of the unique capability of the HiRES electron source of delivering high flux of electrons bunched in femtosecond-long pulses. Such pulses will be carefully manipulated by a series of magnetic and electromagnetic lenses along the optical transport line, in order to deliver the required brightness and dimensions to the sample. If successful, the instrument will provide multiscale characterization both in time, spanning from femtosecond to nanoseconds, and in space, enabling for the first time dynamical studies at nanometer length scales. While the experiments will be carried out in diffraction mode, the pulses produced by the setup could be directly used to enable ultrafast pump-probe STEM or, by adding a copy of the in-vacuum focusing systems, for direct ultrafast imaging.

### **Accomplishments**

During the course of the project we introduced many modifications to the experimental apparatus, crucial to achieve sub-micrometer resolution in the experiments. The laser beamline was upgraded for improved stability and the experimental chamber was modified with high-precision motors and a dedicated in-vacuum focusing system. The magnetic lenses for final focusing had very tight requirement in space and gradient, and were specifically designed and fabricated for this experiment. Within the sample chamber, we installed a sample positioning assembly with two linear and two rotation stages for alignment of the multi-sample cartridge to the laser and electron beams. We actively worked on acquiring, preparing and characterizing materials for electron beam characterization with nanometer precision. Multiple samples were prepared for this purpose: nanometric structures on polycrystalline gold samples were formed by using Focused-Ion-Beam techniques at NCEM and the Molecular Foundry; polycrystalline Ti:Al samples were characterized with Electron Beam Scanning Diffraction at NCEM, to map size and orientations of different grains.

Samples were then loaded in the HiRES sample chamber for characterization with ultrafast pulses. During a first calibration run we were able to achieve 3  $\mu\text{m}$  spot size with 4.5 nm beam emittance. Such values are fully reproduced by electrodynamics simulations. Also, a first scanning experiment on Ti:Al sample was carried out, following the appearance of different diffraction orders as the beam was moved around the boundaries of different crystal grains. We are now starting a second run with enhanced beam brightness. Simulations predict a beam size below 100 nm.

## Computational Design of Smart Complex Oxides with Tunable Quantum Phases

Jeffrey B. Neaton

### *Project Description*

In this project, we develop and use computational approaches for discovery and design of complex functional materials for next-generation energy, computing, and information technologies. We wish to identify new tunable and topological materials of technological relevance. Further, we wish to also understand and develop design rules for how atomic-scale structure and chemical composition conspire to give rise to tunability of novel quantum phases, providing a blueprint for future efforts to synthesize new materials in this and related classes. Nodal semimetals, materials systems with nodal-point or -line Fermi surfaces, are much sought after for their novel transport and topological properties, such as protected surface states, ultra-high mobility, anomalous magnetoresistance, novel quantum oscillations and exotic optical properties. The purpose of this project is to study, predict and tune novel semimetal systems, with the combination of theory, DFT calculations and high through-put work flow.

In particular, we focus on topological materials with electron filling constraints. We develop a new workflow which will greatly reduce the number of materials that actually go through the full DFT calculations. Out of a handful of candidates we find, we will show that these materials have filling-enforced Dirac nodes and their exact locations and the crucial symmetries which are relevant to the nodes. This workflow will enable us to discover and understand more novel topological nodal semimetals, which later can be studied extensively by experiments. In addition to the filling enforced topological semimetals, we will also extend our search to other systems, for examples, topological materials which can be tuned and switched by electric or magnetic field.

### *Accomplishments*

This past year, we have developed a workflow to identify new tunable and topological phases. Through collaborations with the BES-funded Materials Project Predictive Modeling Center, we have built a multi-layer computational screening workflow – including methods to efficiently evaluate wavefunction parity, band structure, and other topological properties – to search for new topological insulators and Dirac semimetals in a large compound space. We have successfully shown how the interplay between electron filling and nonsymmorphic space-group symmetries can guide the search for nodal semimetals which are filling-enforced. We have developed a new workflow to effectively screen materials candidates based solely on their (1) space group, (2) electron count in the formula unit, and (3) multiplicity of the formula unit. This criterion greatly reduces the computation load for discovering topological materials in a database of previously synthesized compounds and works on all the 230 space groups.

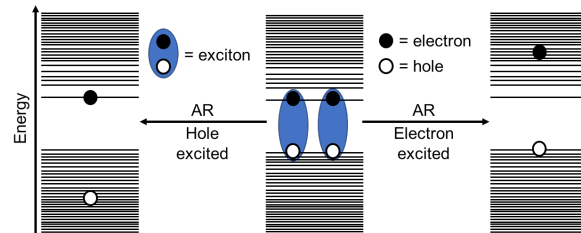
We focused on a few selected nonsymmorphic space groups which are predicted to host filling-enforced Dirac semimetals. Of the more than 30,000 entries listed, our filling criterion alone eliminates 96% of the entries before they are passed on for further analysis. From this guided search, we discover a handful of candidates, including the monoclinic crystals  $\text{Ca}_2\text{Pt}_2\text{Ga}$ ,  $\text{AgF}_2$ , and  $\text{Ca}_2\text{InOsO}_6$ , and the orthorhombic crystal  $\text{CsHg}_2$ . Based on ab initio calculations, we show that these materials have filling-enforced Dirac nodes near the Fermi energy. In addition, we also identify  $\text{CaPtGa}$  as a promising filling-enforced Dirac-ring semimetal candidate. We perform symmetry analysis of these candidates to further ensure their nodal types and calculate their Dirac speed.

## A stochastic approach to calculate Auger recombination and impact excitation rates: Application to core-shell nanocrystals and seeded nanorods)

Principal Investigator: Eran Rabani

### Project Description

Auger recombination (AR) in nanocrystals (NCs) is a fast, nonradiative decay process that limits the efficiency of NC-based displays, photovoltaic cells, lasers, *etc.* AR occurs by an exciton recombining and transferring its energy to a third particle (see Figure). The two primary purposes of this project are: 1) develop a quantitatively accurate computational method for calculating AR rates in NCs of experimentally relevant sizes and of any dimensionality (0D, 1D, 2D) along with 2) to apply our new method to elucidate the underlying physics that will allow nanocrystals to be designed with decreased or enhanced AR rates depending on the application.

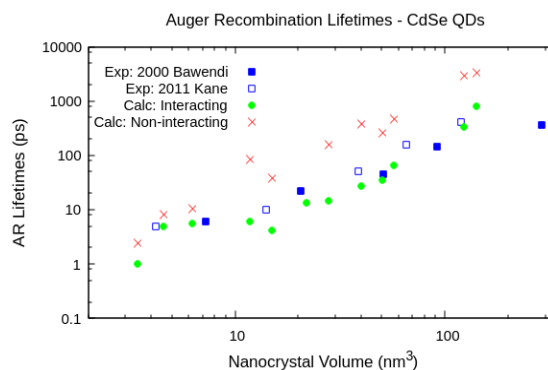


Although there has been much advancement in our understanding of AR in NCs from experimental measurements, all calculations of the AR rates in NCs have used non-atomistic models or have used the non-interacting carrier approximation. It is expected that neglecting the electron-hole interaction will not be valid in systems where the electron-hole interaction energy is comparable to that of the quantum confinement energy (*e.g.*, 1D systems). Our new computational method includes the electron-hole interaction in the initial biexcitonic state such that our method is generally applicable to 0-, 1-, and 2-dimensional NCs, along with NC heterostructures and will allow us to study them systematically.

### Accomplishments

Our most significant accomplishment has been the development of an atomistic model to include the electron-hole interactions in the calculation of AR rates. We have done this by solving the Bethe-Salpeter equation and using the resulting excitonic states in the formation of the initial biexcitonic state.

Additionally, we have also demonstrated that the inclusion of the electron-hole interactions is imperative for quantitatively accurate AR rates in CdSe nanorods (NRs). Surprisingly, we also found that the inclusion of excitonic effects becomes important for CdSe quantum dots (QDs) of moderate size (see Figure). In our systematic study of AR in CdSe QDs and NRs, we found that the non-interacting framework is only able to predict accurate results in the strong confinement regime (very small QDs) while our interacting framework we developed is able to predict quantitatively accurate results for all sizes of CdSe QDs and NRs studied (manuscript in preparation).



We are now beginning to extend our method to study the scaling behavior of AR rates in nanoplatelets in heterostructured NCs – both of which have been found to have very promising uses in NC applications.

## IN-OPERANDO IMAGING OF MOLECULAR ORDER AND DYNAMICS IN SOFT NANOMATERIALS AT RELEVANT LENGTH AND TIME SCALES

Principal Investigator(s): Jim Schuck, Ron Zuckermann, Sujoy Roy

### *Project Description*

The purpose of this project is to develop an unprecedented experimental capability allowing us to directly observe and understand the dynamic interactions between fundamental building blocks in soft materials, including bio-mimetic materials, under conditions in which they function. Because dynamics are crucial to the function of soft-materials (e.g. protein catalysis, membrane separations), high-resolution methods are urgently needed to map their degree of order and their dynamics in functional environments. We need to be able to visualize motion *in operando* at the level of individual chemical building blocks – i.e. a single peptoid polymer chain. Our present inability to directly measure these characteristics is severely limiting our ability to engineer advanced function into next-gen soft materials including peptoid-based nanomaterials. For example, the ability to introduce well-defined pores into peptoid nanosheets or functionalization of a polymer nanotube interior would enable materials capable of the specific transport of ions, gases, drugs or even proteins.

Here, we leverage significant LBNL-unique strengths in nano-optical and scan-probe microscopies, x-ray imaging and spectroscopy, and nanomaterial design and synthesis to invent novel capabilities for mapping the evolution of order and dynamic interactions within soft nanomaterials at critical length and time scales. Most excitingly we aim to observe the dynamics and ordering of bio-mimetic nanomaterials while they are performing their designed function (e.g. binding to a molecular target, responding to an applied force or different environmental conditions). Our team tightly integrates the critical discovery cycle of synthesis-characterization-understanding. We expect the new capabilities developed here to establish LBNL as a hub of soft materials research, discovery and innovation that attracts top researchers with diverse sets of scientific questions and critical technological applications.

### *Accomplishments*

We have made significant accomplishments in a number of key areas. First, we succeeded in optimizing the critical campanile near-field feedback and scanning parameters for operating in non-ambient environments – overcoming a major roadblock/risk anticipated with our novel approach. Second, we have made substantial improvements on creating large-area peptoid nanosheet samples supported on flat substrates suitable for imaging. This is based on a new, and much more generalizable, nanosheet synthesis that builds up nanosheet bilayers one layer at a time exploiting a Langmuir-Schaffer transfer. This is important, as it creates uniform nanosheet preparations suitable for a wide variety of analyses (e.g. TEM, XPCS, GIWAXS, the NanoFrap experiments proposed here). Third, we have successfully demonstrated operation of XPCS in novel environmental and liquid sample cells. Our final major accomplishment has been to use the increased sensitivity in near-field scanning operation to defect-bound exciton emission from a 2D material at room temperature for the first time – discovering a possible path for realizing room-temperature single-photon sources in high-quality 2D semiconductors. This work is now under review at *Nature Nanotechnology*.



## Simulating Excited State Energies and Dynamics with Superconducting Qubits

Principal Investigator(s): Irfan Siddiqi

### *Project Description*

The calculation of molecular properties from first-principles is a classically intractable problem due to the exponential scaling in computation cost with both the number of atoms and basis set size. For these reasons quantum simulations have been the subject of increasing study both theoretically and experimentally, with efforts to develop various approximate approaches that trade off reduced simulation accuracy for a lower burden of computational complexity. While such techniques have benefited greatly from the growth in classical CMOS based computing architectures, they are beginning to run into fundamental physical limits that prevent further scaling. We will develop an experimental platform based upon a new hybrid approach known as the Variational Quantum Eigensolver (VQE) which makes efficient use of both quantum and classical computational resources to store and process data. Initially we plan to apply small scale simulators to model various known problems in quantum chemistry as a proof of concept of both experimental and theoretical techniques. Once completed we hope to scale the system to larger number of qubits allowing us to begin exploring the application of this computing paradigm to cutting-edge problems in the field.

### *Accomplishments*

Our most significant accomplishment has been the first experimental calculation of the full energy spectrum of a given Hamiltonian beyond the ground state within a superconducting architecture. We have additionally demonstrated, for the first time, a recent theoretical extension of the VQE approach based on a Quantum Subspace Expansion (QSE). In particular we have established the technique's ability to partially mitigate stochastic, incoherent errors, allowing us to attain near chemical accuracy ( $1.6 \times 10^{-3}$  H) of the energy levels of the hydrogen molecule. Significant progress has also been made in the design and fabrication of 2D coplanar qubit architecture with greater numbers of qubits. Our fourth generation of multi-qubit processors now provide up to 8 qubits with typical  $T_1$  and  $T_2$  lifetimes in excess of 30 and 50  $\mu$ s respectively. The implementation of robust benchmarking techniques allows us to estimate our single-qubit gate fidelity across the chip as above 99.9% and our two-qubit gate fidelity above 98%. The performance of these chips, which is now at or near state-of-the-art, will allow the demonstration of large scale VQE, with our current focus on bond torsion simulations of ethylene and a better understanding of the scaling properties of the algorithm.

### **Lattice and Carrier Dynamics in Halide Perovskites**

Principal Investigator(s): Peidong Yang, Jeff Urban; Jie Yao; Linwang Wang

#### *Project Description*

Following the rise of perovskite oxides in 1980s, halide perovskites may trigger the next renaissance in condensed matter. The success of organic-inorganic halide perovskite solar cells prompts the investigation on this class of materials. Fascinating properties and novel phenomenon have been predicted in the halide perovskite system. The governing mechanisms behind these remarkable features originate from the dynamics of atoms and charges in the perovskite lattice.

In this proposal, we aim to discover, understand, control, and exploit lattice and charge dynamics in various halide perovskite single crystals and low dimensional nanostructures. We will focus on the fundamental physical properties in the halide perovskite family, including phase transformation, thermoelectrics, ferroelectrics, and charge transport. Inorganic halide perovskite represents an exciting emerging research field with ample opportunities of discoveries for novel materials chemistry and physics. This research project is expected to make significant impact to chemistry, material science, physics, and electrical engineering communities. It will place MSD-LBNL as the leading institute to study this new class of semiconductor.

#### *Accomplishments*

We have achieved facile synthesis of halide perovskite nanowires with high quality and excellent functionalities. We anticipate to gain insight into dynamics of the lattice and charges from the following aspects:

1. Phase Diagrams and Phase Transformation. We have systematically synthesized and studied the rich phase diagrams in various halide perovskites, and investigated the physical properties of different phases as well as the phase transition process.
2. Thermoelectricity. We have investigated the thermoelectric properties of individual single halide perovskite nanowires using our all-in-one thermoelectric platform.
3. Interface Charge Transport. We aim at exploring fundamental physical processes in single crystalline and heterostructured halide perovskites.

## Nanoscale Magnetometry, Electrometry, and Thermometry of Exotic Quantum Materials Using Nitrogen-Vacancy Defects in Diamond

Principal Investigator: Norman Yao

### *Project Description*

The purpose of this project is to develop a quantum sensing platform based upon shallow nitrogen-vacancy (NV) spin defects in diamond. As a solid-state entity localized to within a few lattice sites, the NV center can act as a true point sensor, enabling the imaging of local magnetic, electric and thermal properties of strongly correlated materials. The insights arising from this project will enable diverse applications ranging from a better understanding of magnetic excitons in layered two dimensional materials to the strain tensor mapping of diamond anvil cells. Moreover, the proposed project will also help to generate novel techniques for the control of local fields in applications ranging from energy harvesting to magnetic switching. Data obtained from the direct measurement of spin relaxation times in quantum materials will help to improve hetero-structure design and to enable longer-lived spin coherences for spintronic applications.

We will begin by creating shallow NV centers 3-10nm below the surface of CVD grown, electronic grade diamond samples. To do this, we will perform reactive ion etching in an inductively coupled plasma to remove a 3-5 micron layer of strain damage. Next, we will implant ionic Nitrogen gas at an energy of 2keV. This implantation results in a dilute ensemble of substitutional nitrogen impurities (P1 centers). To create NV centers from these implanted P1 defects, we perform a final high temperature vacuum annealing step. Using a home-built confocal microscope, we will directly image the NV centers resulting from this creation process and find photostable defects with an average spatial separation of 0.5microns. Finally, we will characterize the coherence properties and depths of the NV centers using spin-echo based NMR techniques.

### *Accomplishments*

We have successfully created two dimensional arrays of photostable, shallow NV centers with varying depths and densities. By performing Ramsey spectroscopy, we observe coherence times  $T_2^* \sim 1.4$  microseconds, consistent with being limited by the  $^{13}\text{C}$  nuclear spin bath. In order to determine the depth of individual NV defects, we measure the variance of a fluctuating magnetic field generated by nearby immersion oil protons on the surface of our diamond sample. We utilize a so-called XY8 dynamical decoupling pulse sequence to measure the individual Fourier components of the magnetic resonance signal. By tuning the free evolution time, we measure the signal contrast and indeed observe a narrow dip at the Larmor precession frequency, whose amplitude enables us to directly determine each NV's depth to within 1nm accuracy.

In addition to calibrating the depth of shallow NV defects, we have also made important steps toward utilizing NV centers to characterize signatures of pressure-driven magnetic phase transitions. In particular, we have measured the NV center's zero-field splitting (ZFS) as a function of applied pressure in a custom-built mini-diamond-anvil-cell. We observe a ZFS susceptibility of approximately 15 MHz/GPa, which enables one to use the NV center as an independent probe of the applied pressure. In addition to these magnetic resonance susceptibility measurements, we have also recently observed an extremely intriguing heavy-tailed line-shape for the NV center's ESR spectra. The shape of the line is unlike any other NV spectra we have observed or seen in the literature and we believe is due to the presence of local electric charges in the diamond lattice. By carefully fitting these spectra as a function of P1 density, we have made exciting progress in imaging single charge defects inside the diamond lattice.

## Multimodal Imaging and Spectroscopy of Solid-Liquid Interfaces

Haimei Zheng (MSD, LBNL)

### *Project Description*

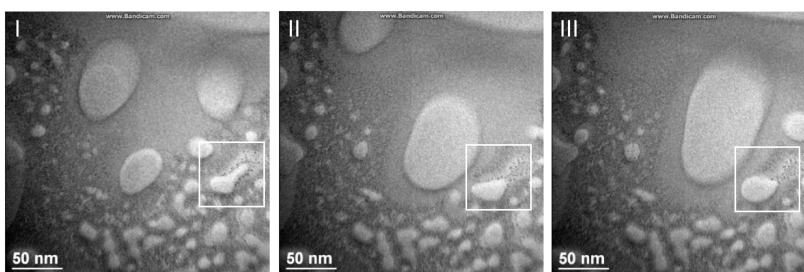
In this project, we aim to study the behavior of liquids (i.e., water or other solvent) in small volumes, i.e.,  $10^{-18}$  (atto)- $10^{-21}$  (zepto) liters, for instance, phase transitions of nanodroplets that are under an external stimulus (e.g., light, electrical, chemical or mechanical means).

We will use transmission electron microscopy (TEM) imaging as the primary approach, other methods, for example, electron or X-ray spectroscopy as complimentary to elucidate the atomic/molecular level phenomena at solid-liquid interfaces.

### *Accomplishments*

Progresses have been made on the study of nanoscale solid-liquid phase transitions and interfaces. We have observed solid/liquid-like phase transitions of Pb nanostructures on SiNx membranes using liquid cell TEM. Reversible phase transitions have been observed. Quantitative understanding of such transitions has also been achieved using in situ X-ray methods and theoretical calculation. This study is highly relevant to a broad of phase transition phenomena at solid-liquid interfaces. A manuscript of this work has been completed and it is ready for submission.

Recently, we have also studied more complex solid-liquid-gas interfaces and their role in nucleation, growth and self-assembly of nanoparticles. As shown in Figure 1, dynamics of bubble formation from electrolysis of water, nanoparticle formation at the edges of a bubble and their movements are observed. More depth understanding of the phenomena will be developed based on more experiments and theoretical calculation.



**Figure 1.** Sequential images from a movie taken from a liquid cell containing a liquid film on SiNx membrane with cobalt precursor where bubbles (white, round) and cobalt oxide nanoparticles are present.

This project effort on the study of solid-liquid interfaces by multimodal imaging and spectroscopy is highly beneficial for fundamental understanding of various materials dynamics and chemical reactions for energy applications. The project achievements have provided future funding opportunities. Currently, I am working on joint proposals for DOE EFRC, NSF center, NIH grants.

## Interfacing Chemical and Biological Catalysis for Solar-to-Fuel Conversion

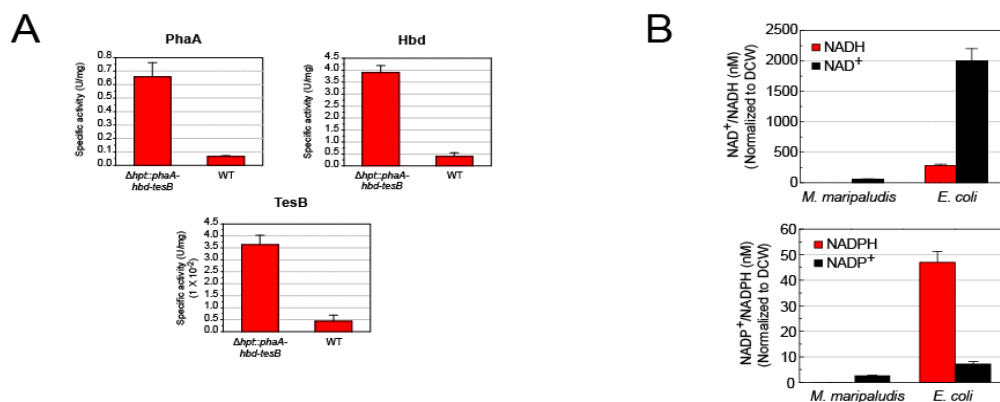
Principal Investigator(s): Michelle Chang

### Project Description

The purpose of this project is to develop approaches to integrate chemical and biology catalysis for solar-to-fuel conversion consisting of light-harvesting nanowires functionalized with hydrogen-producing catalysts and living microbes as an autotrophic chassis for the production of value-added fuels and other chemicals from CO<sub>2</sub> and photogenic H<sub>2</sub>. During the course of this LDRD, we have focused on developing methods to metabolically engineer methanogens to build biosynthetic pathways downstream of acetyl-coenzyme A.

### Accomplishments

We have initiated work with the methanogen, *Methanococcus maripaludis*, which is capable of fixing carbon dioxide to produce methane and biomass as a product. In this pathway, acetyl-CoA serves as a key intermediate and could possibly be tapped for the production a value-added compounds such as isoprenoids, polyketides, fatty acids, and a variety of other targets. In our previous report, we demonstrated that we could express genes for a heterologous pathway to produce 3-hydroxy acids from acetyl-CoA. Quantitation of mRNAs indicated that high expression could be achieved but did not result in protein production. In this reporting period, we have developed strategies that allow us to achieve high protein production, yielding specific activities in cell lysates comparable to model microbes such as *Escherichia coli* (Figure 1A).



**Figure 1.** Developing *M. maripaludis* as a synthetic biology platform. (A) Achieving high protein expression levels in *M. maripaludis* for a pathway to produce 3-hydroxy acids. (B) Analysis of NAD(H) and NADP(H) levels in *M. maripaludis* compared to *E. coli*.

Further analysis of these strains show that although pathway expression is high, product titers remain quite low. Since archaea utilize non-canonical redox cofactors, we measured the level of NAD(H) and NADP(H) in *M. maripaludis*, which indicates that they are substantially below the levels measured for a typical heterotroph such as *E. coli* (Figure 1B). We have thus constructed pathways for the overexpression of NAD biosynthesis for *M. maripaludis* and have successfully transformed them into a host containing the PhaA-Hbd-TesB pathway. We have also initiated experiments to identify NAD(P)(H) utilizing enzymes from this host to assess their affinities for these co-factors. In addition to these studies on basic archaeal physiology, we have also initiated efforts to develop ribosome profiling experiments on this host to explore their translation mechanisms.

Designing Efficient Energy Conversion Pathways for Synthetic Organisms  
Principal Investigator(s): Karen M. Davies

*Project Description*

The purpose of this project is to dramatically increase our understanding of how nature converts sunlight and other natural energy resources into the cellular energy units, ATP and NADPH, required for biomass or biopolymer production. The ultimate aim is to combine the most efficient natural energy converting pathways into synthetic organisms to improve the productivity of designer compounds e.g. Xylene, Polylactic acid, or Ethene, in large-scale industrial growth vats. To achieve this aim, we are comparing how the structure and *in situ* organization of proteins involved in both photosynthesis and oxidative phosphorylation from various species change with different growth conditions and how this influences the efficiency of the energy converting pathways.

Our approach involves two new revolutionary imaging techniques, which have not been routinely performed at LBNL. These techniques are: electron cryo-tomography and electron cryo-microscopy. Electron cryo-tomography allows a researcher to directly visualise the inside of cells at a resolution where both protein structure and membrane morphology is easily observed. This technique enables scientists to assess how proteins interact in cells to execute a function and how the efficiency of this pathway could be improved. Electron cryo-microscopy provides close to atomic details of macromolecular complexes allowing scientists to decipher atomic mechanisms of many enzymatic reactions aiding in the development of synthetic biocatalysts. One of the key aims of this LDRD project is to establish these two novel imaging techniques as a mainstay technique for all LBNL scientists in order to assist in the execution of DOE-directed research.

*Accomplishments*

During FY17 we have installed a new ground-breaking direct electron detector (developed at LBNL) on our high-end transmission electron microscope (TEM). This detector greatly improves the quality of data we can obtain by allowing us to image radiation sensitive samples with minimal dose at close to Nyquist frequencies. In addition to this software upgrade we have employed a new TEM manager to oversee the running of the cryo-EM facility and completely overhauled the alignment of the microscope including installing automatic data collection software. Since February FY17, the cryo-TEM has had 80% uptime allowing the routine collection of data for single particle and electron cryo-tomography.

Using this upgraded technology, we have started to make progress towards our aims of understanding how photosynthetic systems adapt to changing light and environmental conditions for efficient photosynthetic productivity. We have established a number of collaborations with various experts in the field and we are currently collecting data on shared interests. We anticipate that within the next year we will have sufficient results for at least one high-impact publication and several grant applications which will provide us with independent funding to further pursue these projects.

## **Robust Synthetic Membranes for Microbial Electrocatalysis: Separating Electron-Generating Organisms from the Catalytic Reaction Environment**

Principal Investigators: Heinz Frei and Caroline Ajo-Franklin

### *Project Description:*

Biohybrid technologies that combine bacterial and inorganic catalysts have the potential of converting the dilute energy contained in wastewater or solar light to fuels and chemicals. Despite recent leaps forward, biohybrids need several major breakthroughs to become viable and, in particular, scalable at a level that will have impact on chemicals manufacturing or fuel consumption, largely because of limitations at the abiotic/biotic interface. In particular, the macroscale separation of biotic and abiotic components due to the incompatible reaction environments results in crippling (ohmic) resistance losses and device architectures not suitable for large scale manufacturing. The goal of this project is to couple the incompatible inorganic and biological environments on the shortest possible length scale, the nanoscale, under membrane separation. Our approach consists of creating a single integrated biohybrid assembly composed of solid-supported inorganic catalysts separated from microbial catalysts by a nanometer-thick functionalized membrane.

### *Accomplishments:*

We have demonstrated a novel concept for completing the chemical redox cycle between a bacterial catalyst and an inorganic catalyst at the length scale of nanometers while chemically separating their incompatible environments. The biohybrid system is composed of an inorganic substrate, represented by a tin oxide anode, overlaid with a 2 nanometer thick silica membrane containing embedded *p*-oligo(phenylene vinylene) molecular wires, and a microbial catalyst, *Shewanella oneidensis*, on the opposing side. The ultrathin silica membrane with embedded wires blocks small molecule transport including oxygen but readily transmits protons. Electron transport from the microbial catalyst to the inorganic oxide across the silica layer is enabled by the embedded molecular wires whose electronic properties are tuned by functional groups in order to match the energetics of bacterial electrons and the conduction band of the inorganic oxide for facile of electron flow. The flow takes place at sufficient rate to allow the organism to maintain biomass. This is the first demonstration of nanoscale integration of microbial and inorganic catalysts under membrane separation of the incompatible environments.

For demonstrating utilization of the energy stored in waste organic to power the synthesis of useful chemicals, such as hydrogen peroxide from oxygen in air, core-shell microtube arrays of square inch size were developed. Each microtube consists of a metal oxide core whose inner surface provides sites for inorganic catalysis. This inner tube is surrounded by a 2 nm silica shell with embedded molecular wires whose outside surface is loaded with bacterial organisms. Currently, core-shell constructs with tungsten oxide as core tubes are being pursued with the goal of converting oxygen to hydrogen peroxide, an important industrial oxidizing agent, using bacterial electrons generated by waste organic consumption as power source. The microtube array provides separation of the incompatible biotic and abiotic reaction environments on all length scales from nanometers to decimeters and beyond.

The ability to optimize this platform for nanoscale integration of different combinations of incompatible biotic and abiotic catalysts will drive the development of scalable biohybrid systems that harness the energy found in wastewater or sunlight to a variety of industrial chemicals and fuels.

## **Life Science applications of X-ray scattering at ALS-Upgrade**

Principal Investigators: Greg L. Hura & John A. Tainer

### *Project Description*

We see transformative advantages for our field through coordinated upgrades of the Advanced Light Source and its beamlines. We aim to accomplish both short and long term plans for enhancing existing capabilities and introducing new ones for the characterization of structure in biology. Central to our aims is experimentally demonstrating requirements on a light source for optimal implementation. Our proposal further optimizes what we have available now and defines light source upgrades which will have significant impacts. Our goals address the following two biological challenges 1) Building intuition on the large networks and multi-level feedback loops in cellular systems requires many measurements which current capabilities cannot deliver 2) Engineering biologically inspired macromolecules requires a rapid means to compare design relative to reality. By coordinating efforts to address these challenges we will ensure the ALS upgrade has high impact for the biosciences.

### *Accomplishments*

To date our liquid robotics system is twice as fast as prior to our LDRD using a single needle. The robotics we have installed can run with four rather than the one of our system. Thus we anticipate an 8 fold improvement in total speed. We have yet to fully realize this speed as we continue to improve the design for single needle modality. Once this a single needle is functioning without issue we will stage increasing the needles to double and finally quadruple. We have implemented all the code necessary to stage up to four needles.

At the moment our ability to collect samples with a single needle is at an 80% success rate. This continues to improve. Bubbles in the needle remain a challenge. As speed has improved we have invested heavily in automatically detecting and categorizing types of collection failures. Once bubbles form they persist into subsequent samples. Thus our automated detection system is critical so as to not disturb delicate samples without collection. For biology, sample is limiting so significant continued effort is required in this area.

Our newly developed code for error checking is written in python and Tk1. We anticipate being able to collect 100 samples in the span of 30 minutes. Thus error checking will be critical if we are to process hundreds of plates in a week. Our code can track improvements in sample handling historically and is essential for establishing technology. The LDRD funding has been fundamental in establishing our new capacity.



## **Toward Next Generation Gamma-Ray Tracking Arrays: Development of Inverted Coaxial Segmented HPGe Detector Technology**

Principal Investigator(s): Heather Crawford and Reynold Cooper

### *Project Description*

This project is aimed at characterizing a novel next-generation high-purity Ge detector technology, and to better understand the performance limitations for gamma-ray energy tracking detectors based on point-contact designs. The large-volume inverted coaxial HPGe segmented point contact detector has unique properties associated with the low electric field strength, long charge drift times and highly localized weighting potentials within the detector. These characteristics provide potential for discrimination of single vs. multi-site interactions and outstanding position resolution, but also introduce challenges associated with charge trapping along the drift path, and an associated degradation of energy resolution.

Within this LDRD we characterized a prototype inverted coaxial-segmented point contact detector, and explored the performance limitations associated with this technology. We constructed an experimental signal basis corresponding to gamma-ray interactions localized within the crystal volume, based on controlled scanning measurements using highly collimated gamma-ray sources. With this experimental signal basis, we developed pulse shape analysis algorithms to determine, event-by-event, the location of individual gamma-ray interactions. We have explored the limitations on the energy resolution and position resolution of such a detector. In parallel, we pursued realistic simulations for this detector geometry, refining the description of signal shapes, etc. in response to the scanning data sets obtained.

### *Accomplishments*

The most significant accomplishment associated with the second year of this LDRD was the refinement of the experimentally produced set of basis signals and the generalization of the algorithms to fit individual experimental signals, and locate gamma-ray interaction points not only in azimuthal angle and depth (z), but also radially within the cylindrically symmetric crystal. A comprehensive set of collimated beam measurements using a  $^{137}\text{Cs}$  source was made to characterize the detector response in three dimensions, and produce sets of basis signals for all detector segments. The pulse-shape analysis was extended to extract for each event the depth and azimuthal angle, as well as the radial position at which the event occurred. Three-dimensional position reconstruction has been demonstrated for single-site events within the detector volume.

With the algorithms developed, we were also able to make an in-beam test to experimentally measure the position resolution in three dimensions based on the Doppler correction of a gamma-ray emitted from a nucleus moving at 10% the speed of light. This short experiment was performed at the 88" Cyclotron facility at LBNL. Based on this stringent test of performance, a preliminary position resolution of  $\sigma_{x,y,z} = 1.6$  mm was determined. The full results of the developed algorithm, experimentally constructed basis and achieved position resolution are being assembled into a second publication for this LDRD work. It is worth noting that this is the first time that a 3D position reconstruction in a large-volume Ge detector has been possible based on a completely experimental signal basis.

In addition, the extension of signal decomposition to multi-site gamma-ray events within the crystal volume has been started, and very preliminary results are promising. This work will hopefully be continued within our larger collaboration involved with the LDRD, and once the overall performance in this regard is verified, future funding opportunities for next-generation prototypes can be explored.

## **Computational Nuclear Physics Code Development for Fundamental Interactions/Astrophysics, Supporting FRIB**

Principal Investigators: Wick Haxton, Dan Kasen, Thorsten Kurth, NSD  
Ann Almgren, John Bell, Esmond Ng, Sam Williams, Chao Yang, CRD

### *Project Description*

The purpose of this project is to develop next-generation codes to support fundamental nuclear physics important to FRIB, the Facility for Rare Isotope Beams. FRIB's scientific focus is the discovery and characterization of unstable isotopes that are short-lived under conditions found on earth, but stable states in the high-temperature environments of astrophysical explosions. This report describes third-year progress on the project's two foci, the development of a hybrid code capable of integrating supernovae out to late times, and the application of lattice QCD to fundamental symmetries involving one- and two-nucleon systems.

The numerical astrophysics community has made great progress toward developing 3D numerical models of core-collapse supernovae (CCSN) that combine realistic treatments of the nuclear equation-of-state, shock wave generation and propagation, and energy and lepton number transport. These codes, integrated to typically one second after core bounce, reliably compute the initial conditions for the star's subsequent mantle ejection and neutrino-driven neutron-rich wind. Our work focuses on producing an integrated code framework for propagating the explosion to later times, where contact can be made with the nucleosynthetic processes relevant to FRIB as well as to the electromagnetic observables. This is achieved by feeding the output from the explosion code CHIMERA into the compressible hydrodynamics code CASTRO and the radiation transport code SEDONA, tools suited for integrating out to late times.

FRIB's rare isotopes, captured in atom traps, can open up new opportunities to probe fundamental properties connected with weak interactions. To connect FRIB observations to underlying theory, one must derive from a fundamental UV theory the effective low-energy symmetry-violating nucleon-nucleon interactions responsible for the polarization of FRIB nuclei. We are developing the first rigorous methods for doing through numerically exact solutions of the strong interaction by discretizing time and space on the lattice (LQCD).

### *Accomplishments*

The flagship lattice QCD accomplishments were the first sub-1% calculation of the axial vector coupling constant  $g_A$ , and a 1% calculation of the leading short-range two-nucleon operator contributing to double beta decay.  $g_A$  has remained an outstanding benchmark calculation for more than a decade due to the challenge of controlling systematic errors. The lattice community estimated a 2% precision would be possible with next generation computing by 2020. Using a new computational strategy (described in our year two report), we determined  $g_A$  with 1% precision, using computing time provided by LLNL and through CalLat's 2016 INCITE allocation. This work is in the process of being accepted for publication in *Nature*.

The key advance in the astrophysics program was the delineation of uncertainties in supernova post-processing calculations of nucleosynthetic yields. As computational costs limit the complexity of the nuclear networks that can be employed directly in codes like CHIMERA, most calculations employ a more complete and realistic network only in a post-processing step, utilizing Lagrangian tracer particles. The limitations of this approach include poor spatial resolution, inconsistent thermodynamics, and uncertain mass cuts. The impact of such uncertainties was quantified, for supernova progenitors ranging from 12 to 25 solar masses.

## R & D TOWARDS AN ELECTRON-ION Collider

Spencer R. Klein

### *Project Description*

The U. S. Nuclear Science Advisory Committee's 2015 Long Range Plan for Nuclear Science recommended "a high-energy high-luminosity polarized EIC [Electron-Ion Collider] as the highest priority for new facility construction, following the completion of FRIB." This LDRD is for perform R & D on some key aspects of an EIC – the physics case, detector design, and accelerator technology, with a view to establishing a major role for LBNL in a future EIC.

One EIC physics driver is to map the partonic content of heavy nuclei in 3 dimensions, using coherent photoproduction of vector mesons. One LDRD physics focus was to develop a Monte Carlo simulation of vector meson photo- and electroproduction at an EIC. It should simulate the production of many different vector mesons for different ion species, collision energies, etc. It can be used to strengthen the EIC physics case, by introducing mesons that contain the heavy b quarks, and considering exotic QCD final states, like pentaquarks and glueballs.

We are contributing in a couple of ways to detector design. We are developing a set of detector requirements, to facilitate comparison of different designs. Another focus is to understand the capabilities of existing technologies, to study their suitability for an EIC. This work has a special focus on a mid-rapidity charged particle tracking system, including a vertex detector, using MAPS (monolithic active pixel sensor) technology. With these, we will evaluate different detector layouts, with different numbers of layers and separations.

Our accelerator technology work focused on superconducting magnet development for the ion ring of JLEIC, and for the Interaction Regions of both JLEIC and eRHIC. These have strategic value to an EIC to establish key performance parameters (such as collider energy and luminosity), formulate R&D plans, and estimate construction cost for the competing proposals.

### *Accomplishments*

One significant accomplishment was to develop a preliminary version of a Monte Carlo simulation for vector meson photoproduction and electroproduction, and verify its performance against data from the HERA collider. We then calculated the production rates for different vector mesons for two proposed EIC configurations: eRHIC at BNL, and JLEIC from Jefferson Laboratory. We studied the kinematic distributions of the produced vector mesons at both facilities, and found strong arguments for a detector with a very wide acceptance in rapidity. We also studied the rapidity distribution for the  $X^+$  (4430) in a tetraquark model. It could be visible in an EIC detector with acceptance extending to negative rapidities.

We have also begun exploring the performance of different detector configurations; this work has emphasized the importance of having thin (with low amounts of material) to minimize multiple scattering. Additional detector layers made with some of the thicker proposed technologies can actually reduce detector performance; the improved tracking precision is more than offset by the additional multiple Coulomb scattering. We evaluated the MAPS technology used by the ALICE ITS upgrade, and found that it looks very suitable for an EIC detector.

We are directing our magnet effort toward the design of a 6 T arc dipole which would double the JLEIC ion beam energy versus the baseline design. We assessed the performance limits and trade-offs for the JLEIC machine parameters. For the IR regions, we are contributing to the development of a high-field final focus quadrupole. We presented these studies at the JLEIC collaboration meetings and the EIC accelerator workshop.

## ***Topmetal* Charge Readout Plane for Neutrinoless Double-Beta Decay Searches**

Principal Investigator: Yuan Mei

### *Project Description*

The purpose of this project is to develop a direct charge readout plane that is suitable for high-pressure gaseous Time Projection Chamber (TPC), operating in either electron drifting or ion drifting mode, for the search of Neutrinoless Double-Beta Decay ( $0\nu\beta\beta$ ). A positive observation of  $0\nu\beta\beta$  would signal violation of the lepton number conservation, confirm that the neutrino is its own antiparticle, and provide support for the lepton-aided mechanism of generation of the matter-antimatter asymmetry in the early universe. It will also provide insights into the mechanism responsible for non-zero neutrino mass. It has recently been demonstrated that certain high-pressure gas such as Xenon exhibits excellent intrinsic energy resolution in the  $0\nu\beta\beta$  energy range by ionization alone. When instrumented as a TPC, it enables charge track imaging capabilities that provide extra handle for discriminating  $0\nu\beta\beta$  signals against backgrounds. TPCs are also easily scalable to large mass provided there is an accompanying charge readout scheme.

Leveraging the recently developed CMOS direct charge sensor *Topmetal*, we envision the realization of a charge readout plane with a tiled array of CMOS charge sensors, without gas-electron multiplication. Charge collection electrodes, front-end amplifiers, as well as data processing circuits, are integrated in the CMOS sensors placed directly at the site of charge measurement. The plane will simultaneously achieve the necessary low electronic noise for energy resolution and the high spatial resolution for ionization charge tracking, while satisfying the stringent radio-purity and scalability requirements for a future tonne-scale experiment.

### *Accomplishments*

In FY17 the previously designed sensor *Topmetal-S* was produced. Small-scale tests show that the sensors achieved the required  $<30e^-$  noise, which is the most critical performance metric. Other functionalities including in-chip waveform digitization, sensor configuration and data communication have all been verified to function correctly. A yield problem due to instability in the DAC's analog output buffer was identified. A probe-test procedure was established and all produced chips were screened by the procedure. 24% of the chips that are fully functional were selected.

A 19-chip array was designed and produced. The supporting readout system, including an FPGA carrier board that directly couples to the array inside of the TPC, a control and data receiving/processing system outside of the TPC, and the associated firmware/software have been developed and commissioned. Tests show that the array is fully functional and all the chips are well controlled by software over a high-speed Ethernet connection. Data are recorded via the same channel.

We are in the process of characterizing the array in the high-pressure TPC apparatus to extract the energy resolution—the most important parameter for  $0\nu\beta\beta$  searches. Detailed measurements of other performance metric using real radioactive sources are underway as well.

Next Generation Relativistic Heavy Ion Collider  
Principal Investigator(s): Ernst Sichtermann, Barbara Jacak

*Project Description*

The purpose of this project is to investigate the gluonic structure of dense matter. Cold, dense matter will be probed using electron-ion collisions at a future collider. For this purpose we need to simulate and optimize EIC detector performance. Our work aims to establish a leadership role at the EIC and provide a basis for continued and enhanced block funding from DOE/NP.

We can also have a first look at the gluonic structure in cold dense matter by looking at direct photons produced in collisions of p+Pb at the LHC. The main source of such photons is the QCD analog of Compton scattering where an incoming quark and gluon produce a quark and photon in the final state. We do this measurement with the ALICE experiment, in order to produce physics results now, in parallel with preparations for the future. The particle identification developments needed to identify single, isolated photons are useful in p+p, p+Pb and also Pb+Pb collisions, where we can study the gluonic structure of hot dense matter.

*Accomplishments*

We have made several major accomplishments on our two goals. On the ALICE experiment, graduate student Dixit has completed calibrations of the ALICE Electromagnetic calorimeter for Pb+Pb and p+Pb collision data collected in the LHC Run-2. Utilizing this now well-performing detector, Postdoc Lai developed and optimized the performance of a Deep Neural Network to separate the single photon signal from a background consisting of two merged photons, or an overlapping photon and hadron. This method utilizes the TensorFlow package running on NERSC's CORI, and represents a milestone in utilizing Machine Learning techniques for ALICE. Training samples are generated with Monte Carlo, and then the algorithm is run on the data. We began quantifying the performance by comparing to the previously existing photon identification technique in ALICE.

In parallel, Lai developed an easy-to-use data structure (a ROOT ntuple) to enable students to quickly access the data and perform physics analyses using the calorimeter and track data from ALICE. This ntuple includes the DNN output for photon studies. Dixit produced ntuples for the entire p+Pb data set, and these are in use by the group, including by UCB undergraduate researchers.

For the EIC simulations, Sichtermann developed a concept for forward/backward tracking using monolithic active silicon pixel detectors. With two UCB undergrads, he simulated the trackers' performance and presented the results to the EIC community. Studies with this tool were performed for two possible experiment designs at EIC. The fast simulation tool is being compared with a full GEANT-based description of the tracker performance by Sichtermann and Lai.

Sichtermann also quantified event rates expected at both the BNL and JLAB designs of an EIC in order to specify integration times for the amplifier incorporated into the silicon pixel sensor. He determined that a 10 microsecond integration time should be sufficient to anchor the sparse silicon hits to a faster detector located farther from the interaction region.

## **Advancing Germanium Detector Technologies for Sciences and Security**

Principal Investigator(s): Kai Vetter

### *Project Description*

The purpose of this project is to utilize recent developments in the fabrication and operation of High-Purity Ge (HPGe) detectors to improve gamma-ray imaging capabilities relevant for the development and utilization of diagnostic and therapeutic tracers based on new radioisotopes. Emphasis is put on alpha-particle based radio-isotopic tracers to enable highly efficient alpha-particle therapy. Alpha-particle therapy is an emerging treatment modality for cancer which promises high cure rate due its specific characteristics and localized dose. However, one of the challenges in the development and deployment of alpha-particle loaded tracers is the uncertainty in the uptake of them. New gamma-ray imaging modalities are needed to provide sufficient sensitivity and resolution in the localization of these tracers which are associated with gamma-ray energies not normally used in nuclear medicine. Neither positron-emission tomography nor current single photon emission tomography instruments are built for the predominant gamma-ray energies ranging from 200 keV to 1200 keV. HPGe detectors in so-called Double-Sided Strip Detector (DSSD) configuration provide energy and three-dimensional information of individual gamma rays enabling gamma-ray imaging capabilities over a wide range of gamma-ray energies, matching the requirements in the development and ultimately verification of alpha-particle therapy. The Applied Nuclear Physics program has available state-of-the art DSSD HPGe detectors that are utilized to demonstrate the ability to image relevant gamma-ray energies, e.g. from Ac-225, provided by Rebecca Abergel and her team at LBNL.

### *Accomplishments*

Our most significant accomplishment has been to successful imaging of Ac-225 with our DSSD HPGe instrument. We were able to image Ac-225 with several gamma-ray energies associated to the decay of Ac-225 and its daughters. With preliminary data processing we demonstrate a three-dimensional position resolution of about 4 mm. We expect an improvement of 2-4 by refining the signal processing methodology and an improved instrument. The current HPGe detector has been operating for almost 10 years and the reprocessing of the detector and its contacts would provide a more reliable, uniform, and less noisy instrument.

## Theoretical Challenges for Electron-Ion Collider Physics

Principal Investigators: Felix Ringer, Feng Yuan

### *Project Description*

The purpose of this project is to perform theoretical investigations on the electron-ion colliders (EIC) physics to sharpen the message and strengthen the scientific arguments for this machine in the near future. These efforts will be coordinated with the detector R&D, to fully explore the discovery potential and make the EIC physics program even more compelling, and to help ensure that the EIC program stays with time. In particular, two major research areas need significant improvements: gluon orbital angular momentum (OAM) contribution to the proton spin and the hadronization in cold nuclear environments. Both topics belong to the core of the scientific goals of the EIC machine. In this proposal, we will attack these two questions.

### *Accomplishments*

Our most significant accomplishment has been to develop novel experimental observables sensitive to the gluon OAM contribution to the proton spin. In Publ.[1,2], we have demonstrated that the hard diffractive dijet production in lepton-nucleon collisions can provide direct access to the gluon OAM distribution. We have shown that the single longitudinal spin asymmetry in this process depends crucially on the gluon OAM. More over, the spin asymmetry has a nontrivial angular correlation between the jet transverse momentum and the recoiled nucleon momentum. In Publ.[3], the transverse momentum dependent (TMD) parton distributions at small- $x$  are studied in a consistent framework that takes into account the TMD evolution and small- $x$  evolution simultaneously. In Publ.[4,5], we investigated the physics of elliptic gluon distribution in a series of publications. In Publ.[4], we studied its contribution to the rapidity and azimuthal correlations of particles produced in high energy pp and pA collisions. In Publ.[5], we carried out a full evaluation of the deeply virtual Compton scattering cross section in the dipole framework in the small- $x$  region, where the  $\cos 2\phi$  term is generated by the elliptic gluon Wigner distribution. The measurement at the planned electron-ion collider provides an important information about the gluon tomography at small- $x$ .

For jet physics, in Publ.[6], we have presented the first threshold and jet radius jointly resummed cross section for single-inclusive hadronic jet production. We work at next-to-leading logarithmic accuracy and our framework allows for a systematic extension beyond the currently achieved precision. We present the first numerical results for the LHC and observe an improved description of the available data. At a future Electron Ion Collider a similar framework can be used where jets are produced at lower energies which makes higher order QCD corrections potentially even more relevant. In Publ.[7], we studied the transverse momentum distribution of hadrons within jets, where the transverse momentum is defined with respect to the standard jet axis. We present numerical results and compare to available data from the LHC. In Publ.[8], we presented a framework that describes the energy distribution of subjects of radius  $r$  within a jet of radius  $R$ . We plan to perform a phenomenological study of this observable and investigate the impact of the future experiments at EIC. In Publ.[9], we studied the Collins asymmetry and quark transversity distribution from RHIC experiments. We calculate the Collins azimuthal asymmetry for charged pions inside jets using these extractions for RHIC kinematics at center-of-mass energies of 200 and 500 GeV. We compare our results with recent data from the STAR Collaboration at RHIC and find good agreement, which confirms the universality of the Collins fragmentation functions. In Publ.[10], A novel global QCD analysis of charged  $D^*$ -meson fragmentation functions is presented at next-to-leading order accuracy.

## Enabling Big Science with High Throughput Methodologies Year 2

Principal Investigator: Carl Haber

### *Project Description*

This LDRD proposal is aimed at evaluating and acquiring technical concepts and capabilities which could be crucial aspects of future efforts to construct large particle detector systems at the Laboratory. These efforts address, in particular, particle physics and nuclear physics experiments which require large area arrays of precision sensors.

The particular technologies and methods proposed for study here involve precision electrical and mechanical assembly, inspection, and testing, which require high throughput and very repetitive and reproducible procedures. The throughput requirement derives from schedule and cost drivers. Indeed, the labor costs of these large projects could be reduced dramatically as a result of these methods.

The goal of this LDRD project was to identify prototypical processes which are general enough to apply to many future fabrication efforts. Initially, a set of structures were chosen and a corresponding high throughput assembly, test, and inspection process was designed. In Year 2 this was extended into the actual fabrication of the process and its evaluation. For Year 2 we chose to focus on a specific design – the multi-function bias, multiplexer, monitor, and control circuit PCB as an appropriate candidate for integration and production/test/inspection. In Year 2 we also extended our work on 3D metrology applied to precision optics for cosmic microwave bolometry.

### *Accomplishments*

The multi-function board provides a highly efficient low voltage, high current regulation function, remote multiplexed control of high voltage, low current sensor bias, and real-time monitoring and control capabilities. Typical experiments require 10-20 thousand of such elements, which must be of extremely high reliability and radiation resistant.

In Year 1 we designed a full assembly and test process. We began the design work on both the circuits and the floor plan. In Year 2 we completed this design, fabricated the board, loaded it and successfully tested it, initially in single board form. We then developed a design whereby 27 boards were arrayed 3 x 9 on a panel with high density interconnections to enable all the boards to be tested in-mass, without singulation. This now demonstrated a scalable system, our goal, which is what is required for a high-throughput fabrication project. Based upon these results, we intend to continue this approach in later DOE funded activities.

In Year 1 we also developed a variety of inspection and measurement tools which we have applied to sensor module and stave metrology. Most significant here is a full 1.4 meter long optical scanner for both 2D and 3D imaging and metrology. We also studied optical inspection issues for cosmic microwave bolometer arrays: We applied a number of optical profiling techniques to measure the surface quality of ceramic lenses and tested these on a measurement station assembled as part of this work.

In Year 2 we also continued the bolometer scanning work. The CMB team produced a set of spheres with various coatings which we comparatively measured using our 3D metrology tools. We also developed software plug-ins to our analysis framework, specific to the bolometer study. The scanner and the analysis tools remain a capability which the CMB team continues to use.



## **Enabling Technologies for Next Generation Receivers to Measure the Polarization of Cosmic Microwave Background**

Principal Investigator(s): (Akito Kusaka)

### *Project Description*

The cosmic microwave background (CMB) is a unique tool to approach some of the most important questions in cosmology and fundamental physics: inflation, dark energy, dark matter and neutrinos. The P5 subpanel of the HEPAP committee has recommended that the DOE support an ambitious next-generation experimental concept called CMB Stage 4 (CMB-S4), and LBNL is poised to play a leading role in this program. This proposal encompasses key technologies that will enable next generation receivers for such future CMB experiments: a cryogenic half-wave plate (HWP), and advancement in detector technology. These will not only enhance CMB experimental sensitivity, but also minimize project cost and greatly simplify construction of the instruments.

The required detector count for CMB-S4 is more than 20 times of that for experiments under construction, while the cost increase is restricted to only 5-10 times that of current experiments. The goal of this proposed research is to develop three key technologies that will enable a cost effective leap in experimental sensitivity for CMB-S4: (1) A continuously rotating cryogenic half-wave plate (HWP) for maximally efficient polarization modulation. While technically challenging, the cryogenic temperature of the HWP suppresses the excess thermal emission from the HWP and prevents the detectors from sensitivity degradation. (2) Improvement of CMB detectors by reducing the operating temperature of the transition-edge sensors (TES). The TES operating at lower temperature ( $\sim 70$  mK) has a suppressed level of thermal noise, which contributes to lower level of the detector noise as well as higher fabrication yield. We support this technological development via developing a cryogenic test platform.

### *Accomplishments*

The cryogenic HWP development has made significant progress. After successful completion of the small prototype system during the previous year, we have developed a full-scale system that has an inner diameter of 45 cm this year. This system employs mag-lev bearing with high-Tc superconductor ring and an electromagnetic drive, and designed to operate at a cryogenic temperature below 77K. To our knowledge, it has the largest inner diameter fabricated to date for this type of system, and is ready for use in future projects such as POLARBEAR2, Simons Observatory, and CMB-S4. It was demonstrated and evaluated using liquid nitrogen, and we achieved low level of friction and desired rotation stability. The system will go through the final demonstration under mechanical cooler cryostat (importantly, in a vacuum environment) soon.

We have also developed a cryostat as a test-setup for a 70 mK bolometers for the next-generation CMB instrument. The cryostat is equipped with a two-stage pulse-tube cooler to achieve 4 K, and an adiabatic demagnetization refrigerator (ADR) on the 4 K stage to achieve  $\sim 50$  mK temperature. We have completed commissioning and evaluation for the 50K and 4K stages, and achieved satisfactory cryogenic performance. We have installed the ADR in this cryostat and test the sub-Kelvin stage soon. We also made progress designing the detector and readout setup in this cryostat to commence the detector testing.

## Ultrahigh Voltage and Light Collection in Liquid Xenon Dark Matter Experiments

Principal Investigator(s): McKinsey, Daniel

### *Project Description*

Efficient light collection and adequate electric drift field are both essential for achieving the best sensitivity of liquid xenon (LXe) to dark matter interactions. The best evidence that sufficient light collection and drift field can be achieved comes from LUX, where 11% light collection and 200 V/cm drift field were demonstrated. Compared to LUX, the goals for large future detectors are currently more modest for light collection ( $> 7.5\%$ ) and more ambitious for drift field ( $> 700$  V/cm). There is a bit of a tradeoff here; it is believed that the larger LXe detector will result in more light being lost due to finite reflectivity and absorption by impurities in the LXe, while it is also believed that the LUX drift field was limited by dust or asperities on the cathode and anode grids, and that additional engineering and quality control will allow better high-voltage (HV) performance. At the same time, there is little basic understanding of what fundamentally limits light collection or HV. This lack of basic understanding creates additional risk: if it is not known what physical mechanisms actually limit light collection and drift field in practice, then there is a danger that that incorrect quality control and quality assurance metrics will be applied, and final detector performance could suffer. At the same time, a better understanding of these topics may enable enhanced performance above baseline assumptions. In this LDRD project, both of these topics are studied so as to enable optimization of LXe-based dark matter experiments. Berkeley is a leader in dark matter experiments using LXe, and this work will help maintain Berkeley's leadership role.

### *Accomplishments*

The xenon gas handling and purification systems have been designed and built. The high voltage testing apparatus has been designed, purchased, and assembled, including electric field simulations of the overall apparatus and Rogowski electrodes. The high voltage delivery system for this apparatus has been designed, built, and tested. An existing cryostat has been modified for this study. Lead x-ray shielding for the cryostat has been designed and built. A purity monitor has been designed, built, and successfully tested; this will be used to verify that electron lifetime in the LXe is sufficiently high for high-voltage breakdown tests to be meaningful. Photomultiplier readout systems for use in both liquid argon and liquid xenon have been built.

The light collection apparatus has been fully designed, including an optical cell that can be filled with LXe, and into which 175 nm light may be introduced. An existing cryostat has been modified to suit this experiment. A test of the optical cell vacuum seal has been planned, and will be carried out in 2018. Measurements of internal reflectivity from PTFE surfaces covered with water and mineral oil have been compared to measurements without liquid, in preparation for studies in which PTFE will be immersed in LXe. Analysis of room-temperature data has been completed, leading to a model of immersed PTFE reflectance that may be now applied to LXe.

We are now focusing on the exploitation of both of these systems. HV studies will quantify the effects of electrode gap size, electrode size and shape, electrode surface treatment, and liquid purity. Reflectivity studies will quantify the dependence of reflectivity on wavelength of light, surface treatment, angle of incidence, and LXe purity. We also plan to study fluorescence of PTFE for VUV light, as evidence from LUX and other existing LXe time projection chambers indicates that PTFE fluorescence may be a source of unwanted single-photon and single-electron noise in LXe-based dark matter experiments.

## CONFRONTING BEYOND THE STANDARD MODEL THEORIES WITH NEW LHC AND ASTROPHYSICAL DATA

Principal Investigator: *Michele Papucci*

### *Project Description*

The purpose of this project is to leverage the present and upcoming data coming from the Large Hadron Collider, Dark Matter detection searches and particle astrophysics experiments to gain knowledge of new particle physics beyond the Standard Model (BSM). The use of novel software tools the PI is currently developing will improve the effectiveness of comparing theoretical models to the LHC data and allow more extensive studies of the implications of the experimental results for BSM models. In particular this project will focus on searches for models of Dark Matter, models addressing the naturalness of the electroweak scale and any possible new physics signal that may show up in the upcoming data.

### *Accomplishments*

The work supported by this LDRD produced various results for collider BSM searches, flavor physics and dark matter model building. We have identified a complete set of simplified models that can be used as a benchmark of searches for Dark Matter at the LHC involving a gauge boson, a top/bottom quark or a Higgs and missing transverse energy (“mono-X”) and identified the cases where these searches are optimal. We also have devised novel strategies both for triggering and for reconstruction that will allow LHC experiments to search for new physics models which were eluding current and past searches due to their difficulty to be separated from backgrounds. In particular we found trigger strategies that can allow to detect low-scale conformal hidden valleys (“soft bombs” signals) and reconstruction strategies for searching for “Quirks” (heavy particles confined by a new macroscopic strong force). Postdoc I. Mould devised new techniques to detect whether a jet is originating from the hadronic decay of a boosted gauge boson. Such techniques are crucial for searching for heavy particles decaying into gauge bosons and Higgs at the LHC. Further work on the software development of tools Atom and Fastlim has been performed and development efforts for another package, EWKfast, for the fast computation of gauginos/higgsinos production cross-sections in the general (N)MSSM has been mostly done. A publicly available code and publication will be produced in the near future.

We have also proposed the concept of a new sub-detector for the LHCb experiment dedicated to the searches of new long lived particles which are ubiquitous in many hidden sector models. This idea has produced enough interest to sparkle preliminary feasibility studies and R&D within the LHCb collaboration. Motivated by recent discrepancies reported by the Belle and LHCb collaborations between experimental measurements of  $B \rightarrow D^{(*)} \tau \nu$  branching ratios and their Standard Model predictions, we have performed a general analysis of the modification predicted by BSM models taking into account the full tau polarization information. This has also led to the development of a software package called “Hammer”, that allows efficient reweighing of MonteCarlo event samples of semileptonic decays, with full new physics and form factor parameterization uncertainties. This package, whose first public version will be released in the first quarter of 2018 has already been requested by Belle II and LHCb experimental groups for the integration in their analysis codebase. Other results produced by this LDRD have been an investigation of viable models for ultra-light Dark Matter and further progress in the control of power corrections in soft collinear effective theory for reducing theoretical uncertainties in the predictions of the Higgs production cross-section for the LHC.

## Germanium CCDs

Principal Investigators: (David Schlegel, Steve Holland)

### *Project Description*

The purpose of this project is to develop scientific charge-coupled devices (CCDs) using the semiconductor germanium as the substrate material. This work builds upon our existing expertise in silicon CCDs that includes deployment of fully depleted CCDs in DOE cameras and spectrographs including the Baryon Oscillation Spectroscopic Instrument, the 570 Mpixel Dark Energy Camera, and the upcoming spectrographs for the Dark Energy Spectroscopic Instrument.

Germanium CCDs have been listed as a technology of interest in the Cosmic Visions Dark Energy: Technology white paper (<https://arxiv.org/abs/1604.07821>). Ge has a smaller bandgap when compared to silicon, and this results in a longer wavelength cutoff, i.e. 1.4 eV versus 1 eV in Ge and Si, respectively. This increased wavelength response into the near infrared would greatly enhance Dark Energy science by allowing for the study of high-red shift galaxies and other astronomical objects. The development of Ge CCDs is the next logical next step in the realization of high performance image sensors for Dark Energy science.

### *Accomplishments*

In the first year of the project, we have developed a Ge-compatible process flow and produced CCD and test structure designs for fabrication at the LBNL MicroSystems Laboratory. We have identified the gate insulator and gate electrode structure as major areas for development. A primary issue for Ge devices is the water soluble insulator GeO<sub>2</sub> and the degradation of this material at post-oxidation temperatures exceeding 400C.

We have identified polycrystalline Ge as a potential gate electrode material based on the ability to in-situ dope the material during the deposition for sufficient conductivity, and the ability to etch the layer in conventional plasma etching tools. We are utilizing fabrication equipment in the UC-Berkeley Marvell Nanofabrication Laboratory for this work. In addition, we are working with the LBNL Molecular Foundry to use electron-beam lithography to develop a gate electrode structure with submicron-wide gaps between the electrodes.

At present there is only one supplier of 150 mm diameter Ge wafers, and one concern is that extremely low levels of contaminants in the Ge could be detrimental to CCD operation. We partnered via the SBIR program with a company that grows large diameter, high purity Ge (HPGe) for gamma-ray detection applications. HPGe is analogous to the high-resistivity silicon used in LBNL CCDs, and features the desired low levels of detrimental impurities in the starting material. Work is ongoing to produce HPGe wafers.

## Optimizing Silicon Photomultipliers for Detection of 175 nm Photons in Liquid Xenon

Principal Investigator(s): Peter Sorensen

### *Project Description*

Identifying the nature of non-baryonic dark matter is one of the major outstanding challenges in astrophysics. World-leading experiments use liquid xenon as a target medium. Liquid xenon scintillates in the ultraviolet, so these experiments would benefit enormously from an improvement in their ability to detect ultraviolet photons – the expected signal from a dark matter scattering event. The purpose of this project is a significant improvement in vacuum ultraviolet 175 nm photon sensing capabilities of silicon photomultipliers. The state of the art is about 35% detection efficiency, and we would like to double that number. Because of the weak interaction between dark matter and normal matter, any improvement must also be accompanied by extremely high radio-purity and chemical inertness.

Silicon photomultipliers do not effectively detect ultraviolet photons, because the photons are stopped in the first 10 nanometers of material. We pursued two approaches to this problem, both of which began with commercially available silicon photomultiplier devices. The first approach was to modify the front side of the device, by applying a few hundred nanometers coating of wavelength shifting compound. The compound shifts ultraviolet photons to visible photons, which can pass into the device. Such compounds are not chemically inert so we planned to encapsulate the compound with an ultraviolet-transmitting window ( $\text{MgF}_2$ ). The second approach was to modify the backside of the device. The device would be thinned to allow ultraviolet photons to pass into the active sensing layer. Then, a very thin 5 nanometer electrical contact would be deposited via Molecular Beam Epitaxy (LBL is one of very few labs which have such a facility).

### *Accomplishments*

We built a test bed to compare the processed silicon photomultipliers against a known benchmark, traditional photomultipliers. At the Molecular Foundry facility at LBL, we developed a process of purifying and evaporating the wavelength shifting compound onto the front side of the silicon photomultipliers. We iterated several times on this process, and obtained a smooth deposition profile of the wavelength shifter. We benchmarked the device performance using the test bed, and found that the photon detection capabilities using the wavelength shifter were not significantly better than the traditional photomultiplier. Faced with these data, we shifted our focus to the backside modification approach.

There are several manufacturers of silicon photomultipliers worldwide. Despite initially encouraging correspondence, we found that most of the manufacturers were ultimately unable to collaborate on this approach due to their own intellectual property issues. Each manufacturer has a slightly different process for making their devices, and these processes are closely guarded. One company (based in the U.S.) did send us bare devices along with information about their silicon doping profile. We were able to thin them and apply the MBE contact, but the device structure was not ideal and the results were not encouraging.

The most significant accomplishments of this project were a fresh look at the production and trajectory of scintillation in liquid xenon. We realized that liquid xenon is likely also producing infrared photons, which may be easier to detect. We also realized (critically) that, similar to wavelength shifting molecules, materials in our dark matter detectors may be producing unwanted fluorescence photons. A separate project will address that subject.



## Publications List

AF-Huang LB17036 Femtosecond Synchronization for Small-Scale Pump-Probe Ultrafast Experiments

### **Papers and Presentations from Workshops and Conferences**

G. Huang , K. Campbell , L. Doolittle, Q. Du, J. Jones, C. Serrano, V. Vytla, S. Babel, M. Boyes, G. Brown, D. Cha, G. Dalit, J. DeLong, B. Hong, A. McCollough, A. Ratti, C. Rivetta, R. Bachimanchi, C. Hovater, D. Klepec, D. Seidman, B. Chase, E. Cullerton, J. Einstein-Curtis, O. Kumar, “LCLS-II gun/buncher and APEX LLRF development”, LLRF2017, Barcelona, Oct. 2017

AF-Ji LB16001 Development of a Compact Laser-Driven Ion Beam Accelerator for Discovery Plasma Science

### **Papers and Presentations from Workshops and Conferences**

S. S. Bulanov, S. V. Bulanov, T. Zh. Esirkepov, M. Kando, S. Rykovanov, F. Pegoraro, C. B. Schroeder, E. Esarey, and W. P. Leemans, “Strong field electrodynamics of a thin foil”, AIP Conference Proceedings 1812, 090001 (2017); doi: 10.1063/1.4975897

S. S. Bulanov and F. N. Beg, “Summary report of working group 6: Laser-plasma acceleration of ions”, AIP Conference Proceedings 1812, 030006 (2017); doi: 10.1063/1.4975845

J. Li, A. V. Arefiev, S. S. Bulanov, M. Bailly-Grandvaux, G. M. Petrov, C. McGuffey, and F. N. Beg, “Ionization injection of highly charged copper ions for laser driven acceleration from ultra-thin foils”, draft

Q. Ji, S. Steinke, S. S. Bulanov, F. Treffert, K. Nakamura, C. Toth, J. J. Barnard, T. Schenkel, E. H. Esarey, W. P. Leemans, “High Intensity Laser Matter Interactions with the BELLA PW Laser Facility”, High Energy Density Science 2017, April 18-21, 2017, Yokohama, Japan

S. Bulanov, D. Seipt, T. Heinzl, M. Marklund, Q. Ji, S. Steinke, C. Schroeder, E. Esarey, W. P. Leemans, “Electromagnetic cascades and the depletion of intense fields”. 58th Annual Meeting of the APS Division of Plasma Physics, October 31–November 4 2016; San Jose, California

S. Steinke, Q. Ji, S. Bulanov, J. Barnard, T. Schenkel, E. Esarey, W. P. Leemans, “Isochoric heating of solid gold targets with the PW-laser-driven ion beams”, 58th Annual Meeting of the APS Division of Plasma Physics, October 31–November 4 2016; San Jose, California

S. Steike, Q. Ji, S. S. Bulanov, J. Barnard, H. Vincerti, T. Schenkel, E. H. Esarey, W. P. Leemans, “First results on ion acceleration with BELLA PW laser”, SPIE Optics + Optoelectronics, April 24-27, 2017, Prague, Cze Republic

S. Steinke, “Isochoric Heating of Solid Gold Targets with PW-Laser-driven Ion Beams”, Sixth International Conference on High Energy Density Physics (ICHED2017), June 5-9, 2017, Shirahama, Wakayama, JAPAN

S. Steinke, “Towards isochoric heating of solid gold targets with the laser-driven ion beams, First results on ion acceleration with BELLA PW”, 3rd European Advanced Accelerator Concepts Workshop, September 24-30, Elba, Italy

S. Steinke, Q. Ji, K. Nakamura, F. Treffert, J. H. Bin, S. S. Bulanov, M. Roth, C. Toth, E. H. Esarey, T. Schenkel, W. P. Leemans, “Laser-driven ion acceleration at BELLA”, 5th High-Power laser workshop, Menlo Park, USA, Sep. 27-28, 2017.  
<https://app.certain.com/profile/web/index.cfm?PKwebID=0x92900649e7&varPage=home>

AF-Wilcox LB15001 A New Concept for High Average Power Ultrafast Lasers

**Journal Publications**

T. Zhou, T. Sano, and R. Wilcox, “Coherent Combination of Ultrashort Pulse Beams using Two Diffractive Optics”, *Optics Letters*, 42, 4422 (2017),  
<https://www.osapublishing.org/ol/abstract.cfm?uri=ol-42-21-4422>

AL-Guo LB16003 High Pressure Soft X-ray Spectroscopy for Chemistry and Structure of Fluids

**Journal Publications**

Ruimin Qiao, Yujian Xia, Xuefei Feng, James Macdougall, John Pepper, Kevin Armitage, Jason Borsos, Kevin G. Knauss, Namhey Lee, Arnaud Allézy, Benjamin Gilbert, Alastair A. MacDowell, Yi-Sheng Liu, Per-Anders Glans-Suzuki, Xuhui Sun, Weilun Chao, Jinghua Guo, “Soft X-ray Spectroscopy of High Pressure Liquid”, *Rev. Sci. Instrum.*, Accepted (January 5th, 2018)

AL-Roy LB16004 Probing Spatially-Resolved Intermittent Chemical Kinetics in Confined Spaces Using X-ray Photon Correlation Spectroscopy

**Journal Publications**

tY. Chen, S. Roy, et al, “Tracking silver nanoparticle using coherent X-ray” (in preparation)

AL-Shapiro LB16005 High-Dimensional Ptychographic Imaging for Studying Nanoscale Dynamics, Chemistry and Morphology at the ALS and ALS-U

**Journal Publications**

Park, J. et al, The Origin and Function of Multimodal Spatio-Assembly within Metal Oxide Aggregates, in preparation.  
Y.-S. Yu, M. Farmand, C. Kim, Y. Liu, C. P. Grey, F. C. Strobridge, T. Tyliczszak, R. Celestre, P. Denes, J. Joseph, H. Krishnan, F. R.N.C. Maia, A. L. D. Kilcoyne, S. Marchesini, T. Leite, T. Warwick, H. Padmore, J. Cabana, and D. A. Shapiro, “Three-dimensional localization of nanoscale battery reactions using soft X-ray tomography”, *Nature Communications*, accepted, 2018.  
X. Zhu, et al, Measuring spectroscopy and magnetism of extracted and intracellular magnetosomes using soft X-ray ptychography, *PNAS*, 113 (51), E8219-E8227, 2017.

BE-Bissell LB17005 Identifying Bioactive Compounds Across the Tree of Life: from Bacteria, to Plants, to Human Organoids

**Journal Publications**

T. Eng, R. Herbert et al., and A. Mukhopadhyay, Screening Rhizobacteria for Production of Novel Bioactive Compounds. In preparation.



- R. Herbert, et al., and J. Mortimer, A Synthetic Terrestrial Ecosystem for Bioactive Compound Identification. In preparation.
- M.H. Stoiber, J. Quick, R. Egan, J.E. Lee, S.E. Celniker, R. Neely, N. Loman, L. Pennacchio, J.B. Brown. De novo Identification of DNA Modifications Enabled by Genome-Guided Nanopore Signal Processing. Under Review at Nature Communications (preprint at: <https://doi.org/10.1101/094672>)

BE-Mao LB17006 Impact of Gut Microbiome on Genetic Susceptibility to Chemically Induced Colon Cancer

**Journal Publications**

- Mao JH, van Diest PJ, Perez-Losada J, Snijders AM. Revisiting the impact of age and molecular subtype on overall survival after radiotherapy in breast cancer patients. *Scientific Reports*, 7: 12587 (2017).
- Chen EG, Wang P, Lou H, Wang Y, Yan H, Bi L, Liu L, Li B, Snijders AM, Mao JH, Hang B. A robust gene expression-based prognostic risk score predicts overall survival of lung adenocarcinoma patients. *Oncotarget*, [http://www.oncotarget.com/index.php?journal=oncotarget&page=article&op=view&path\[\]=23490](http://www.oncotarget.com/index.php?journal=oncotarget&page=article&op=view&path[]=23490).

BU-Hong LB16016 Urban Integrated System (URBIS): A Data and Computing Platform for Urban Systems

**Journal Publications**

- Y. Chen, T. Hong, M.A. Piette. Automatic Generation and Simulation of Urban Building Energy Models Based on City Datasets for City-Scale Building Retrofit Analysis. *Applied Energy*, 2017.
- C. Weissmann, T. Hong, C.A. Graubner. Analysis of heating load diversity in German residential districts and implications for the applications in district heating systems. *Energy and Buildings*, 2017.
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BU-Taylor LB17008 Advancing Innovation Decision Science: Mapping Theory to Technical Change in Clean Energy

**Journal Publications**

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CH-Ahmed LB16006 In Situ Multi-modal Probing of Chemical Reactions via Windowless Micro-reactors

**Journal Publications**

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CH-Toma LB16007 Spotlighting Catalysis: In situ and Operando Characterization of Photoelectrochemical Assemblies

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- J. Eichhorn, J. K. Cooper, L. Hess, D. Larson, M. K. Gilles, I. D. Sharp, F. M. Toma, Quantifying intra- and intergrain inhomogeneities in BiVO<sub>4</sub> thin films by photoconductive AFM, June 2017, Technical University of Munich, Germany.

CH-Wilson LB17011 Probing Reactive Intermediates in Microenvironments

**Journal Publications**

- R.D. Davis, M.I. Jacobs, F.A. Houle, and K.R. Wilson, "Colliding-Droplet Microreactor: Rapid On-Demand Inertial Mixing and Metal-Catalyzed Aqueous Phase Oxidation Processes." *Analytical Chemistry* 2017, 89, (22), 12494-12501.
- M.I. Jacobs, J.F. Davies, L. Lee, R.D. Davis, F.A. Houle, and K.R. Wilson, "Exploring Chemistry in Microcompartments Using Guided Droplet Collisions in a Branched Quadrupole Trap Coupled to a Single Droplet, Paper Spray Mass Spectrometer." *Analytical Chemistry* 2017, 89, (22), 12511-12519.

CE-Ceja Navarro LB15016 The Soil Metazoan Microbiome: A Compartment of Importance to Soil Nutrient Cycling

**Journal Publications**

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CE-Jones LB16039 Ultra High Resolution Climate Projections to Support Climate Readiness in the San Francisco Bay Area

**Journal Publications**

- P. Vahmani, A. Jones, "Water Conservation Benefits of Urban Heat Mitigation", *Nature Communications*, 8:1072, doi: 10.1038/s41467-017-01346-1

CE-Keenan LB16045 Predicting the Maximum Rate of Carbosylation Based on Optimal Leaf Resource Allocation

**Journal Publications**

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- H. Wang, C. Prentice, T. Keenan, T. Davis, I. Wright, W. Cornwell, et al. "Towards a universal model for carbon dioxide uptake by plants", *Nature Plants*, 2017, 3, 734–741

- S. Niu, Z. Fu, Y. Luo, P. Stoy, T. Keenan, et al. “Interannual variability of ecosystem carbon exchange: From observation to prediction”, *Global Ecology and Biogeography*. 2017 DOI: 10.1111/geb.12633.
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CE-Tas Baas LB16024 Assessing Microbial Functions at Terrestrial-Aquatic Interfaces by Metagenome-Based Metabolic Flux Analysis

**Journal Publications**

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- N. Tas, K. Wickland, H. Garcia Martin and K.H. Williams “Aquatic microbial metabolic responses to terrestrial carbon inputs resolved via multi-omics approaches”, in preparation

CE-Wu LB17009 Remote Monitoring of Soil-Plant Biome Responses to Water and Metal Stress

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- Y. Wu, C. Chou, L. Peruzzo, W. Riley, Z. Hao, P. Petrov, G. Newman, E. Blancaflor, X. Ma, R. Versteeg, B. Dafflon, E. Brodie and S. Hubbard, “Life in the Dark: Roots and How They Regulate Plant-soil Interactions”, AGU annual meeting, Abs# B12B-04, Dec 11, 2017

CR-Baden LB17037 Automated Translation of Applications to Large Scale Programming Systems

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- S. Martin, M. J. Berger and S. B. Baden, “Toucan - A Translator for Communication Tolerant MPI Applications,” 31st International Parallel and Distributed Processing Symposium, IPDPS’17 (2017)

CR-Calafiura LB16008 Exploring the Limits of Low-Energy, Real-Time, Streaming Data Processing with Neuromorphic Computing

**Journal Publications**

- R. Carney et al, “Neuromorphic Kalman filter implementation in IBM's TrueNorth”, *Journal of Physics, Conference Series*, Vol 898, No 4, 2017  
<http://iopscience.iop.org/article/10.1088/1742-6596/898/4/042021>

CR-Carter LB17013 Enabling Extreme-Scale Many-Query Computational Physics

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- M. J. Zahr, P.-O. Persson, “An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions,” *Journal of*

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CR-Chan LB16009 ExaGrid: Large-Scale, Asynchronous Co-Simulation of Advanced Electric Grid Systems

**Papers and Presentations from Workshops and Conferences**

- Wang, J. Bachan, C. Chan, “ExaGridPF: A Parallel Power Flow Solver for Transmission and Unbalanced Distribution Systems”, IEEE Conference on Innovative Smart Grid Technology (ISGT), 2018

CR-Day LB16010 Exploiting Physics-Based Concurrency in Time-Dependent Extreme-Scale Multiphysics Simulations

**Journal Publications**

- F. Hamon, M. Day, M. Minion, “Concurrent Implicit Spectral Deferred Correction Scheme for Low-Mach Number Combustion with Detailed Chemistry,” submitted to *Combustion Theory and Modeling*, 2017

CR-Johansen LB16012 Modeling the Earth's Hydrological Cycle from Watershed to Global Scales

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- A. Rhoades, (2017) *Understanding 21st Century Hydroclimatic Trends in Western USA Mountain Ranges using Variable-Resolution CESM*. U.C. Davis, Ph.D. dissertation in Atmospheric Science

CR-Li LB17014 High Performance Computing for Large-Scale Mobility Modeling

**Journal Publications**

H. Zhan, G. Gomes, X. Li, K. Madduri, A. Sim, and K. Wu, “Consensus Ensemble System for Traffic Flow Prediction”, IEEE Transactions on Intelligent Transportation Systems, accepted Dec. 2017

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J. Ugirumurera, X.S. Li, J. Thai, G. Gomes, A. Bayen, “High Performance Computing in Large-Scale Traffic Engineering Problems”, Women in HPC Workshop at Supercomputing Conference, SC17, Nov 12, 2017, Denver

#### CR-Lin LB15007 Fast Numerical Methods for Green's Function in Mesoscale Simulation

##### **Journal Publications**

- X. Li, L. Lin, J. Lu, PEXSI-\Sigma: A Green's function embedding method for Kohn-Sham density functional theory, Ann. Math. Sci. Appl. in press 2017  
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- L. Lin, “Localized spectrum slicing”, Math. Comp. 86, 2345, 2017  
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- L. Lin, Z. Xu and L. Ying, Adaptively compressed polarizability operator for accelerating large scale ab initio phonon calculations, SIAM Multiscale Model. Simul. 15, 29, 2017 <http://arxiv.org/abs/1605.0802>

#### CR-Marques LB15005 Unconstrained Functionals for Massively Parallel Scaling of Conjugate Gradient Eigensolvers

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S M. Del Ben, O. Marques and A. Canning, “Unconstrained Functionals for Massively Parallel Scaling of Conjugate Gradient Eigensolvers”, in draft form

#### CR-McClean LB16011 Design of Quantum Chemistry Simulations for Superconducting Circuits

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CR-Michelogiannakis LB17015 Continuing Digital Computing Performance Scaling Post Moore's Law

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- D. Vasudevan, G. Michelogiannakis, and J. Shalf, "CASPER - Configurable Design Space Exploration of Programmable Architectures for Machine Learning using Beyond Moore Devices", IEEE/ACM International Symposium on Nanoscale Architectures (NANOARCH), July 2017  
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- G. Michelogiannakis, D. Donofrio, and J. shalf, "Modeling of Novel Transistors, Manufacturing Technologies, and Architectures to Preserve Digital Computing Performance Scaling", First international workshop on post Moore's era supercomputing (PMES), November 2016  
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CR-Minion LB17016 Acceleration of Temporal Integration for Real Time - Time Dependent Density Functional Theory

**Journal Publications**

- B. Krull and M. Minion, "Parallel-in-Time Magnus Integrators for Isospectral Flow Problems", In preparation

CR-Moore LB15041 Solving Problems in Materials Theory via Quantum Networks

**Journal Publications**

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CR-Perez LB17017 Scaling Interactive Science for Data-Intensive Discovery

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CR-Wu LB16014 Open Framework for High-Performance Streaming Analytics

**Journal Publications**

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CR-Yang LB16015 Neuromorphic Image Analysis and Pattern Recognition

**Journal Publications**

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GO-Ajo-Franklin LB17025 Dark Fiber and Distributed Acoustic Sensing : Opportunities for Critical Infrastructure and Environmental Monitoring

**Journal Publications**

Lindsey, N.J., Martin, E.R., Dreger, D.S., Freifeld, B., Cole, S., James, S.R., Biondi, B.L., and J.B. Ajo-Franklin, “Fiber-optic network observations of earthquake wavefields”, Geophysical Research Letters, 2017, Vol. 44, No. 23, pp. 11,792-11,799

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Ajo-Franklin, J.B., Dou, S., Lindsey, N., Freifeld, B.M., Daley, T.M, Tracy, C., and I. Monga, “Dark Fiber and Distributed Acoustic Sensing: Applications to Monitoring Seismicity and Near-Surface Properties”, Session S013, American Geophysical Union, Fall Meeting, Dec.11-15, 2017, New Orleans, LA

GO-Arora LB16020 Multi-Scale Modeling of Geochemical Impacts on Fracture Evolution

**Journal Publications**



S. Molins, B.Arora, D. Trebotich, C. Steefel, “Multi-scale model of reactive transport in fractures– An adaptive embedded-boundary approach” Draft manuscript to be submitted to Transport in Porous Media

GO-Christensen LB16022 Identifying the Source and Magnitude of Redox Related Metal Isotope Fractionation: An Essential Tool for Earth System Science

**Journal Publications**

Brown, S.T., Basu, A., Ding, X., Christensen, J.N., and DePaolo, D.J. "Uranium Isotope Fractionation by Abiotic Reductive Precipitation" In preparation for PNAS

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GO-Guglielmi LB16021 Advanced In-Situ Experiments for Understanding Induced Seismicity

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Y. Guglielmi (Invited speaker, 29 March 2017), In Situ Experiments in Fault Zones, ICDP Workshop on Scientific Exploration of Induced Seismicity and Stress (SEISMS, Lamont-Doherty Earth Observatory, Columbia University, USA)

Yves Guglielmi, Paul Cook, Pengcheng Fu, Joe Morris, and the EGS Collab Team (2018), In-Situ Monitoring of a Hydraulic Fracture Initiation using an intelligent straddle packer tool. 52nd US Rock Mechanics/Geomechanics Symposium (Seattle, Washington), 24-27 June 2018

GO-Nico LB17004 Developing Science Based Scalable Approaches to Groundwater Banking

**Journal Publications**

G, Newman, et al., “Full Waveform Seismic Imaging of Groundwater Recharge Location” manuscript in preparation

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P. Nico, et al, “Impact of Subsurface Stratigraphy on Water Migration during On-Farm Water Recharge” United States Committee on Irrigation and Drainage, Sacramento, October 2017

- P. Nico, et al, “Importance of Subsurface Sediments on Water Movement” Almond Conference, Sacramento, December 2017
- C. Ulrich, et al “On-Farm, Almond Orchard Flooding as a Viable Aquifer Recharge Alternative” American Geophysical Union Meeting, New Orleans, December 2017

GO-Stringfellow LB16023 Characterizing the Environmental Impact of Chemical Compounds Used in Oil and Gas Development

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- W. T. Stringfellow, M. K. Camarillo, J. K. Domen, W. L. Sandelin, C. Varadharajan, P. D. Jordan, M. T. Reagan, H. Cooley, M. G. Heberger, and J. T. Birkholzer.  
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- M. K. Camarillo, J. K. Domen, and W. T. Stringfellow. “Physical-chemical evaluation of hydraulic fracturing chemicals in the context of produced water treatment.” J. Environ. Management 183: 164 – 174 (2016)
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- S. B. C. Shonkoff, W. T. Stringfellow, and J. K. Domen. “Preliminary Hazard Assessment of Chemical Additives Used in Oil and Gas Fields that Reuse Their Produced Water for Agricultural Irrigation in The San Joaquin Valley of California.” Technical Report. PSE Healthy Energy, Inc. Oakland, CA. (2016, September)
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- W. T. Stringfellow, M. K. Camarillo, N. Spycher, and P. Nico. “Produced water from oil & gas fields as a potential source of irrigation water.” Toward Sustainable Groundwater in Agriculture – An International Conference Linking Science and Policy, Burlingame / San Francisco, CA, June 28-30 (2016)
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- Shonkoff, S. B. C., J. Domen, M. K. Camarillo, and W. T. Stringfellow. (Invited Presentation). "From 'fracking' to oil and gas development: chemical constituents and potential implications for the beneficial reuse of produced water." Symposium on Environmental Aspects of Unconventional Oil and Gas Production and Hydraulic Fracturing, 251st American Chemical Society National Meeting & Exposition, San Diego, CA, March 13-17 (2016)

ED-Joo LB16019 The Grid Initiative - Data Driven Approach for Monitoring and Control of Distribution System Assets

**Journal Publications**

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#### **EB-Celniker LB15022 Microbiome Adaptation in Response to Environmental Challenges**

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EB-Northen,Trent R LB17020 Eco-FAB: Discovering of the Genetic Basis of a Beneficial Microbiome to Improve Crop Productivity

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- A. Fernandez-Bravo, K. Yao, E. S. Barnard, N. J. Borys, E. S. Levy, B. Tian, C. A. Tajon, L. Moretti, M. V. Altoe, S. Aloni, K. Beketayev, F. Scotognella, B. E. Cohen, E. M. Chan, P. J. Schuck, "Continuous-Wave Upconverting Nanoparticle Microlasers", Submitted (2017), under revision.

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- J.P. Philbin, D. Skubitz, E. Rabani, “Excitonic Effects Control Auger Recombination in CdSe Quantum Dots and Nanorods”, 2017, in preparation.
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- Franziska K. K. Kirschner, Felix Flicker, Amir Yacoby, Norman Y. Yao, Stephen J. Blundell, “Proposal for the Detection of Magnetic Monopoles in Spin Ice via Nanoscale Magnetometry”, arXiv:1711.00408, <https://arxiv.org/abs/1711.00408>
- Norman Y. Yao, Michael P. Zaletel, Dan M. Stamper-Kurn, Ashvin Vishwanath, “A Quantum Dipolar Spin Liquid” (in press, *Nature Physics*)
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MS-Zheng,Haimei LB17030 Multimodal Imaging and Spectroscopy of Solid-Liquid Interfaces

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NS-Haxton, Wick C LB15027 Computational Nuclear Physics Code Development for Fundamental Physics/Astrophysics

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PH-Kusaka,Akito LB16037 Enabling Technologies for Next Generation Receivers to Measure the Polarization of Cosmic Microwave Background

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PH-Papucci,Michele LB15031 Confronting Beyond the Standard Model Theories with New LHC and Astrophysical Data

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