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Report on
Ernest Orlando Lawrence
Berkeley National Laboratory

Laboratory Directed Research and Development Program

FY 2012

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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, and general sciences in a manner that ensures employee and public safety and 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 to 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 support DOE's Strategic Themes that are codified in DOE's 2006 Strategic Plan (DOE/CF-0010), with a primary focus on Scientific Discovery and Innovation. For that strategic theme, the Fiscal Year (FY) 2012 LDRD projects support each one of the three goals through multiple strategies described in the plan. In addition, LDRD efforts support the four goals of Energy Security, the two goals of Environmental Responsibility, and Nuclear Security (unclassified fundamental research that supports stockpile safety and nonproliferation programs). Going forward in FY 2013, the LDRD program also supports the Goals codified in the new DOE Strategic Plan of May, 2011. The LDRD program also supports Office of Science strategic plans, including the 20-year Scientific Facilities Plan and the Office of Science Strategic Plan. The 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 LDRD program also play 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 Work For Others (WFO) sponsors. Among many directions, these include a broad range of health-related science and technology of interest to the National Institutes of Health, breast cancer and accelerator research supported by the Department of Defense, detector technologies that should be useful to the Department of Homeland Security, and particle detection that will be valuable to the Environmental Protection Agency.

The *Berkeley Lab Laboratory Directed Research and Development Program FY2012* 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.

The Berkeley Lab LDRD program is a critical tool for directing the Laboratory's forefront scientific research capabilities toward vital, excellent, 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 capability, and permits exploration of exciting new opportunities. All projects are work in forefront areas of science and technology. Areas eligible for support include the following:

- 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 maintain compliance with DOE Orders, in particular DOE Order 413.2B Admin Chg 1 (dated January 31, 2011). 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 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 FY2012, Berkeley Lab was authorized by DOE to establish a funding ceiling for the LDRD program of $23M including General & Administrative (G&A) overhead, which equated to ~3.4% of Berkeley Lab's FY2012 projected operating and capital equipment budgets. This funding level was provided to develop new scientific ideas and opportunities and allow the Berkeley Lab Director an opportunity to initiate new directions. Budget constraints limited available resources, however, so about $20.0M was expended for operating expenses (3.05% of actual Berkeley Lab FY2012 operating and equipment costs excluding ARRA funding).

In FY2012, scientists submitted 204 proposals, requesting about $40.4M in funding prior to assessing laboratory overhead. Ninety two projects were funded, with awards ranging from $36K to $630K. These projects with final costs are summarized with in the Table of Contents.

LB12038

Free-Electron Laser Soft X-Ray Self-Seeding

Principal Investigator: Paul Emma

Project Report for 2012:

Project Description

The purpose of this project is to demonstrate self-seeding of soft x-rays in the Linac Coherent Light Source (LCLS) Free-Electron Laser (FEL) at the SLAC National Accelerator Laboratory using a grating-based monochromator. These data will enable the use of a similar seeding system for the Next Generation Light Source (NGLS) at LBNL in the future.

We are developing and designing a grating-based monochromator and set of x-ray mirrors to channel the FEL radiation from the first half of the existing LCLS magnetic undulator into seed the second half in order to reduce the FEL bandwidth and provide longitudinally coherent soft x-ray pulses in the 500-1000 eV range. The work involves LBNL (mechanical design), SLAC (magnets, controls, and integration), and the Paul Scherrer Institute in Switzerland (procuring the x-ray optics).

Accomplishments

We have developed a mechanical design for the monochromator, in collaboration with SLAC, which includes motorized remote controls of the various mirrors and grating position. The x-ray optics (variable-line spacing grating and 3 different x-ray mirrors) are being procured at PSI with specifications provided by SLAC and LBNL. We have also developed a design for overlap diagnostics in order to spatially overlap the electron and photon beams during commissioning and have drawn up a commissioning plan, appropriate machine protection logic, and designed the chicane dipole magnets which are used to set the temporal overlap.

We are in the process of procuring the grating and mirrors through PSI and will begin purchasing hardware starting in the new calendar year. The installation at LCLS should begin in August, but will depend on the timely procurement of this quite specialized grating. With on-time delivery we should be commissioning the new self-seeding system on the LCLS at SLAC in October or November of 2013.

LB12037

Antihydrogen Research for Advanced Studies in Matter-Antimatter Asymmetry

Joel Fajans PI; Jonathan Wurtele co-PI

Project Description

The goal of this LDRD was both to develop experimental capabilities of the Berkeley Ultra-low Energy Trap in ultra-cold plasmas, to develop methods for measuring the gravitational force of the Earth on antihydrogen with the constraints imposed by current and near-term experimental capabilities, to apply these methods to current experiments, and to develop computational tools for assessing possible methods of mixing antiprotons with positrons to enhance the antihydrogen production rate on the ALPHA-II experiment.

Accomplishments

The Berkeley Ultra-low Energy Trap studies the dynamics of cold, highly magnetized pure electron plasmas, with a focus on understanding cooling mechanisms for plasmas in the ALPHA antihydrogen apparatus. We completed construction of the apparatus, trapped electron plasmas in a 3T field and performed temperature measurements. We expect to publish multiple publications this year regarding the dynamics of plasmas in this trap.

Measurements were taken to test the feasibility of 3D-printed materials for use in an ultrahigh-vacuum environment. The use of these parts in a laboratory environment is highly desirable since they can be rapidly produced and are much cheaper than an equivalent machined part. We found that printed sterling silver parts had sufficiently low out-gassing that, after a low temperature heating cycle, chambers containing these materials were capable of being pumped to pressures below 10^{-9} mbar.

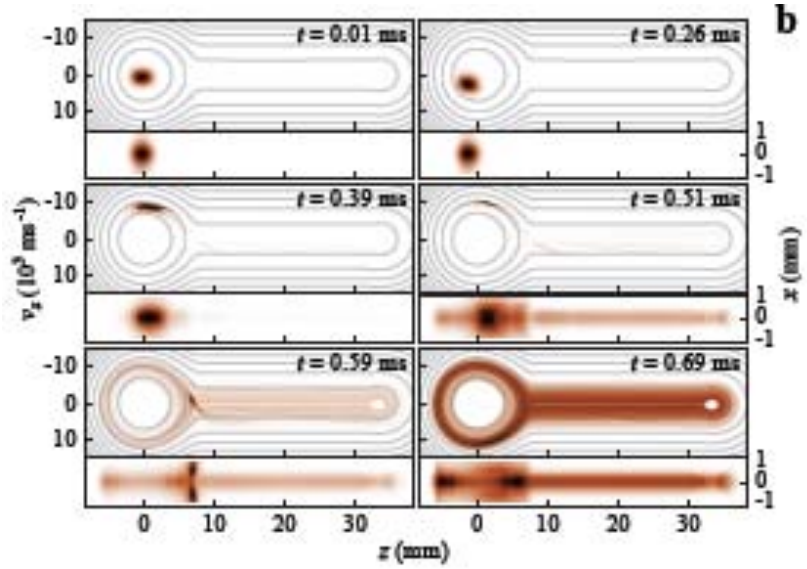


Figure: We improved and utilized a Vlasov simulation to study particle dynamics and plasma physics during the mixing of antiprotons and positrons. The longitudinal (z,v_z) phase space and the (x,z) density are plotted at various times in the mixing.

We prepared and submitted to a refereed journal a paper on our new methodology for measurement of the gravitational force of the Earth on antihydrogen. We developed a new simulation to study antihydrogen dynamics in existing and proposed experiments and prepared a paper that will soon be submitted. Follow-on funding will be pursued through NSF and DOE.

LB10031

Novel Accelerator & Engineering Strategies for Ion Beam Cancer Therapy
Principal Investigator(s): David Robin

Project Description

The use of carbon-ion beams to kill tumor tissue has been a promising avenue of cancer research since the initial experiments were conducted at Berkeley Lab's Bevalac from 1977-1992. However, because of the extraordinarily high cost of carbon ion-beam facilities (~$250 million), only a handful have been built worldwide since the Bevatron was closed; none are in the United States. Presently the only ion used in the United States is protons. Compared with carbon, proton facilities are smaller and less expensive (~$125 million).

Driving up the cost of such carbon ion-beam treatment facilities are the huge, 600-ton gantries required to focus a high-energy carbon-ion beam precisely on the tumor site. Gantry size is directly related to the enormous weight of focusing magnets used to guide the beam from the accelerator to the patient. In particular carbon beams have three times the magnetic rigidity compared with proton beams thus requiring significantly larger gantries. While most proton facilities are being built with gantries, there exists only one carbon gantry in the world (in Heidelberg) whose size is nearly double that of a proton gantry and at 660 tons is 5 times heavier than proton gantries. The purpose of this project was to explore the use of high field superconducting magnets to reduce the size, weight, and cost of gantries.

Accomplishments

Gantry size is directly related to the enormous weight of focusing magnets used to guide the beam from the accelerator to the patient. We reduced the weight of the largest of these magnets by 80 percent by using an unconventional magnet design – we call a Canted Cosine Theta (CCT) superconducting magnet. Critical to the new CCT magnet design is the placement of a pair of overlapping solenoid coils. When the coils are chilled to superconducting temperatures and a current is applied, they create very strong magnetic fields strong enough to bend the ion beam.

The year before last, the focus of our work was the use of intensive computer modeling in determining the winding path of the coils around the toroidal mandrel to create the required magnet fields. The construction and performance of a CCT magnet is critically dependent upon the mandrel. So this past year our effort was focused on the design of the toroidal mandrel to support the coils. In the process a key lamination concept was developed. This lamination solved many of the most fundamental challenges of a CCT magnet – the ability to analyze, construct, and quickly ramp the magnetic fields. The mandrel also is very important for managing the large stresses of the magnet. A half scale rapid prototype model was constructed of the mandrel. It appears this lamination concept for CCT magnets may make them attractive not only for gantry magnets but also for very high field magnets.

LB10012

Ion Beam Driven Fusion and Fusion-Fission Hybrids

Principal Investigator: Peter Seidl

Project Description

We assessed the potential of ion-beam driven fusion, fusion-fission reactor hybrids and accelerator-driven energy producing systems. Parametric studies on a variety of thorium-fueled, liquid-salt cooled pebble bed and other subcritical fission blankets were performed in the first year of this LDRD. Ion beam accelerators capable of providing the needed high average beam power and high power efficiency were investigated to identify R&D needs and possible paths forward. In the second year, we studied the beam physics for the creation of high-charge state beams in a gas jet stripper for high-current heavy-ion accelerators to drive inertial fusion energy targets. We concluded transverse emittance growth due to space charge is significant, but magnetic separation of charge states after the stripper can lower the emittance growth. We also contributed to presentations and reports to the National Academies of Sciences and Engineering review of "Prospects for Inertial Confinement Fusion Energy Systems." LBNL has been a leading institution for heavy ion driven inertial fusion (HIF) in the US.

Our most significant accomplishments this year are a survey paper and two collaborations to address HIF beam physics issues. The paper (submitted to Phys. Rev. ST-AB) identifying near-term (<5 years) and longer range R&D needed to make a strong case for an aggressive HIF research campaign supported by the DOE. This will be a more likely prospect when, or if, the National Ignition Facility at LLNL succeeds in demonstrating ignition and a self-propagating fusion reaction with high yield. NIF ignition experiments will continue for the next several years.

To initiate new research in the interim period, we collaborated with two universities where high-impact, low-cost experiments may be performed to illuminate beam physics pertinent to HIF, using Paul Trap simulators and low-energy, high space-charge electron beams. They are summarized below. Paul Traps, or a quadrupole ion trap uses DC and RF fields to trap and store ions. The ion dynamics mimic those in strong focusing accelerators. We developed a concept to upgrade the very impressive Paul Traps at Hiroshima University to enable measurements with a significant space charge tune depression characteristic of the transverse dynamics anticipated in heavy ion fusion accelerators. The application of Paul Traps in this space charge dominated regime would enable the experimental "simulation" of the transport of high-current ion beams through thousands of lattice periods at a very modest cost, within a space of < 1 meter.

In collaboration with colleagues at the University of Maryland Electron Ring (UMER), we have modeled and developed prototype electronics for a novel beam dynamics experiment for HIF: To amplify the ion beam current, a velocity chirp and strong confining pulses established by induction cells, the ion beams are to be longitudinally compressed by a large factor against space charge fields. Using the Warp particle-in-cell code, we simulated the UMER beam compression from the 100-ns initial bunch by a factor of 2-3 in about six turns within the 12-meter circumference ring. We have also developed and prototyped pulser circuits to demonstrate the needed voltage rise time (~100 V/ns) by leveraging circuit designs developed for the NGLS. The beam-confining waveforms, which must change for each turn, precisely balance the space-charge field at the end of the beam bunches to prevent particle loss and emittance growth. We have made a strong case for this and related experiments which would provide a most very opportunity to test the compression of the fusion driver beam at a very economical scale using low energy electrons – a beam manipulation that would, at full HIF driver scale, require ~100 meters.

LB11035

Experimental Realization of a High-Harmonics-Seeded, Laser-Plasma-Accelerator Driven Free-Electron Laser

Principle Investigator: Jeroen VAN TILBORG

Project Description

The purpose of this project is to experimentally realize soft X-rays (30-100 eV) seeding into a laser-plasma-accelerator (LPA) driven free-electron laser (FEL). The proposal contains two stages: (1) Construction and characterization of an ultra-short high-power seed source of soft X-rays through means of high harmonics generation (HHG) from a near-infrared laser. (2) Efficient coupling of the seed pulses and LPA-based electron beams in the undulator to optimize FEL output flux, stability, and temporal coherence. The T-Rex laser at LOASIS will be used to produce and deliver both the high-power HHG seed and the high-current electron beam into the THUNDER undulator. The proposed system will benefit the non-linear X-ray community and serve as a test-bed for seeded FEL's.

Accomplishments

During 2011 & 2012, several properties of LPA e-beams critical to an FEL application were verified. Through measurement of coherent optical transition radiation it was measured that the slice energy spread of LPA e-beams could be as low as <0.5% [Lin *et al.* PRL **108**, 094801 (2012)], whereas the spectrum of betatron-produced X-rays provided an excellent upperbound to the e-beam source size and e-beam emittance [Plateau *et al.* PRL **109**, 064802 (2012)]. During 2012, improvements were made to the delivery line of the LPA to the undulator. Detailed scans of the two quadrupoles allowed for determination of the exact field strength, enabling us to control the e-beam delivery. Also, we were able produce first XUV light out of the LPA-driven undulator. Although the e-beams used in these studies were of broad-bandwidth nature (and hence the undulator radiation was expected and measured to be broad-bandwidth), the XUV spectra were recorded with a low-spectral-resolution transmission grating and with a high-spectral-resolution reflective concave grating covering a large bandwidth.

In terms of the proposed seed source for the LPA-based FEL, we selected HHG from a spooling tape in the so-called CWE regime (Coherent Wakefield Emission). The idea is to put the tape at the undulator entrance, in order to 1) provide an HHG source without need for XUV transport optics, and 2) have the tape act as an e-beam and seed combiner. We have measured the surface roughness of our tapes through X-ray reflectometry at the ALS, and have found that all tapes meet the surface conditions for CWE (roughness <15 nm). During 2012, we built a CWE test setup. Using gratings and MCP's, we were able to measure the harmonic yield for various tape materials and laser conditions (compression, focal location, and energy). We recorded the XUV spatial profile and divergence. Harmonics up to the 17th harmonic were recorded. In independent calibration efforts at the ALS we have obtained an absolute photon-to-count calibration of our MCP imaging setup. Currently we have recorded a conversion efficiency of $5x10^{-7}$ for the 15th harmonic, which is less then our goal of $5x10^{-6}$, although our measured divergence is much better (7 mrad instead of the anticipated >30 mrad). The extensive data set has given us detailed physics insight, and we are investigating how to further improve the seed parameters. Even with the current seed power (estimated to be 2.5 MW peak power) we would be well above undulator spontaneous power of ~0.1 MW, allowing us to confidentially move forward with the integrating of the seed arm onto the LPA undulator line.

LB12007

Soft X-Ray Spectroscopy for In-situ Electronic Structure Study of Artificial Photosynthesis

Principal Investigator: Jinghua Guo

Project Description

This proposal is to develop an in-situ photon-in/photon-out soft x-ray detection system for electronic structure study of artificial photosynthetic catalysts. Such development is crucial for studying the inorganic and biological catalysts, especially in the dilute aqueous systems. The goal is to extend the advantages of soft x-ray spectroscopy into the catalytic, environmental, and biological communities in order to understand the mechanism of the multi-electron catalytic reactions. Catalytic reactions such as water oxidation, H_2 production, and CO_2 reduction are all multi-electron reactions, where several intermediate states are involved in the reaction cycle. Therefore, a holistic study of the entire course of the reaction, including the intermediate states of the catalytic cycle, holds the key for discovering novel efficient photocatalysts. The proposed effort will have the significant impact on the renewable and carbon-neutral energy technologies that require us to understand, predict, and ultimately control chemical reactivity, bonding, and charge transfer at the electronic, atomic, and molecular levels. The resulting systems will serve the need from JCAP and broad general user community.

The hierarchy of goals in the approach to these systems in the soft x-ray energy range will be:

1) To detect the weak signal from dilute samples by using an efficient detection scheme that collects fluorescence signal from a large solid angle.

2) To mitigate the radiation damage by using a bending magnetic beamline (BL631) with fast scanning capability and very stable photon beam, and cooling and liquid flow cell will also be applied.

3) To record soft x-ray spectra from a flow sample cell to probe the intermediate states of catalytic reactions in time-scale (~μs to ms) in a dilute (≤1 mM) and wet environment.

The collaborators are Per-Anders Glans, Elke Arenholz, Catherine Jenkins, Zahid Hussain (ALS), Junko Yano, Vittal Yachandra, Heinz Frei (PBD, JCAP)

Accomplishments

In the first year, we have designed and constructed an endstation for photon-in/photon-out soft x-ray spectroscopy on BL6.3.1. The postdoc, Debajeet Bora was hired for the LDRD project. The endstation was assembled offline for vacuum test, and installed on BL6.3.1 in August. It has been operated for JCAP's scientists and general users to carry out a number of XAS experiments.

A four elements Vortex detector was ordered with the JCAP funding, and the detector has been arrived recently and will be tested in January. The high throughput fluorescence detection systems will be useful for the study of dilute systems as found in environmental sciences and other fields. In-situ cells have been fabricated with two types: static electrochemical liquid cell (successfully operated) and flow electrochemical liquid cell (under commissioning), which will be well suited for the study of the electronic structure of artificial photosynthetic catalysts.

The automation of the sample control is under developing. We are starting to design a high throughput soft x-ray fluorescence spectrograph. Optical design is under way, and soon will start the mechanical design and request the quote of optics (mirror and grating).

A few possible efficient catalysts for photoelectrochemical water splitting reactions are to measured. The results are expected to be crucial in design and control of photocatalysts.

LB10009

Long-range Ordering of Block Copolymers on Faceted Silicon
Principal Investigators: Alexander Hexemer
co-PI Howard Padmore, Ting Xu, Thomas P. Russell

Project Description

The purpose of this project was to generate an ultradense array of addressable nanoscopic elements over macroscopic length scale by using ordered block copolymers (BCPs). The self-assembly of block copolymers, two chemically dissimilar polymers covalently bond together, has become a promising route to generate templates and scaffolds for the fabrication of nanostructured materials. In general, BCPs in thin films self-assemble into grains, a few microns in size, of laterally ordered nanoscopic microdomains. We have shown that the surface reconstruction of single crystalline wafers, cut along specific crystallographic planes, can be used to generate nanoscopic surface facets that can guide the self-assembly of BCPs into a highly ordered, single grain array of nanoscopic elements with a well-defined orientation over large areas. While similar results can be obtained on the surface of reconstructed silicon, drawbacks to this approach are the rigidity and cost of sapphire or silicon. It is highly desirable to develop routes by which long-range ordered structures could be generated on inexpensive, flexible substrates. One of the easiest ways to accomplish this is to make polymeric replica of the faceted surface of reconstructed sapphire or silicon. We used this approach to imprint different commercial polymers.

In order to quantitatively determine the crucial parameters for the perfection of BCP ordering on faceted surfaces, we will further develop grazing incidence small angle X-ray scattering (GISAXS). Currently, GISAXS is the only technique to examine nanoscopic elements in large area because of its great sensitivity. These GISAXS results will also be combined with computer simulation to understand how faceted surface function.

Accomplishments

We have discovered a simple, versatile approach to the directed self-assembly of block copolymers into a macroscopic array of unidirectionally aligned line patterns on reconstructed faceted single crystal surfaces or on flexible, inexpensive polymeric replicas. High fidelity transfer of the line pattern generated from the microdomains to an imprint mold, i.e. a secondary master, was also shown.

We have discovered that a simple reconstruction of BCPs can provide etching contrast and allows the patterning of BCP masks for subsequent pattern transfer into the underlying silicon substrate. Using a highly selective cyro-ICP etching densely packed, sub-15 nm, silicon nano-trenches were fabricated. These nano-trench patterns were used as a nano-imprint master to pattern polymeric materials. Oriented silicon nano-trenches were created using graphoepitaxy directed self-assembly. The methodology was used to pattern silicon holes from a patterned surface-perpendicular cylinder forming PS-b-PEO block copolymer.

We have also accomplished to generate ultradense nanoscopic lines by means of directed self-assembly (DSA) of BCPs on defect-free faceted substrates, resulting in a film with long range ordering and orientation of line patterns with an amplified areal density over large distances. We also proposed a new method that controls the direction of well-aligned and oriented nanolines by the facet geometry. This methodology may provide an easy way to prepare ideal templates and scaffolds for the fabrication of magnetic storage media, optical devices, and arrays of conducting wires.

LB11020

New opportunities in Hard X-ray Tomography– High Temperature and Elemental Imaging

Principle Investigators: Alastair MacDowell(ALS), Stephano Marchesini (ALS), Jonathon Ajo-Franklin (ESD), Ho-YingHolman (ESD), Peter Nico (ESD), Eleanor Blakely (LSD), Al Thompson (LSD) Joe Gray (OHSU) , Peter Denes(LDEG), Rob Ritchie (MSD, UCB)

Project Description

We have identified two unique areas of instrument development involving the technique of hard x-ray 3 dimensional (3D) tomographic imaging that can provide novel measurements relevant for the CC2.0 initiative. The 2 instruments are:-

1) A High Temperature micro-Tomography load cell that can image in 3D the condition of materials when under tension or compression in-situ at up to 2000^{o}C.

2) A novel 3D imaging detector with elemental specificity.

The High Temperature Load cell has been applied to the problem of investigating 3D crack propagation within silicon carbide composite ceramics whilst operating at high temperature. Silicon carbide (SiC) composites are proposed materials that show the ability of maintaining strength whilst at very high temperatures (~1700C). Typical applications include critical components in hyper sonic aircraft, space re-entry vehicles and high temperature turbines for jet propulsion and power generation. In the latter case, turbines are Carnot engines where higher efficiency is achieved by operating at higher temperatures. This is of significant relevance to the CC2.0 initiative.

The 3D elemental imaging camera is based on encoded aperture technology and is intended to image fluorescent x-rays from a sample irradiated by excitation x-rays. It will use the new high speed energy resolving CCD detectors being built at LBNL. A range of demonstration experiments for this new detector relevant to CC2.0 are planned. These include characterizing iron carbonate precipitation during CO_2 sequestration, chromium and uranium remediation at DOE sites, effect of chemical and structural factors in plant materials and their deconstruction by cellulolytic microorganisms and metal tagging in mice to track metastatic pathways for spread of cancer

Accomplishments

The High Temperature micro-Tomography load cell has been designed, assembled and commissioned. A series of SiC composite materials made by Teledyne Inc. have been imaged while undergoing strain to failure at 1750C. The samples were imaged in 3D with a resolution of 1-2 micron at high temperature showing crack propagation. The data is undergoing analysis and will be used in modeling code being developed at Univ of Florida. Preliminary experiments have been carried out in other fields to expand the range of technique. These include magma evolution (understanding volcanos), crystal growth from melts, Carbon Preform Space vehicle re-entry heat shields.

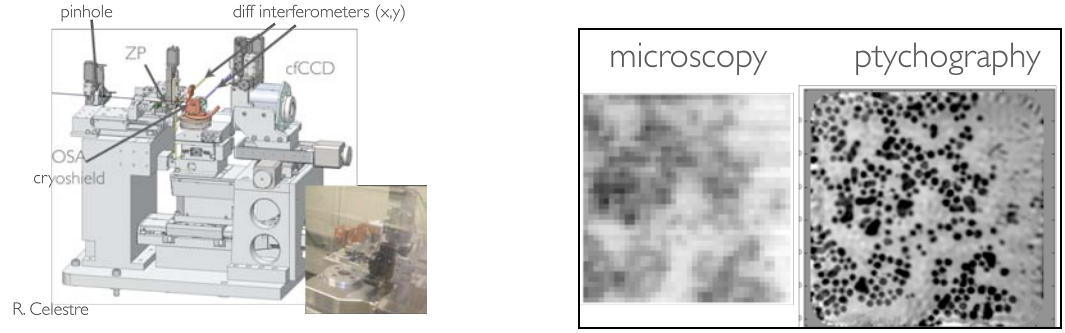
3D Elemental imaging camera. Coded apertures were constructed and elemental test samples imaged to demonstrate elemental selectivity and the re-construction algorithms. Preliminary data taken with an intiail version of the fast energy resolving LBNL CCD, final version is scheduled for Spring 2013.

LB10014

The Nanoscale Surveyor
Principle Investigator: Stefano Marchesini (Advanced Light Source)

Project Description:
This project aims to develop a high-throughput Terapixel x-ray camera to study nano-materials at a few-nanometer resolution in three dimensions with chemical sensitivity. The purpose of this camera is to establish a user community interested in nanoporous materials that fits the ALS strategic plan (COSMIC) and the future of X-ray science at the lab. Materials based on nanoparticles offer opportunities in energy applications ranging from solar cells, hydrogen storage, batteries and fuel cells.

The subject of this proposal is a new x-ray imaging method, Ptychography. In a scanning x-ray microscope, the intensity of light transmitted through an object is recorded point by point in the image. The Ptychographic version simply replaces the point intensity detector with a 2d imaging detector such as a CCD camera, so that point by point, the diffraction pattern of the local object can be recorded.
Accomplishments:
In fiscal year 2012, we focused on developing a fast instrument suitable for ptychographic tomography with soft x-rays on samples in vacuum that can be measured at high or low temperatures. A zone plate forms a coherent illumination spot of the order 300nm diameter on the sample and diffraction patterns are recorded, along with accurately encoded values of the sample position, as the sample scans in x and y over a region of interest of the order 10 microns. A novel differential interferometer scheme is employed measuring the zone plate lens with respect to the sample in x and y, reflecting one of the x beams from a cylindrical sample chuck through a cylindrical lens. Sample encoding within an x/y scan is accurate to about 10nm. Figure 1 shows a CAD drawing of the NANOSURVEYOR instrument and a demonstration of the current imaging



(left) The Nanosurveyor instrument with cryo-sample rotation stage and interferometer position sensing. (right) show the a STXM image and ptychographic reconstruction of a random aggregation of nanoparticles. The smallest visible features are 10 nm gold nanoparticles.

capable using a STXM enhanced with ptychography at 800eV x-ray energy. We also developed an augmented Lagrangian alternating direct ion method (ADM) for solving the phase retrieval problem, developed scalable HPC code for high throughput analysis, and an augmented projection scheme to compensate for instabilities in the acquisition system such as vibrations.

LB12018

Lensless X-ray Imaging of Orbital Order Bragg Plane

Principal Investigator: Sujoy Roy (ALS)
Co-PI**:** Weilun Chao (CXRO), Stefano Cabrini (Molecular Foundry), Stefano Marchesini (ALS)

Project Description

Complex oxide provides the paradigmatic example of how correlated interplay between spin, lattice and orbital can give rise to exotic new phases and material properties. A prototypical example of such a material are the manganite compounds that are of the general formula $R_{1-x}A_xMnO_3$ (R = rare-earth metal, A = divalent element) and show colossal-magnetoresistance (CMR) properties near the Curie temperature T_C, which make them a leading candidate for the next generation oxide based electronic devices. Particularly interesting is the charge/orbital order phase in which an electronically ordered phase appear due to arrangement of Mn^{3+} and Mn^{4+} atoms over mesoscopic length scale. Resonantly tuned coherent x-ray scattering studies on the orbital order peak show speckle pattern that indicate presence of electronic texture in the Bragg plane. The question therefore is, what are these structures due to? Are there charge/orbital order domains and if so, what is their origin? How do they form and evolve? To address these questions we propose to employ x-ray holography technique that will enable us to directly image the Bragg planes in real space. The experiment will use coherent x-rays from the synchrotron and employ reflection geometry that will allow us to probe area of interest in the reciprocal space.

Accomplishments

We have made significant progress towards achieving an image of the electronic order Bragg plane. Getting a high quality nanostructured pinhole is critical for the success of the project. Together with Molecular Foundry and Center for X-ray Optics we have developed a method to fabricate high quality non-circular nano-apertures. We were also successful in fabricating a special nanostructured aperture to directly measure 2D transverse coherence length of x-ray beam in a single shot.

We have developed important collaboration with Prof Y. Tokura from University of Tokyo who is a world renowned expert on single crystal growth physics. This collaboration has resulted in us getting high quality single crystal and thin film samples that are essential for the success of our experiment. We have successfully developed a method to physically put apertures on these single crystal in a non-destructive manner. The sample is currently being tested.

We are using an epitaxially grown rare earth element Dysprosium to image magnetic Bragg plane. Dysprosium is a helical antiferromagnet with a Néel temperature of 180 K and undergoes ferromagnetic transition at 85 K. We have been successful in getting a hologram out of the antiferromagnetic Bragg peak of a helical rare earth magnet Dy. Inversion of the hologram shows structure in the cross correlation terms. This is a promising result and we are currently doing further experiments.

A postdoc has been hired and has joined the group in February 2012. He has experience in resonant x-ray magnetic scattering and we think the progress will be accelerated with his addition.

LB10023

Ambient Pressure Photoemission Spectromicroscopy
Principal Investigator(s): Tolek Tyliszczak, Hendrik Bluhm, Zahid Hussain

Project Description

The goal of this project is to design and construct a scanning ambient pressure photoemission microscope with a spatial resolution of 100 nm or better for the investigation of heterogeneous chemical reactions at solid/vapor interfaces under conditions relevant to atmospheric/environmental science, energy research and heterogeneous catalysis.

Synchrotron based ambient pressure photoemission spectroscopy (APPES), which was developed at LBNL 12 years ago, has shown its utility for the investigation of solid/vapor and liquid/vapor interfaces at pressures up to 5 Torr (the equilibrium water vapor pressure at 0 °C is 4.6 torr). In particular in the fields of heterogeneous catalysis and atmospheric/environmental science, the investigation of surfaces under realistic conditions of temperature, gas composition and pressure is essential for a fundamental understanding of the molecular processes at liquid/vapor and solid/vapor interfaces that govern interfacial chemistry. Many of the most relevant solid/vapor interfaces are spatially and chemically inhomogeneous. In current APPES experiments this aspect cannot be adequately evaluated since the measurements average over the whole sample area that is illuminated by the incident X-ray beam, which is usually 100 μm in diameter or larger.

Accomplishments

We implemented the scanning ambient pressure spectromicroscope in the new APPES endstation at beamline 11.0.2 at the ALS. This endstation features a 3rd generation differentially pumped electrostatic lens system with an acceptance half angle of better than 10 deg and a high performance hemispherical electron energy analyzer. We have designed and built a modular scanning microscope, which can be attached to the electron energy analyzer.

We were able to measure spatially-resolved XPS spectra from various micro fabricated, spatially heterogeneous sample surfaces, proving the validity of the technical approach to the mapping of the chemical composition using zone-plate focusing. due to lack of coherency in the X-ray photons illuminating the zone plate. Due to lack of coherency in the X-ray photons illuminating the zone plate at the XPS branchline of beamline 11.0.2 the predicted spatial resolution of 100 nm or better could not be achieved; the best resolution is currently about 300 nm. The Kirkpatrick-Baez mirrors at this branchline are distorting the coherence of the beam. We developed a plan for a redesign of the branchline to provide fully coherent X-rays to the APPES endstation and have applied to the DOE for the funds for this beamline upgrade. Tests of the microscope setup on another branchline showed that the zone plate optics delivers the spatial resolution according to the theoretical prediction.

LB12022

Grazing Incident Soft X-ray Scattering of Organic Photovoltaics

Principal Investigators: Cheng Wang, Alexander Hexemer, Howard Padmore, Yi Liu, Rachael Segalman, Jeff Kortright, Harald Ade, Thomas Russell

Project Description

The development of solution-processable organic electronic materials has enabled the use of low-cost deposition methods such as roll-to-roll print to make organic solar cells. The world record organic photovoltaics cells (OPVs) shave efficiency of more than 10% that is now reaching commercial viability. X-ray scattering methods have recently been widely used as high resolution, nondestructive probes for characterizing mesoscale structure of organic photovoltaics. The scattering represents a statistical average over a large sample area, therefore a great complementary to direct imaging techniques such as electron microscopy and scanning probe microscopy. X-ray scattering is the only research tool that allows high-throughput and in-situ characterization. It provides the capability to determine the fundamental connection between how organic electronic materials organize on small length scales during the device fabrication and how that translates into their operation in OPV device. This project is focusing on developing grazing incident soft x-ray scattering (GISoXS), a mesoscale structure probe, to study the OPV devices in the real device geometry and in-situ analysis during operation. GISoXS combines the conventional x-ray scattering with x-ray spectroscopy thus offers enhanced scattering contrast and chemical sensitivity by tuning x-ray photon energy close to the absorption edge of constituent materials. The goal is to develop a unique and powerful approach with this 3D mesoscale chemical structure probe that targets at high throughput realtime device characterization, which is currently unavailable with other techniques, therefore achieve better understanding of the correlation between nano-morphology and electronic structure for optimizing the OPV performance.

Accomplishments

During this LDRD, we have started the general method development of GISoXS with existing high performance OPV materials including polythiophene/fullerene and all polymer systems. Some of the results were published in high profile journals. Based on the existing scattering setup at BL11.0.1.2, we are optimizing the instrument to accommodate GISoXS experiment with the goal of high throughput operation as well as in-situ real device characterization with new matreials. Thermal electric based sample environment will be developed and implemented for in-situ study of the effect of thermal treatment and solvent annealing during the device fabrication. Soft x-ray scattering data will be collected as a function of incident angle, and photon energy which should be selected to provide different depth information and resonant enhancement for the different polymer components at various time scale. Customized instrumentation, established experimental protocol and advanced data analysis package is currently being developed for GISoXS that will be applied to a few applications on new OPV materials developed at LBNL. We anticipate it becoming a standard tool for high throughput organic thin film structure characterization, which will lead to faster discoveries of the best OPV materials for photovolatics and thereby contribute toward CC2.0's vision of reducing carbon emissions.

LB10026

Test Monochromator/Spectrometer Systems with Prototype High Density Gratings for High Resolution X-ray Scattering

Principal Investigator: Tony Warwick

Project Description

Resonant Inelastic soft X-ray Scattering (RIXS) measures the energy scales of soft excitations which are normally obscured by lifetime broadening. The main technical issue is to achieve the high energy resolution needed (1meV – 10 meV) at the photon energies required to access relevant core levels (500 eV – 1.3 keV). The goal of this work is to design, build and operate small, novel, test monochromator-spectrometer systems to precisely evaluate the x-ray dispersive quality of prototype high-density multilayer diffraction gratings. These systems will transform the instrumentation for ultrahigh resolution RIXS from extremely large spectrometers to smaller instruments, able to perform at even higher spectral resolution within the space of the ALS floor.

A simple high resolution multilayer-grating test monochromator will be designed and constructed to measure the efficiency and the precise dispersive and optical properties of prototype high resolution multilayer gratings.

Multilayer (ML) coated blazed gratings will be developed with a high groove density operating in a high diffraction order. A chemical etch of assymetrically cut silicon substrates will be developed to produce the smooth facets on which multilayer deposition can be made to produce gratings with high efficiency. Prototype gratings constructed by various techniques will be measured. Numerical simulations of grating errors will be performed.

Accomplishments

1. A process of fabrication of high quality blazed gratings with anisotropic wet etch of silicon has been developed.
2. Optimization of growth conditions of multilayers on saw-tooth substrates has been performed for magnetron and ion beam sputtering. The optimized process provided good replication of saw-tooth profile by a multilayer interfaces.
3. Fabricated test Multilayer Blazed Gratings (MBGs) demonstrated world record efficiency in EUV and soft x-rays.
4. Ability of MBGs to deliver high diffraction efficiency in a high diffraction was demonstrated. It is very promising for ultra-high resolution EUV and soft x-ray spectroscopy applications.
5. Fabrication of practical diffraction gratings is underway. Substrates have been procured and delivered. Optics and instrumentation for spectroscopic testing has been designed.
6. This work is summarized in four additional publications this year. This program has produced a coherent line of ten publications detailing the successful development of etching and coating techniques for Multilayer Blazed Gratings and detailing their performance with measured record making efficiencies.

LB11039

Soft X-ray Spectroscopy of Lithium-ions and Electrons for Li-ion Batteries

PIs: Wanli Yang, Yi-de Chuang, Zhi Liu, Arthur L Kilcoyne, Gao Liu, Lin-wang Wang

Project Description

Developing efficient electrical energy storage through Lithium batteries has become one of the most critical challenges for enabling the effective use of the intermittent green energy sources, as well as for allowing the expansion of hybrid electric vehicles to all-electric vehicles. At this time, the importance of obtaining and understanding the critical electronic states in battery materials has not been widely realized, and soft x-ray spectroscopic tools have not been commonly employed for helping/guiding the advance of the field. The goal of this proposal is to provide strong impacts on linking the two isolated fields of battery-material developments and soft x-ray spectroscopy. The accumulated spectroscopic information will clarify many conceptual controversies to improve both our fundamental understanding and the rationality of material development for achieving high battery performance. .

Experimental techniques in this proposal include in-situ X-ray absorption (XAS), X-ray emission (XES), resonant inelastic X-ray scattering (RIXS), ambient pressure X-ray photoelectron spectroscopy with spatial resolution of 15 microns (ap-μ-XPS), and scanning transmission X-ray microscope (STXM) from four soft X-ray beamlines at the ALS. The combination of the soft x-ray techniques provides the thorough information on both the valence and conduction states on the surface and in the bulk. These key electron states in the vicinity of the Fermi level often defines the electric properties of the interested materials, and are sensitive to the subtle but important phenomena induced by lithiation.

Accomplishments

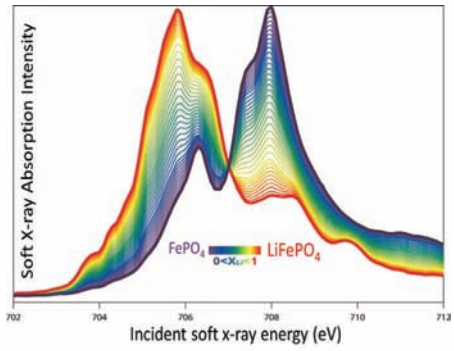


Figure: Soft x-ray absorption spectroscopy of Li_xFePO_4 cathodes at different lithiation levels. The spectra provide abundant information on how the electron states evolve in the Li-ion intercalation process, such as, valency, spin state, charge transfer and phase transformation.

We have demonstrated the power of soft x-ray spectroscopy on providing detailed information of the key parameters that defines the battery performance. We established several spectroscopic data-analysis methods to tackle subtle but critical effects related to battery operations, e.g., the deviation from the two-phase transformation in LiFePO4 systems, the relative electron state energy levels in Fe-, Mn-, and CO- based positive electrodes. In particular, we have further showcased the uniqueness of soft x-ray techniques for clarifying the origin of the high capacity and performance problems in Mn- based cathode materials.

A dedicated mobile endstation has been commissioned for running both in-sit and ex-situ soft x-ray experiments on battery materials at different synchrotron beamlines.

LB12001

Global Transcriptome, Deletome and Proteome Profiling of Yeast Exposed to Radioactive Metal Ions: A Tool to Distinguish Radiation Induced Damage from Chemical Toxicity

Principal Investigator: Rebecca Abergel

Project Description

The goals of this project are to investigate the biological effects of exposure to actinides and lanthanide fission products and to distinguish the chemical toxicity of the investigated metal ions from the radiation-induced damage due to their radioactive properties. Specific aims are to 1) investigate toxicity gene expression signaling pathways following exposure to selected *f*-elements and 2) elucidate the mechanisms of metal cellular uptake and deposition.

The consequence of exposure to radioactive and non-radioactive f-block metals will be examined on a systematic level, using a combined functional genomic, biochemical and spectroscopic approach on the powerful eukaryote model organism *Saccharomyces cerevisiae*. We anticipate the establishment of the metal-responsive transcriptomic and proteomic profiles following exposure to equi-toxic concentrations of the selected metal-ions. The identification of genes and proteins with altered expression upon actinide and lanthanide fission product exposure will permit the subsequent characterization of metal-protein complexes and the establishment of deletome genomic profiles.

Accomplishments

The homozygous diploid *S. cerevisiae* strain BY4743 was used for initial viability/cytotoxicity assays, with Eu as a model contaminant. Protocols were established to define equi-toxic concentrations of contaminants by monitoring cell growth (OD_{650} readings) and determining cell viability after metal exposure (cell counts and Trypan Blue viability assay). All protocols from cell culture to RNA and genomic DNA purification were adapted for subsequent use of radioactive materials.

We also started to establish protocols for spectroscopic characterization. The iron-transport protein transferrin (Tf) was used as a model species and its interactions with the actinide ^{248}Cm (chosen for its inherent luminescent properties) were characterized by liquid chromatography, UV-Visible and luminescence spectroscopy. Three different Cm-Tf complexes were investigated, providing the first example of the sensitization of Cm(III) luminescence by a protein through an energy transfer process known as the antenna effect.

We are in the process of applying our protocols to exposure with a series of radioactive metals and will complete the functional genomic analysis for the Eu samples. We also continue to explore the use of liquid chromatography coupled to mass spectrometry and luminescence spectroscopy to identify and characterize protein-metal species formed as a consequence of external exposure.

LB11004

Scientific Tools in Multi-Dimensional X-ray Spectroscopy and Coherent Diffractive Imaging

Principal Investigators: A. Belkacem, R. Falcone, O. Gessner, S. Leone, C.W. McCurdy, D. Neumark, R. Schoenlein, and Th. Weber

Project Description:

The purpose of this project is to carry out proof-of-principle studies that will establish some of the critical experimental concepts in multi-dimensional x-ray spectroscopy and time-resolved coherent diffractive imaging. All-x-ray techniques can probe multiple core and inner valence transitions within the same experiment, introducing atomic specificity to nonlinear spectroscopy techniques and allowing for coherent mixing schemes with dramatically enhanced signal-to-background contrast. Multi-dimensional spectroscopy in the x-ray regime will be a major breakthrough for understanding the correlation effects and many-body processes that underlie the properties of complex materials. Coherent diffractive imaging is one of the most active fields of current x-ray based research. The prospect of translating the outstanding achievements of static structure determination with x-rays into the time domain continues to inspire hopes that one day one will be able to literally "watch" the atomic-scale details of processes such as protein folding, the binding of viruses to receptors, and ultrafast structural dynamics in nanomaterials.

The proposed studies will be carried out using two of the UXSL high harmonic sources. These include a low repetition rate high-intensity high-harmonic system, a high repetition rate moderate-intensity high-harmonic system. Each one of these systems will focus on a different aspect of the proposal.

Accomplishments:

Both projects made significant progress over the past year. State-of-the-art experimental setups are fully designed, built and interfaced with the corresponding high harmonic systems. Two postdoctoral fellows lead these two parallel efforts. We use a combination of photoelectron spectroscopy and fluorescence measurement as a signature of two-photon absorption by a neon atom in the non-linear x-ray optics experiment. Two separate coatings on the same face of a single focusing mirror with different multilayer structures that reflect the 17^{th} and 29^{th} harmonics, respectively facilitate the critical spatial and temporal overlap between the two different XUV pulses. The near-edge coherent diffractive imaging (CDI) project has led to the first demonstration of element-specific contrast enhancement in tabletop CDI employing an ultrafast extreme ultraviolet (XUV) light source with tunable photon energy. By combining two measurements performed at energies below and above the Al $L_{2,3}$ absorption edge, the spatial autocorrelation function of a micron-scale double pinhole in a 300 nm thick aluminum foil has been retrieved in excellent agreement with a scanning electron microscopy (SEM) measurement and despite a dominant background signal from directly transmitted light across the entire range of detectable diffraction angles. The results have been published in *Optics Express* (F. Weise et al., *Differential near-edge coherent diffractive imaging using a femtosecond high-harmonic XUV light source*, Opt. Express **20**, 26167 (2012)).

LB12006

Photo-switchable Metal Organic Frameworks for CO_2 Sequestration
Principal Investigator(s): Mary Gilles

Project Description

Smart materials that combine high surface areas with the ability to undergo controlled nano- and macro scale structural changes offer creative approaches for CO_2 capture/release, sensors, and development of responsive materials. This project will construct metal-organic frameworks (MOFs) containing chromophores that undergo reversible conformational and/or chemical changes upon photon absorption. We will utilize *in situ* soft X-ray spectroscopies to examine changes in physical properties (chemical bonding, oxidation states, and gas absorption) of the chromophores before and after photon (UV/Vis) absorption. The gas uptake of the MOFs before and after photo switching will be probed *in situ* by a variety of synchrotron based soft x-ray spectroscopies that examine bulk and interfacial properties.

Accomplishments

A powder form of trans dicarboxylic acid substituted Cu based MOFs was synthesized and its crystallinity verified by x-ray diffraction (XRD). Near edge x-ray absorption spectra were measured at the carbon and copper edges using scanning transmission x-ray microscopy (NEXAFS) as well as photoelectron spectra (PES). By directly irradiating the dicarboxylic acid solution the cis version of the framework was synthesized. Photo switching between the trans and cis isomers showed very small changes in XRD patterns. This arises because photo switching would occur only on the outermost portions of the powder, creating a scenario of measuring a small change in signal (photo switched MOF) over a large background (non-photo switched MOF). Hence, further experiments have worked on developing MOF thin films.

MOF thin films were grown for several days on a functionalized silicon substrate inserted upside down into a solution containing the trans azobenzene and copper precursors. PES experiments indicated that the sample inhomogeneity posed a significant obstacle for future experiments examining the more subtle spectral changes that would occur during gas uptake. Hence, we proceeded with layer-by-layer synthesis of HKUST-1, one of the most well characterized MOFS, to obtain expertise in this method. HKUST-1 films were synthesized as function of: temperature; Cu metal precursor and concentration; self assembled monolayer (carboxylic acid or alcohol terminated); and substrate (Au or SiO_2). Synthesized films were examined for roughness (atomic force microscopy), for elemental homogeneity (scanning electron microscopy with elemental analysis), for orientation (synchrotron based x-ray diffraction), and for carbon bonding homogeneity (PES). Oriented and homogeneous films of HKUST-1 are now routinely synthesized and the current focus is on incorporating azobenzene into the HKUST-1 MOF and synthesis of a trans azobenzene Cu MOF thin film for soft x-ray studies on the effects of photo switching on gas uptake.

LB12010

Mechanisms of Metal-Catalyzed Reactions within the Carbonic Anhydrase Matrix

Principal Investigator: John F. Hartwig

Project Description

The emerging field of artificial metalloenzyme catalysis has largely grown without the support of mechanistic investigations of the catalytic systems of interest. Yet, such insight would be important for the development of small-molecule transition metal catalysts. The purpose of this project is to develop methods for the rigorous analysis of transition-metal catalyzed reactions within a protein matrix. The most commonly reported artificial metalloenzyme systems involve an organometallic complex anchored to the active site or exterior of a protein, either via a covalent cysteine linkage or through a non-covalent interaction between the metal complex and the protein. An alternative method that we envision is the direct substitution of a non-native metal into a metalloprotein whose active site resembles a typical small molecule ligand. For example, the tri-histidine zinc-binding site in carbonic anhydrase bears resemblance to the known Tp and Timm ligand classes. Direct substitution of a transition metal into the active site of a protein has the potential to increase the influence of the primary and secondary coordination sphere of the active site over the selectivity of reactions occurring at the metal center.

Accomplishments

We have prepared two variants of carbonic anhydrase in high purity (>95% by SDS Page Gel) and reasonable yield (15-65 mg/L *E. coli* culture). One variant (9*His) lacks all nine native surface histidine residues, but expresses in lower yield and exhibits lower stability in liquid solution than the native protein. The other variant (3*His) has been prepared (in higher yield) by removing only three of the nine native surface histidine residues. Although we have found that the remaining surface histidine residues of the 3*His variant can be protected by DEPC, this protection results in a mixture of products in which several lysine residues have also been modified. Dialysis of the apo-variants of these mutants against solutions of cationic Rh(I) complexes in aqueous buffers have not resulted in rhodium substitution at the active site, as analyzed by nanoelectrospray ionization mass spectrometry as assumed in the work reporting catalytic reactions of Rh-carbonic anhydrase systems. Poor solubility of the rhodium source may limit this method of preparing Rh-carbonic anhydrase complexes. Therefore, other methods to introduce rhodium are currently under investigation. Upon preparation of Rh-CA variants, we plan to determine the reactivity of these complexes toward the oxidative addition of Si-H bonds, a reaction that we showed to occur readily in model TpRh(I) complexes.

In parallel with this direct metal substitution methodology, we are investigating artificial carbonic anhydrases prepared from the introduction of entire organometallic complexes into the active site of the enzyme. The strong affinity of the carbonic anhydrase active site for aryl sulfonamides has led us to target several bis-nitrogen ligands used in Shilov-type C-H activation bearing sulfonamide groups to anchor the complex within the protein active site. Preparation of sulfonamide-bearing diimine ligands were complicated by poor nucleophilicity and solubility of electron-poor anilines, but we have recently prepared a sulfonamide-substituted bipyridine ligand, whose CA-binding properties are currently under investigation.

We envision that NMR spectroscopy will be critical to our mechanistic investigations, and ^{15}N NMR spectra of model Tpm'Rh complexes has shown that the ^{15}N signal for the Tpm'Rh complex is much less intense than the analogous signal for the free ligand. This finding could assist in the location of rhodium within the carbonic anhydrase active site, which cannot be determined by mass spectrometry alone.

LB12020

Developing f-electron Soft X-ray Spectroscopy Simulation, Theory, and Experiment for Clean Energy Materials

Principal Investigator(s): David K. Shuh, David Prendergast, and Andrew Canning

Project Description

The objectives of this project couple experiment to the development of robust density functional theory (DFT)-based simulation tools for soft x-ray absorption spectroscopy (XAS) of f-electron systems and make these user-friendly methods available. Examples of where soft x-ray spectroscopy at the Advanced Light Source and the corresponding theory and simulation understandings could be used to design improved lanthanide (Ln) materials, are for energy applications such as photovoltaics, batteries and lighting, as well as to actinide (An) materials such as potential separations ligands and advanced materials for nuclear energy. Selected candidate materials identified through a materials design process will be synthesized and characterized, followed by soft XAS and comparison to theory/simulation. New DFT-based methods will be developed for understanding soft XAS of Ln and An materials. Theory capabilities coupled with experiments will enable the design of new f-electron materials and/or modification of existing materials related to clean energy technologies, that perform better and are more economically viable than existing materials. Coupled with simulation and theory, soft x-ray f-electron priorities will be established for current and future ultrafast light sources.

Accomplishments

DFT-based simulation tools for Ln and An soft XAS are being developed and validated by experimental results, and will soon be made available. These DFT methodologies differ from standard approaches based on approximations of the electronic excited states and representation of the spatial extent of such excited states. A working LSDA+U interface to XAS simulations for a connection between structural models and measured spectra has been established using the Prendergast software. This methodology will now be adapted to utilize advanced functionals for treating f-state systems more accurately such as hybrid and dynamical mean-field theory.

There is great interest in ligands with soft donor atoms such as N and S, rather than ligands with a hard O donor atom for new multi-purpose separations ligands. A suite of C and N K-edge spectra have been recorded from a series of related U complexes with the N donor ligand 2,6-bis(2-benzimidazyl)pyridine with a increasingly Cl-substituted equatorial coordination sphere replacing two pyridines. Simulated N K-edge spectra generated by the Prendergast approach are in excellent agreement with the experiment. This is the first investigation of the N K-edge replicating the approach used for the O K-edge to understand f-electron bonding. Similarly, O K-edge XAS spectra are being simulated from maltol and bromomaltol Pu complexes plus the respective bare ligands. The Pu complexes exhibit dissimilar pre-edge features presumably arising from differences in the degree of f-orbital hybridization induced by the electron-withdrawing characteristic of the Br substituent compared to the unsubstituted maltol ligand. DFT has successfully validated the crystal structures.

The Materials Project software has been used to predict new f-electron materials relevant to clean energy and advanced nuclear energy (U materials for storage or fuels). Using the structure predictor a new UB_2O_5 (monoclinic) and the first two U aluminosilicates (triclinic, hexagonal) have been predicted. First principles calculations have been performed to determine their properties and suitability for applications. Np, Pu, Ce, Pr, Eu, and Tb based materials of a similar nature are being investigated with this approach.

LB12029

A Multi-Investigator Approach Towards Chemoenzymatic Catalysis

Principal Investigator(s): F. Dean Toste, Kenneth N. Raymond, Robert G. Bergman

Project Description

We intend to develop processes that merge biological catalysts such as enzymes with soluble transition metal catalysts, offering opportunities to carry out reactions that would not be possible using either type of catalyst independently. Despite the potential for innovation encompassed by this approach, relatively few examples of chemoenzymatic catalysts exist. This is in part due to the fact that enzymatic and chemical catalysts often operate under drastically different conditions. Most notably, enzymatic catalysts tend to work best in aqueous environment, while many of our most powerful homogenous catalysts prefer organic solvents and require the exclusion of moisture. In this program we will investigate a novel approach towards this goal: chemical catalysts are transformed into 'nanozymes' by incorporation into a supramolecular assembly. As such they are able to mimic many of the features of enzymatic catalysts, including the ability to operate in aqueous environments.

Towards this goal, we propose to investigate reactive metal cations contained within water-soluble molecular tetrahedra as catalysts. More specifically, gold catalysts will be initially investigated. Like many cationic metal complexes, these catalysts have only modest stability and activity in aqueous solution and therefore, their application into chemoenzymatic processes requires stabilization of the catalysts towards water. We envision that this can be accomplished with an aqueous host-guest complex. We propose to combine theoretical studies with our experimental work, in order to provide a strong foundation for future catalyst development. As such, we believe that the concepts and insights developed in these studies can be applied to other reactive catalysts systems, with the ultimate goal of developing a tool-box of water-active homogenous catalysts that can be coupled with enzymatic processes.

Accomplishments

We showed that cationic phosphinegold(I) complexes are readily encapsulated by an anionic Ga_4L_6 tetrahedral supramolecular host in water. The resulting host-guest complex was employed as a catalyst for the intramolecular hydroalkoxylation of allenes. The 67 catalytic turnovers observed for hydoalkoxylation reaction catalyzed by Me_3PAu^+ encapsulated in Ga_4L_6 represents one of the highest turnover numbers recorded to date for an encapsulated transition metal complex. Importantly, initial rate kinetics found that the catalytic activity of Me_3PAuBr was *increased* 8.7 fold by encapsulation, and thus constituted the first example of acceleration of a gold-catalyzed process in which reactivity and lifetime of the catalyst are enhanced by supramolecular encapsulation.

Based on these initial finding, we have studied the use of encapsulated phosphineAu(I) complexes as catalysts in a variety of one-pot tandem reactions employing esterases and lipases. Additionally, we have shown that the strategy can be extended to the combination of alcohol dehydrogenases with Ru(II) complexes encapsulated in the Ga_4L_6 tetrahedral supramolecular cluster. Notably, this combination is viable independent of whether the enzymatic or metal-catalyzed reaction proceeds first. The host-guest complexes are well-tolerated by the enzymes and in a few cases show improved reactivity relative to the free cationic guest. We infer that in these cases, supramolecular encapsulation of organometallic complexes prevents diffusion of these complexes into the bulk solution, where it can interact unfavorably with biological catalysts.

LB12030

Oxidative Transformations of Organic Aerosol
Principal Investigators: Kevin R. Wilson and Allen Goldstein

Project Description

Organic aerosols play critical roles in the radiative balance of the atmosphere with far ranging impacts on climate and human health. New molecule-based analytical approaches are required to achieve a fundamental description of the atmospheric oxidation of organic aerosols, which are comprised of thousands of individual molecular species. By combining synchrotron vacuum ultraviolet (VUV) photoionization mass spectrometry (MS) with gas chromatography (GC), a new experimental technique was developed to probe the complex photochemical reaction pathways that transform organic aerosol. This new analytical tool will be used to achieve previously unattainable chemical separation for the analysis of complex aerosol particles containing primarily hydrocarbons. This approach provides a new way to construct molecule-based descriptions of the oxidation chemistry of multi-component organic aerosols and provide new data that is needed for accurately assessing the impact of particulate pollution on air quality, human health and climate. These measurements form the basis for improving parameterizations of organic aerosol chemistry in computer models in broad support of Carbon Cycle 2.0's goal of understanding, assessing and predicting the environmental impact of fossil energy use.

Accomplishments

The viability of the proposed GC/VUV-MS technique was demonstrated for the analysis of diesel fuel—a prototypical environmental pollutant whose chemical complexity itself is a stringent test of any new analytical technique. Traditional GC electron impact ionization mass spectrometry or two dimensional GC analysis of diesel fuel can identify only a fraction of the molecular species in the fuel leaving a substantial amount of material as an "unresolved complex mixture" (UCM) composed primarily of hydrocarbons. The UCM, a common feature in urban organic aerosols and other environmental samples, has yet to be quantified or described molecularly and originates from the enormous number of possible aliphatic isomers with similar mass spectrometric signatures. The strong molecular ion peak in VUV mass spectra allows new molecular structures previously buried within UCM to be observed and assigned. Alkanes, cycloalkanes, bicycloalkanes, etc. can be resolved and quantified. Furthermore, within a specific alkane series, branched vs. linear isomers are clearly separated and quantified. Despite the thousands of possible isomeric configurations only 8-10 major isomers are observed for alkanes in diesel fuel, with a strong preference for methyl branched isomers (vs. ethyl or propyl). This specific isomeric pattern, which is only observable using GC/VUV-MS, could be used to fingerprint various diesel products or be used to understand more subtle aspects of the petroleum refining process and environmental degradation pathways.

Building on these results, we will use isomeric analysis of oxidized motor oil aerosol to develop new molecule based parameterizations of organic aerosol. Motor oil aerosol is a good proxy for diesel particulate emissions in urban environments. This allows detailed analysis of aerosol oxidation chemistry for classes of compounds that goes well beyond what is currently achievable using conventional aerosol analytical techniques. Our objective is to describe how hydrocarbon structure (rings vs. chains) influences oxidation reaction pathways—with the overall aim of delivering a predictive model of the organic chemistry of aerosols in urban environments.

LB10001

Enabling HPC Workflows on Cloud

Deborah Agarwal (PI), Valerie Hendrix, Lavanya Ramakrishnan, and Keith Jackson

Project Description

The promise of on-demand large-scale 'personalized' computing capacity has attracted many DOE science applications to the commercial cloud offerings. . Utility, or "cloud", computing is quickly becoming the dominant paradigm for delivery of cost-effective, scalable, energy-efficient computing resources. Clouds promise to deliver the ability to submit an application from a desktop and take advantage of personalized on-demand resources all over the world. Data-intensive science is quickly gaining more momentum and requiring large-scale resources such as HPC and cloud environments. Thus, it is important to consider the similarities and differences in these environments from the perspective of scientific workflows.

Cloud computing is still early in its development and a wide array of cloud computing paradigms have emerged. As clouds become more ubiquitous, it is essential that DOE scientific applications be able to take full advantage of them. In this project we have worked with a representative set of science applications to identify what is needed to adapt existing application software to the cloud and identify new software needed to enable science applications to readily utilize cloud resources.

Accomplishments

This year we focused on the design, implementation and evaluation of an end-to-end pipeline for the reprojection of MODIS satellite data as the prototype science application. The MODIS satellite project exhibits many of the characteristics of typical data-intensive workflows that need large-scale resources. The MODIS data is important to a wide array of scientific analyses. Data procurement and processing is challenging and cumbersome for the user communities and the data processing is computationally intensive requiring thousands of computational hours. This leads to few scientists being able to do analyses with the data. The intent of the MODIS satellite project is to enable scientists to easily analyze MODIS data in the cloud.

We have three major accomplishments from this project. First, we have researched and developed a prototype data-processing pipeline that downloads the MODIS products and reprojects them on large-scale systems such as HPC and cloud environments. We have overcome a number of challenges of HPC data processing pipelines in the areas of a) orchestration of data from NASA and appropriate storage models for the output data b) validation and versioning of data throughout the pipeline c) failure recovery across steps of the pipeline.

In the second accomplishment, the resulting reprojected MODIS data is being made available to the scientific user community through a front-end web portal (http://portal.nersc.gov/modis). The portal allows users to download reprojected land data (~1TB/year) for the land and atmosphere products: aerosol, water vapor, clouds, atmosphere profile and land surface temperature emissivity. Through the portal we will be able to better understand user behavior.

In the third accomplishment, the MODIS reprojection pipeline has allowed us to understand many of the challenges that other data-intensive pipelines will need to address when using HPC resources. Data from current and future experimental facilities such as the Advanced Light Source (ALS) and Joint Genome Institute (JGI) and Next-Generation Light Source (NGLS) are beginning to be processed in HPC environments. The lessons from the MODIS pipeline provide useful insights for these projects.

This new pipeline will provide a stepping stone to pursuing proposals for big data projects.

LB12009

An Optimization-Based Strategy for Computational Design of Nanoporous Carbon-Zero Materials

Principle Investigator: Maciej Haranczyk

Project Description

The aim of this project is to develop a new strategy for the computational design of porous materials, which will lead to faster discovery of carbon-zero materials for energy-related and industrial applications. In this strategy, high-performance computational methods are used to rapidly measure properties of designed materials, and mathematical optimization methods are used to automatically make modifications to the materials and improve the measured properties. As such, rather than designing many hundreds of thousands of materials and testing each one, one can begin with any random materials, and quickly identify high performing materials through iterative modification of their structure.

We explore the key components of this strategy: 1) developing mathematical optimization algorithms that quickly identify optimal materials; 2) producing tools to rapidly calculate relevant material properties during optimization; and 3) creating novel techniques for representing materials by their shape and chemistry so that they can be automatically tuned during optimization. Although our approach is general in nature and is appropriate for any porous material design requirements, our work will focus on designing metal-organic frameworks (MOFs), a class of material in which the organic components permit a large degree of variation in shape and chemistry. Furthermore, we will apply our method to identify MOFs with optimal properties relevant to specific applications, principally carbon dioxide capture and natural gas storage.

Accomplishments

Our most significant accomplishment to date is successfully identifying many previously unexplored materials whose pore properties suggest they are promising candidates for gas storage, using a prototype of our material design method. We have designed materials to achieve the highest possible surface area per unit mass, an important property for gas storage applications. Our materials are designed by imposing limits on their complexity, and optimizing within this space, in order to identify materials which are both computationally predicted to be high-performance, and also likely to be synthetically achievable.

As a result of this work, several design rules for achieving high surface area materials were revealed, which indicate that the present estimated limits for high surface area can be exceeded. Most significantly, the organic components of our optimal materials are molecules with branches; as organic molecules are low in mass, branching allows the molecule to grow in size and provide additional surface area, without adding significantly to the mass of the material. As such, it was discovered that molecules with high mass shapes but which permit significant branching may be more efficient overall, despite the initial mass penalty.

It was also discovered that certain types of MOF present less challenging targets for achieving high surface area. MOFs constructed from as few metal components as possible typically achieve the highest surface areas per unit mass due to the low number of heavy, metallic components. The consequence of this observation is that low-complexity, and easy to synthesize organic molecules can be used in these MOFs and high surface areas can still be achieved, making them promising targets for breaking the present records of high surface area materials.

LB11018

Next Generation Computing for X-ray Science
Principal Investigator(s) : Xiaoye Sherry Li

Project Description

We propose to develop new high performance computing (HPC) algorithms, codes, and software tools for the analyses of X-ray scattering data collected at the ALS. In conjunction with the development of new physical principles for analyses of novel scattering data, this approach will provide state-of-the-art capabilities for deducing the structure-function properties of materials for photovoltaic, carbon capture and sequestration, battery, and fuel cell devices that directly advance the goals of Carbon Cycle 2.0. The newly developed HPC tools will consequently lead to increased data analysis productivity and more intelligent design of experiments for rapid scientific discovery at both ALS and NGLS.

We will develop the new simulation algorithms understanding the underlying physical principles and the parallel codes to increase the data analysis throughput. We will develop the massively parallel GISAXS and Reverse Monte Carlo codes on the Cray XE6 at NERSC and Titan at OLCF. We anticipate three to four orders of magnitude speedups through this effort. We will apply extensive code optimization techniques to increase both on-node and internode communication performance. We expect this to yield an additional 25x decrease in computing time. We will develop a user-friendly interface by leveraging the other software tools developed at LBNL, such as NERSC Web Toolkit (NEWT) and the newly proposed LDRD project for end-to-end solution for light source data.

Accomplishments

We have developed flexible massively parallel GISAXS simulation software "HipGISAXS" based on the Distorted Wave Born Approximation (DWBA). The software computes the diffraction pattern for any given superposition of custom shapes or morphologies in a user-defined region of the reciprocal space for all possible grazing incidence angles and sample rotations. This flexibility allows a straightforward study of a wide variety of possible polymer topologies and assemblies whether embedded in a thin film or a multilayered structure. Hence, this code enables guided investigations of the morphological and dynamical properties of relevance in various applications. The current parallel code is capable of computing GISAXS images for highly complex structures and with high resolutions and attaining speedups of 200x on a single-node GPU compared to the sequential code. Moreover, the multi-GPU (CPU) code achieved additional 900x (4000x) speedup on 930 GPU (6000 CPU) nodes.

We have performed a series of tests to validate the accuracy of our GISAXS simulation code for a variety of systems. Our computations provided excellent agreement with the experimental data for a variety of structures submitted to us by materials scientists and engineers.

We have engaged in collaborations with several research groups to use HipGISAXS to simulate systems such as high aspect ratio silicon trenches from block copolymer templates (Russell's Group, UM Amherst), hybrid organic-inorganic PbS-TTFTA nanoparticle films (Alivisatos' Group, UC Berkeley, ALS) and gold nanoparticle assemblies in thin nanocomposites films (Xu's Group, UC Berkeley) to name a few.

LB11025

Nyx: The Lyman Alpha Forest Cosmology Simulator
PI: Peter Nugent

Project Description

In recent years astrophysics has undergone a renaissance, transforming from a data-starved to a data-driven science. A new generation of experiments including Planck, BOSS, DES, BigBOSS & LSST will gather massive data sets that will provide more than an order of magnitude improvement in our understanding of cosmology and the evolution of the universe. Given that several of the next generation cosmology experiments are focused on baryon acoustic oscillation (BAO) measurements, the time is ripe to expand and channel the current expertise of LBNL's Computational Cosmology Center to tackle this promising area of research.

To properly simulate the observations from the DOE-led SDSS-III project BOSS and the proposed BigBOSS surveys, we need a fair statistical representation of our universe. Our ultimate goal is to calculate absorption spectra caused by neutral hydrogen in the cosmological environment, with all the relevant physical processes. This requires more than 1000 trillion particles in a single run. At 100 bytes per particle we need 10^5 TB RAM. Such memory-limited computations can be performed only on future Exascale systems. Our approach is to modify the Compressible ASTROphysics code – CASTRO – to perform these simulations. This new code is called *Nyx*, primordial goddess of the night. *Nyx* is a new, multi-dimensional, Eulerian AMR radiation-hydrodynamics code designed for astrophysical simulations.

Accomplishments

In the past year this effort has seen an incredible push forward and some remarkable results. Due to the tremendous interest in BAO cosmology we have attracted a strong suite of collaborators from UC Berkeley, Gottingen University and Brookhaven National Laboratory. During this time we have been able to improve the code for a wide variety of astrophysical calculations and to mine the output of our simulations for direct comparison to observation through a BoxLib reader in the *yt* software package which allows us to perform most, if not all, of the visualization and cosmology analysis for the data produced by *Nyx* (see http://yt-project.org). This effort has been essential in carrying out code comparisons as well as verification and validation of our cosmology simulations.

Nyx has been designed to efficiently utilize tens of thousands of processors; timings of the code this past year on up to almost 50,000 processors show excellent weak scaling behavior. Validation of Nyx in pure dark matter runs and dark matter with adiabatic hydrodynamics has been presented in a recently accepted paper to the *Astrophysical Journal*. Future papers will give greater detail on the implementation in Nyx of source terms, and will present results from simulations incorporating different heating and cooling mechanisms of the gas, as needed for increased fidelity in different applications. Scientific studies already underway with Nyx include studies of the Lyman-α forest and galaxy clusters. In addition, we plan to extend Nyx to allow for simulation of alternative cosmological models to ΛCDM, most interestingly dynamical dark energy and modifications of Einsteins gravity.

LB12035

Interlinkage of Cross-Disciplinary Mathematical Technologies

Principal Investigator(s): J. Donatelli, M. Haranczyk, S. Marchesini, B. Preskill, R. Saye, D. Ushizima, J.A. Sethian

Project Description

Applied and computational mathematics can steer discovery in the DOE facilities, providing advanced algorithms and computational methodologies to efficiently extract data, interpret results, and guide experiments. Given the high cost of these facilities, often in the tens and hundreds of millions of dollars, modest investments can create sophisticated state-of-the-art mathematics that will yield tremendous cost savings in terms of numbers of experiments, data extracted, and materials used. As examples, new mathematics will be instrumental in providing tools to reconstruct structure and properties from synchrotron light sources, direct the hunt for new materials for batteries and gas separation, and model and optimize steps in the production of biofuels. We have been building mathematical models, algorithms, and technologies to attack problems within LBNL and DOE that are brand-new, and require core advancements. The particular focus has been on mathematical advances needed in support of the DOE facilities. We have targeted work in four areas: (i) New Reconstruction Methods for the Advanced Light Source; (ii) Fast Throughput Screening in the Design of New Materials; (iii) Mechanical Modeling of Biological Cell Clusters; and (iv) Advanced Imaging Capabilities in Segmentation and Reconstruction of Material Structures.

Accomplishments

Following on our FY11 work, we have accomplished the following:

In new reconstruction methods, we have focussed on crystallography, nanocrystallography, and single particle resconstruction. We have had remarkable preliminary success with an approach that combines ideas from statistical data analysis, common line analysis, Bayesian probability, spectral geometry, and graph theory in an innovative way and addresses all of these issues in a more computationally efficient manner. We are now using this to build a complete system for nanocrystallographic reconstructions.

In biological modeling, we built a complete simulation of cell cluster dynamics, evolving under the combined effects of hydrodynamic, elastic, and geometric forces, including the interaction of growth dynamics with elastic basement membranes, studying rupture.

In materials modeling, we have developed a new method for tracking multiphase interfaces in materials, including applications to grain metal boundaries, liquid and solid foams, and in semiconductor failures. These new techniques rely on a Voronoi Implicit Interface Method, which combines aspects of level set methods with geometric Voronoi reconstructions to provide a robust, consistent, and accurate technique to track interconnected multiphase multiphysics problems under the combined effects of mechanics, hydrodynamics, and geometry. The methods use a single distance function plus an indicator, defined on a regular mesh, using upwind finite differences. Combined with a new formulation and numerical algorithmic technology for drainage, and coupled to core second order projection methods for incompressible flow, we are able to compute a full macro-scale evolution cycle for liquid foam drainage, rupture, and rearrangement.

We have been in involved talks with DOE about long-term support for mathematics in service of the DOE facilities.

LB12036

LPAR: Low-Power Architecture Research for Exascale Computing
PIs: John Shalf and David Donofrio (CRD)

Project Description

DOE mission needs in energy, national security and science require a thousand-fold increase in supercomputing technology during the next decade, under stringent power and reliability constraints. As high-performance computing systems approach the exaflops scale, their designers are confronting enormous electrical power requirements. Traditional HPC system design methodologies have not had to account for power constraints or parallelism on the level designers must contemplate for exascale systems. In particular, data movement has become the most critical impediment to energy efficiency for future processor technology.

The Low-Power Architecture Research (LPAR) project is creating new hardware innovations that reduce energy consumption by more efficiently controlling data movement. To accomplish those goals LPAR is developing new simulation technology that will enable the development of energy efficient and effective processor and memory architecture essential for future HPC platforms. LPAR is developing novel language constructs that make data movement features easy to use, accessible, and will lead to more efficient programming models. LPAR uses multi-scale architectural simulation coupled with mini- and skeleton- applications to demonstrate the effectiveness of these approaches on a range of system realizations in the following research areas.

1) Language assisted cache coherence: We will demonstrate a software assisted coherence protocols to reduce energy cost and complexity of intra-node cache-coherence systems, and offer dramatically improved control of data movement within the node.
2) Local Stores: We will quantitatively demonstrate efficiency benefits offered by software managed vs. automatically managed processors.
3) Coordinated Data Movement for Manycore: We will demonstrate a hardware approach to coordinating the data-movement activities across many processors in a manycore chip architecture, to improve memory access efficiency.

The simulators enable us to quantify both the performance benefit and the energy improvements offered by these innovations. Through this activity, we can provide a systematic means to evaluate design alternatives from baseline hardware changes all the way up to implications for language design. New, more effective, and more programmable mechanisms for data locality management will have a pervasive benefit for future manycore computing technology.

Accomplishments

Through our FY12 LDRD funding, we hired George Michelogiannakis as a postdoc from Bill Dally's group at Stanford University to work on our Coordinated Data Movement for Manycore thrust area.

The Coordinated Data Movement for Manycore thrust area deals with re-architecting the memory subsystem to support chips that have hundreds to thousands of independent processing elements. Future performance improvements for HPC processors have shifted from clock frequency scaling towards exponential increases in on-chip parallelism. Performance improvements for parallel applications require domain-decomposition of the data arrays from a contiguous arrangement in memory to a tiled layout for on-chip L1 data caches and scratchpads. However, memory performance suffers when subjected to the non-streaming access patterns generated by many independent cores. We propose a collective DMA mechanism, coordinated DMA (CDMA). For stencil applications, we show that CDMA reduces execution time by up to 40% for reading data arrays and 25% for writing compared to base- line DMA, while at the same time alleviating congestion in the on-chip network and reducing DRAM power.

This work has resulted in two papers. The first will be published in IEEE Transactions on Computer Architecture Spring 2012. The second has been submitted to the IEEE Micro 2013 conference.

LB12021

Quantitative Image Analysis for Computational Modeling

Principal Investigator(s): Daniela Ushizima

Project Description

Scientific community is facing hundred to thousand fold increases in data volume from high-throughput instruments, and supercomputers, compared to volumes generated only a decade ago. While these technologies allow acquisition and recording of ever more image data, reasoning and analysis of massive image datasets are lagging behind. Combating this flood of data requires algorithms and computational tools to be tailored to specific science domains. Our focus is on multi-disciplinary research that requires numerical schemes to extract patterns, structure, and quantitative information from digital images, mainly those acquired within LBNL and DOE. The algorithms and software we expect to develop will provide (1) quantitative measurements; (2) initialization for sophisticated numerical modeling; (3) check points for numerical simulations to see if proposed mathematical models match experimental data; (4) the groundwork for analysis software that embed expert domain knowledge; and (5) techniques for data exploration, data summarization and global view of experiments.

Accomplishments

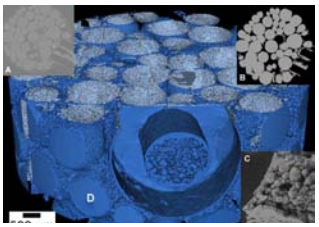


Figure 1 Micro CT segmentation using Quant-CT

Following on our FY11 work, in which we demonstrated volume segmentation results for a set of materials, we developed algorithms adapted to two purposes: (1) analysis of porous materials (Fig. 1), and (2) tracking of cells *in-vivo* (Fig.2).

In collaboration with ALS and ESD personnel, we addressed high-resolution tomographic images, aiming at obtaining timely feedback from experiments. In the first year, we proposed and implemented tools that filter, segment and extract features from porous media, with potential applications to carbon sequestration research. We built a new algorithmic and software framework, Quant-CT, which processes and quantifies structures from the micro CT cross-sections, and uses VisIt for visualization (Fig.1). Datasets range from soil samples, rocks, glass beads and simulated data. The current algorithms are able to differentiate high-density material from void (background) using a graph-based approach (statistical region merging) for Boolean classification, and to extract features such as volume, surface area, granularity spectrum, porosity, and flow curves.

In collaboration with LSD, we have designed a quantitative image analysis pipeline to process HMEC from time-lapse LSCM data, comprising three mains steps: (1) identify protein fluorescence associated to cell structure as F-actin and DNA and eliminate regions corresponding to non-specific binding; (2) estimate the position of the structure boundaries at each time frame; (3) calculate structural changes over time. We focused on sub-cellular protein localization to recover aspects of cyto-mechanics from LSCM imagery, and built algorithms to extract time-varying cell boundaries during key critical early stages of growth and division of HMECs. We quantified cell-spinning velocity during acinus formation (Fig.2), which is typical of non-malignant tissue. These projects are ongoing, and we propose to continue them under this LDRD, and to extend our capabilities across the laboratory, including collaboration with other divisions.

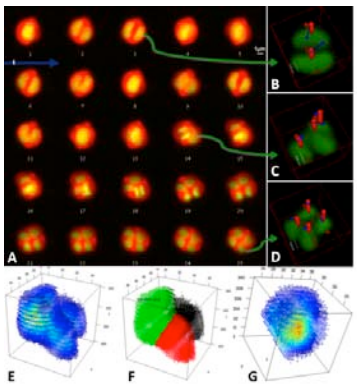


Figure 2 Human mammary epithelial cells spinning

LB10029

Computational Techniques for Non-crystalline X-ray Diffraction Imaging
Principle Investigators: Chao Yang (Computational Research Division), Stefano Marchesini (Advanced Light Source)

Project Description:
The major goal of this project is to develop computational techniques and tools that can be used process diffraction imaging data to elucidate 3D structures of nanomaterials and biological molecules. Non-crystalline X-ray diffraction imaging (Miao, 1999) provides a complementary technique for revealing molecular or cellular structures that are difficult to obtain through other existing techniques such as X-ray crystallography, X-ray tomography, and electron microscopy. Since this imaging technique does not rely on building high-quality lenses or growing crystals, it is suitable for structure studies using a wide variety of light sources including the Next Generation Light Source that is under preparation at LBNL.

Accomplishments:
In fiscal year 2012, we focused mainly on developing fast and more robust algorithms and implementations for phase retrieval. In particular,

1) We developed an augmented Lagrangian alternating direction method (ADM) for solving the phase retrieval problem. The ADM can be viewed as a generalization of the existing projection algorithms such as the alternating projection algorithm and the hybrid input-output (HIO) algorithm for solving the phase retrieval problem. It is more flexible and has been shown to be more efficient and robust. We examined some theoretical convergence properties of the algorithm, and applied the new algorithm to a number of classical and ptychographical phase retrieval problems. Our numerical examples show that ADM produces better reconstructions at a much faster speed. In addition, it is also robust with respect to noise.

2) We also examined the possibility of using Newton's method to solve the phase retrieval problem. We analyzed the Jacobian associated with the nonlinear equations that describe the phase retrieval problem and showed that its spectral radius can be bounded by 1 when the initial guess is sufficiently close to the solution. We developed a hybrid scheme in which the HIO algorithm and the Newton's method are applied in an alternating fashion. The HIO algorithm is mainly used to escape from a local minimizer of the residual. This hybrid scheme works well when the measurement contains a modest level of noise. When the noise level is too high, the Jacobian cannot be computed accurately, and the hybrid scheme may fail.

In addition, we compared several iterative refinement algorithms for solving the single-molecule diffractive imaging problem. In particular, we pointed out the similarity between the projection matching (PM) algorithm, which is commonly used in single-particle analysis in cryo-electron microscopy, and a number of expectation maximization (EM) algorithms. We showed that the use of a Gaussian likelihood function yields the same equation produced by the Poisson likelihood. The key to a successful implementation of the EM algorithm is a proper choice of the metric used to measure the difference between two diffraction images. We also pointed out that the PM algorithm is stochastic in nature because the assignment of one particular orientation to an image depends not only on the signal but also on the amount and the nature of the noise.

LB12024

Numerical Algorithms and Mathematical Software Tools for Computational Material Science and Chemistry

Principle Investigators: Chao Yang (Computational Research Division)

Project description:
The goals of this project are to develop efficient and reliable numerical algorithms and mathematical software tools for computational material sciences and chemistry. Such tools are becoming increasingly important in the design of new materials for harvesting alternative energy and the development of efficient catalyst to separate greenhouse gas from fossil plants. I will focus on two fundamental problems in computational chemistry and materials science: the electronic structure calculation for metals, and the nuclear quantum effects in water and ice.

Accomplishments:
In fiscal year 2012, we developed acceleration techniques for solving the Kohn-Sham density functional theory (KSDFT) problem, which can be formulated as a system of nonlinear equations. We focused on two areas:

1) We developed a fast density evaluation method that is based on the technique of pole expansion and selected inversion (PEXSI) of the Kohn-Sham Hamiltonian. The complexity of this approach is O(N) for quasi-1D systems (e.g nanowires), $O(N^{1.5})$ for quasi-2D systems (e.g. graphene) and $O(N^2)$ for general 3D systems. We integrated this technique with an electronic structure code that is based on discretizing the Kohn-Sham equation through local atomic orbital expansion. We demonstrated linear scaling for large nanotubes.

2) We analyzed the Kohn-Sham fixed point map satisfied by the electron density associated with the solution to the Kohn-Sham problem, and developed a unified framework for constructing preconditioners for accelerating a fixed point iteration for solving the Kohn-Sham problem associated with both insulating and metallic systems. The unified framework requires solving an elliptic partial differential equation, which can be done efficiently by a number of techniques such as the fast multiple method, multigrid etc. Moreover, the unified treatment of metals and insulators also allows us to construct effective preconditioners for hybrid systems that contain both a insulating and a metallic component.

3) We developed a novel discretization scheme called the adaptive local basis functions (ALB), which adaptively and systematically builds the rapid oscillations of the Kohn–Sham orbitals around the nuclei as well as environmental effects into the basis functions. The resulting basis functions are localized in the real space, and are discontinuous in the global domain. The continuous Kohn–Sham orbitals and the electron density are evaluated from the discontinuous basis functions using the discontinuous Galerkin (DG) framework. Numerical examples indicate that our method can reach very high accuracy (less than 1 meV) with a very small number (4–40) of basis functions per atom. We developed the element orbitals, and optimized local basis functions, which further improved the performance of the adaptive local basis functions in terms of reducing the degrees of freedom, and increasing the accuracy of the force calculation which is important for geometry optimization and molecular dynamics simulation.

LB11043

DEFINING AN ECOSYSTEM TO SUPPORT DATA-INTENSIVE SCIENCE

Principal Investigator: Shane Canon and Co-PI: Lavanya Ramakrishnan

Purpose

Scientists are struggling with a tsunami of data across multiple scientific domains. Emerging sensor networks, more capable instruments, and ever increasing simulation scales are generating data at a rate that exceeds our ability to effectively manage, curate, analyze, and share it. This data overload directly impacts our ability to address problems of scientific and national significance, including problems related to climate, energy, and scientific competitiveness. Unlike the hardware, algorithm and software models that currently exist for modeling and simulation, there is no complete ecosystem around data-intensive scientific computing.

This project explores the needs of data intensive computational scientists and the role that many new, potentially disruptive, technologies can play in accelerating discovery. This requires direct engagement with a broad class of scientists to understand their workflows, algorithms, current challenges, and future needs. These engagements also offer an opportunity to build up key success stories that can serve as a model for other applications.

Accomplishments

Our accomplishments this year builds on our last year's efforts and is focused on three areas a) evaluation of Big Data technologies such as NoSQL databases b) prototype development, deployment and evaluation of the end-to-end data-packaging and movement pipeline from experiment facilities (e.g Advanced Light Source) to HPC centers (e.g., NERSC) and, c) strategic collaborations and seeking funding opportunities for gaps identified for a data ecosystem

In the previous year, we evaluated Hadoop, an open source implementation of MapReduce, with specific scientific data patterns (e.g., filter, merge, reorder). In this year, we evaluated existing NoSQL databases on NERSC systems. We used the Yahoo! Cloud Serving Benchmark, a cloud benchmarking toolkit, to evaluate Hypertable, HBASE, MongoDB and Cassandra. Our initial studies show the performance and scalability of these NoSQL databases. Additionally, we evaluated the use of Hadoop as an analysis framework for data stored in these NoSQL data stores to understand the scalability and fault-tolerance limits. In the next year, we plan to evaluate applicability of each of these NoSQL technologies in the context of specific scientific datasets that we have identified from our interactions with science teams.

The goal in our second year was to understand how data-intensive applications from experimental facilities might be able to leverage resources at HPC centers (e.g., NERSC). We continued our work with both ALS and JGI to facilitate their data storage and processing on HPC systems. Specifically, in this year we focused on the data packaging and movement pipeline for the ALS Tomography beam-line. The initial prototype revealed a number of aspects of the software data ecosystem that are needed at the data source and at facilities such as NERSC including services for automated packaging, metadata management, and failure handling. The ALS packaging pipeline will be further explored in the context of a separate funded LDRD.

Finally, this year we established key collaborations to further explore and address identified gaps in the data software ecosystem. We submitted three proposals to the ASCR Collaboratories program and two were funded. PI Canon will be participating in both projects in an advisory role and Co-PI Ramakrishnan is a Co-PI on these new projects.

LB12004

Developing a mechanistic high-latitude biological soil carbon and nitrogen cycle module for site, regional and global land models.

Principal Investigator: Nicholas Bouskill
Other Investigators: Bill Riley, Jinyun Tang (Climate Science, ESD) & Eoin Brodie (Ecology, ESD)

Project description:

This LDRD integrates existing ESD expertise in ecosystem modeling and environmental microbiology to develop a modeling capability for the carbon (C) and nitrogen (N) cycle in high-latitude soils. High-latitude permafrost soils underlie approximately 26 % of terrestrial ecosystems and have the potential to significantly impact the future balance of Earth's C and N cycles. Several models suggest that up to 90 % of the near-surface Arctic permafrost could thaw by 2100 affecting the structure and function of the microbial communities that mediate the majority of biological C and N cycling. These thermal, hydrological, geochemical and biological changes could lead to substantial increases in atmospheric CO_2, CH_4 and N_2O. The efflux magnitudes of these gases from thawing permafrost are largely dependent on complex feedbacks centering on the *in situ* diversity of C- and N-cycling microorganisms, the availability of N, and the physical changes that occur as permafrost thaws. Therefore, the development of a framework for simulating the emergence of microbial community structure based on a few physiological and genomic traits is a critical first step towards predicting how microbial communities will respond to the geochemical, thermal and hydrological changes accompanying permafrost thaw. A further outcome of understanding community emergence is the accurate prediction of rates (e.g., decomposition or N_2O production) that is a consequence of the emergence of particular microbial communities.

Accomplishments

Our approach to modeling microbial diversity has centered on developing a model to capture the physiological and functional diversity of microorganisms involved in nitrification, the rate limiting step in the N-cycle and a significant source of N_2O. To this end we have developed and published (Bouskill et al., 2012) a trait-based model representing the diversity of different organisms mediating nitrification by parameterizing multiple guilds spanning a range of trait-space. The traits represent enzyme kinetics, growth rates, and substrate use efficiencies, and responses to ecological factors (e.g., temperature, pH and organic N). We field-tested this model against observational data from Alaskan tundra (nitrifier community composition, and nitrification rate measurement) and accurately simulated both the emergence of community structure and trends in nitrification under simple the geochemical conditions provided in the original study.

We are currently developing an analogous, though more complex, approach to represent C-cycling heterotrophic organisms. This approach represents the production of exo-enzymes responsible for the breakdown of complex carbon compounds and the subsequent uptake of monomers (with associated CO_2 production) that fuels the growth and development of the heterotrophic community. At the present time, we have finished coding the model and are currently testing across different field conditions.

LB12005

High-throughput Isolation and Functional Screening (HIFS) of Microbes Relevant to Today's Carbon Cycling and Bioenergy Needs

PI: Romy Chakraborty

Project description:

The goal of this project is to unravel structural and functional diversity of microbial communities by developing a high-throughput technology that enables rapid isolation and cultivation of microbes based on their metabolic function. We are taking an innovative approach to overcome the bottlenecks that exist in studying 'unculturable' microbes. Microbial isolates provide information about microbial communities and metabolisms that cannot be obtained directly from genomic- dependent efforts alone. We are developing a rapid high-throughput phenotypic screen and isolation tool that will integrate several time-consuming batch culture-based techniques and yield high number of microbial isolates from any environment. This technique will then be employed to elucidate the cultivable microbial community dwelling in the rhizosphere of Switchgrass with a special emphasis on the microbes capable of 'fixing' nitrogen. Plants rely heavily on nitrogen-fixing bacteria living in the rhizosphere to provide them with a form of nitrogen they can assimilate. Switchgrass is being extensively explored as a feedstock for bioenergy production. Thus, we propose to determine the effect of climate change (elevated temperature and elevated salinity) on the rhizobial microbial population of this plant and study the ability of the rhizobial diazotrophs to survive environmental fluctuations.

Accomplishment:

The proof of concept pipeline for high throughput isolation strategy was developed. Results show that while commercial techniques offer high throughput for functional screening, our isolation strategy provided a better microbial isolation platform. Different redox-based dyes such as tetrazolium salt WST-1, different Biolog dye mixes were tested and results indicated that no one universal dye works for all sample types. The high-throughput technique was employed for three diverse environmental samples to determine whether a broad range of bacteria could be obtained and cultivated using this approach. As many as 30 different microbial isolates were obtained from a single microtiter plate- including fermenters, nitrate reducers, lactate oxidizers and elusive toxic metal tolerant bacterial strains from only 0.1ml sample, at a fraction of cost of traditional isolation methods and only within two-three weeks from Hanford 100H groundwater samples. Multiple oil-degrading isolates were obtained from oil-contaminated ocean water samples, few of them unique species of bacteria. Some of these results are being incorporated into manuscripts. Finally, Switchgrass samples were obtained and microtiter plates were set up to enrich and isolate for N_2-fixing microbes from rhizobia. Initial results show differential substrate utilization of the rhizobia. Isolation of these microbes is underway.

LB10033

Enhanced Subsurface Fluid Characterization Using Joint Hydrological and Geophysical Imaging

Principal Investigator: Michael Commer,
Co-PIs: Michael B. Kowalsky, Stefan A. Finsterle, Gregory A. Newman

Project description:

Within this LDRD project, joint imaging methodologies for advancing the understanding of fluid flow and transport in large-scale complex geologic formations are developed. The methods aim at using field-scale geophysical data in order to enhance the information content of sparsely distributed hydrological (wellbore) measurements. The joint inversion methods have strong practical relevance for a variety of characterization and monitoring cases, such as for CO2 sequestration, geothermal reservoir and remediation-related monitoring.

Accomplishments:

We have completed a coupled joint inversion framework for combining hydrological and geophysical data. A two-level parallel framework addresses the high computational needs of multi-dimensional inversion problems. Both the hydrological and geophysical simulator are multi-threaded. Moreover, computing-intense steps in the optimization framework have been parallelized. The scheme has been successfully applied to inverse problems with a pixel-based parameterization, highly relevant for field-scale applications. For environmental geophysics applications, it could be demonstrated that multi-dimensional hydrogeophysical inverse problems can be solved within reasonable computing times. This is a large advantage compared to stochastic methods, which are statistically more rigorous, yet still face prohibitive computing costs in the presence of highly parameterized models in real-world applications.

Hydrogeophysical inversion needs a proper linkage between hydrological and geophysical attributes. This is usually accomplished through petrophysical relationships. We have implemented the capability of inverting for both hydrological and petrophysical unknowns on pixel-based parameter grids. Given the required data coverage and resolution, this scheme provides for a large degree of flexibility by eliminating the need for prior information, such as variograms to describe spatially correlated attribute fields in geostatistical inversion.

Interest in the final product of this LDRD project has been expressed by the oil industry, where reservoir monitoring applications involve combined analysis of geophysical and hydrological wellbore data. We are working on bringing the product to a more commercial stage by preparing a software disclosure. Advantageous will be that the geophysical component treats a number of data types relevant for the energy industry that can be combined with the hydrological simulator.

LB11007

Effect of Secondary Mineral Coatings on Biogeochemical Processes
Principal Investigator: James A. Davis

Project Description

The goal of the project is to establish a fundamental understanding of how secondary mineral grain coatings affect the rates and equilibria of biogeochemical processes occurring in porous media. We are conducting some of the first investigations that combine controlled reactive experiments with nanoscale characterization of natural and synthetic grain coatings.

Many important reactive phenomena that affect the environmental transport of contaminants occur at the mineral-water interface, including sorption, dissolution, and redox reactions. Fundamental knowledge of these phenomena are primarily based on observations with ideal mineral-water systems, in particular, studies of molecular scale reactions on single crystal faces or macroscopic observations of reactions with pure minerals. However, there is little knowledge of the impact of secondary mineral coatings on reaction rates and equilibria in aquifer sediments. Secondary mineral coatings usually contain multiple phases that depend on local biogeochemistry. The layered structures and variable compositions of the coating regime are important in the development of conceptual models for reactive contaminant transport, because coatings provide reactants, reactive surfaces, and diffusion barriers that may govern process kinetics. New experiments devoted to this topic are needed to advance interpretations of geochemical processes in environmental systems. The research will improve our understanding of how mineral-water interfacial processes affect field scale behaviors of consequence to DOE.

Accomplishments

Progress in 2012 included the completion of long-term laboratory reaction experiments between Savannah River (SR) and Cape Cod (CC) aquifer sediments with solutions containing the tracers (bromide, strontium, arsenic, and uranium), with focus on the sorption and electron transfer aspects of the project. Thirty micron thin sections were prepared with reacted samples and coating compositions were studied by SEM and micro-focused XAS at SSRL, APS, and ALS. FIB samples were prepared at the Lawrence Berkeley NCEM and studied by TEM.

The research has demonstrated the following: 1) hematite nanoparticles within quartz grain coatings at SR control the sorption of uranium in subsurface regions that are low in fine-grained sediments; 2) Fe oxides in fine-grained sediments at SR are dominated by goethite, while in the grain coatings they are dominated by hematite, likely due to the fact that the mechanisms of iron oxide nucleation and crystal growth differ within and outside the coating domain, 3) batch uranium sorption kinetics onto SR sediments are controlled by the rate of diffusion into an internal pore network of grain coatings, 4) goethite-dominated coatings on quartz grains in CC sediments control sorption of arsenic(V) and arsenic(III), and 5) arsenic(III) is oxidized to arsenic(V) at a slow rate within CC sediment coatings.

The research has yielded excellent results at the μm scale and raised new questions that can only be solved at the nm scale. Pore throat sizes in the nm range, in addition to mineral surface charge, likely control the diffusion rates of solutes to reactants within coatings, and thus exert a significant impact on macroscopic rates of sorption and dissolution reactions. The nm scale questions are being addressed in the 2013 research. Mapping the concentration gradient of U within FIB sections at the APS nanoprobe is a major goal, an experimental approach that has never been attempted. To better characterize multi-scale porosity within the coatings, nanoscale tomography at the APS to map pore size distributions will be studied in 2013.

LB11011

CyanoAlkanes:
Engineering Cyanobacteria for Phototrophic Production of Advanced Biofuels
Principal Investigator: Christer Jansson

Project Description

Photosynthetic organisms, like plants, algae and cyanobacteria, offer the potential to convert sunlight and CO_2 directly to transportation fuels, bypassing the need for biomass deconstruction. Cyanobacteria are Gram-negative bacteria and well suited for synthetic biology and metabolic engineering approaches for phototrophic production of various desirable biomolecules, including high-density liquid biofuels such as alkanes and isoprenoids. Many cyanobacteria also thrive in high CO2 levels such as those in flue gas from coal-fired power plants. The main objective of the CyanoAlkane LDRD project is to develop a strong platform for photosynthetic conversion of pointsource CO2 to advanced biofuels using freshwater and marine cyanobacteria.

Accomplishments

We have produced more than 30 engineered strains of a cyanobacterium with enhanced accumulation of precursors for alkane and FA methylester biosynthesis. By constructing an artificial operon with encoding genes, we demonstrated a substantial increase in the endogenous accumulation of alkanes in a cyanobacterium. We also showed that the artificial operon could direct biosynthesis of alkanes in a non-cyanobacterial microorganism. Together with Cheryl Kerfeld and the GEBA-Cyano project at JGI, we have demonstrated the production of a wide array of alkanes by combining genes from different cyanobacteria.

To optimize the activity of the combined enzymes, and to allow for different substrate specificities, we have engineered an artificial enzyme harboring all of the enzymatic activities. We have named this novel enzyme alkane synthase (AS). We consider this first version of AS as a reference parent for further optimization. This optimization strategy is a collaboration with Novici Biotech, employing their proprietary GRAMMR technology.

Together with Hoi-Ying Holman, we have established synchrotron radiation Fourier transform IR (SR-FTIR) spectromicroscopy as a high-throughput diagnostic tool for realtime, single-cell metabolic analysis of genetically engineered cyanobacteria. SR-FTIR data showed accumulation of functional groups in agreement with the GC/MS/NMR results. Multivariate analysis of FTIR spectra revealed that the different strains were phenotypically segregated, but that the stochasticity in the populations gave rise to a high degree of cell heterogeneity within the population for each strain. These findings point to the importance of single-cell approaches to unravel the mechanisms that control specific traits in individual cells. Since SR-FTIR spectromicroscopy is a non-invasive tool, cells can be selected for downstream processing and omic investigation based on FTIR data.

LB10017

CO_2 as Cushion Gas for Compressed Air Energy Storage in Subsurface Reservoirs
Principal Investigator: Curtis M. Oldenburg

Project Description

We have investigated the use of CO_2 as a cushion gas for Compressed Air Energy Storage (CAES) in porous media (PM) systems such as aquifers and depleted gas reservoirs (referred to here as PM-CAES). The advantage of using CO_2 as a cushion gas is that CO_2 compresses in a non-linear and advantageous fashion such that it acts like a super-cushion when the reservoir is operated around the critical pressure of CO_2 (74 bar). The main goal of the project was to assess the feasibility of using CO_2 as a cushion gas for enhancing energy storage.

The approach we used involves simulation of the coupled processes involved in PM-CAES. Many of the processes associated with CO_2-enhanced PM-CAES can be modeled with reservoir simulation capabilities developed by us at LBNL (e.g., T2Well (Pan), and TOUGH2/EOS7C (Oldenburg)). Through use of existing simulation capabilities, we investigated processes of air injection in the well and in the reservoir including the effects of repeated compression and decompression cycling and displacement of water.

Accomplishments

In FY12, we applied our simulation capabilities to prototype 2D and 1D radial systems to investigate the performance of PM-CAES with and without CO_2 as a cushion gas. Our simulations revealed a conflict between maximizing the beneficial effects of the CO_2 cushion and minimizing the negative effects of mixing. Specifically, as shown in Figure 1, when the CO_2 cushion is placed close to the injection well, the non-linear compressibility of CO_2 acts to minimize pressure rise, but in that location close to the well, pore velocities are large and dispersive mixing leads to CO_2 being produced out of the well. Our overall conclusion is that CO_2 is an excellent cushion gas, the use of which may be profitable for an individual PM-CAES facility through future carbon credit or tax policies. To minimize mixing, CO_2 needs to be placed far from the injection/production well. In this position far from the well, the super-compressibility properties of CO_2 will not be exploited.

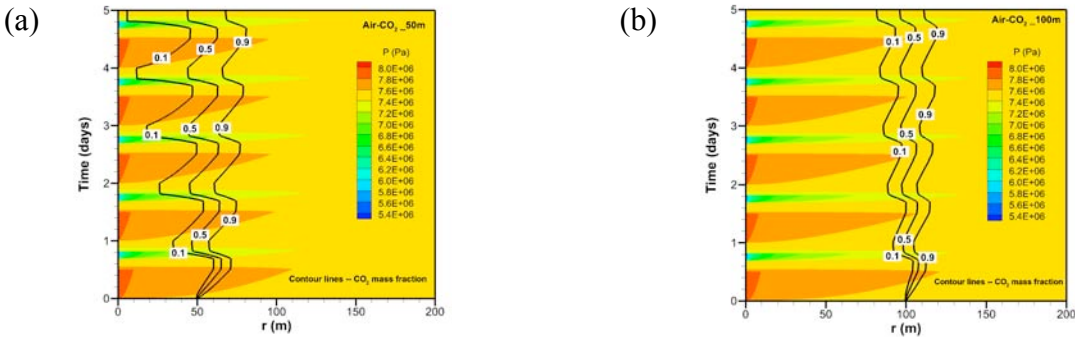


Figure 1. Pressure (color contours) and CO_2 mass fraction (black lines) as a function of time and radius for five cycles of PM-CAES with CO_2 as cushion gas for (a) the cushion gas interface placed initially at r = 50 m (close to well) and (b) the cushion gas placed at r = 100 m (farther from well). As shown, the cushion effect of CO_2 is greater (pressure propagates less far into reservoir) when the cushion is at 50 m, but the mixing is also greater (larger spread in black CO_2 mass fraction lines).

LB11044

Interactions among Cloud Processes, Convection, and Climate Change
Principal Investigator: David Romps

Project Description

Clouds have a significant effect on earth's heat budget. Clouds provide a powerful feedback on climate change, and they have remained the largest uncertainty for almost twenty years in the the study of earth's climate sensitivity. The goal of this project is to address the interplay between atmospheric convection and climate. This will involve work to quantify climate sensitivity to CO_2, understand tropical variability, characterize past climate regimes, and interpret many paleoisotopic records.

While climate modelers have recognized the uncertainty of cumulus convection for a long time, the treatments of convection in global climate models (GCM) are typically *ad hoc* and empirical in nature. This produces considerable uncertainty in climate projections, including simulations from the DOE-NSF Community Earth System Model (CESM). The basic reason is that we do not know how to formulate a rigorous statistical mechanics for convection since it involves processes with no known first-principles solutions (i.e., anisotropic buoyancy-driven turbulence coupled to a phase change). A promising approach is to replace the empiricism in GCMs with explicit numerical solutions to the equations of motion at the native scales of convective systems. With the advanced computational capability afforded by DOEs facilities including NERSC, this approach is now becoming feasible.

Accomplishments

In a collaboration with colleagues at U Albany, we have analyzed observations from hurricanes in the Atlantic. The goal of this work was to ascertain why hurricanes exhibit a strong asymmetry in their production of lightning: the downshear (roughly, downwind) half of the hurricane has several times more lightning events than the upshear half. By using temperature and humidity soundings obtained by dropsondes, we determined that differences in *entraining* convective available potential energy (CAPE) were responsible. This work was published in the Journal of Atmospheric Sciences.

Another line of research evaluated supradomain-scale (SDS) schemes for single-column models. These schemes parameterize the large-scale dynamical interaction between a column of the atmosphere and its surrounding environment. The two schemes – WTG and WPG – were studied from an analytical perspective and also using high-resolution numerical simulations. This led to a pair of papers in the Journal of Atmospheric Sciences that highlighted the advantages of using the WPG scheme over the WTG scheme.

Another study has looked at a parameterizations of convective momentum transport that is currently used by the Community Atmosphere Model (CAM). It was found that this scheme is identical to a simpler scheme devised several decades ago, but with an artificially reduced convective mass flux. This led to a recommendation that CAM change one of its parameters to zero to emulate the earlier, and simpler, model of convective momentum transport.

LB11034

Testing Soil Carbon Sequestration Through Gypsum Treatment

Principal Investigators: Young-Soo Han and Tetsu K. Tokunaga

Project Description

The purpose of this study is to help control adverse effects of increased atmospheric concentrations of CO_2 by decreasing rates of CO_2 emitted from soils through microbial respiration. Soils comprise the third largest global carbon pool, are readily accessible, and hence are potentially economical managed for C storage. This study is investigating a new strategy for increasing C retention in slightly alkaline soils through addition of calcium sulfates. These moderately soluble amendments can reduce microbial respiration, accelerate calcite ($CaCO_3$) precipitation, and promote soil organic carbon (SOC) complexation on mineral surfaces.

Moderate elevation of soil water osmotic potential from $CaSO_4$ dissolution can slow down rates of microbial decomposition of SOC. Increased Ca^{2+} concentrations in soils with pH > 8 (often found in arid and semi-arid regions), can accelerate calcite precipitation. Calcium also promotes SOC binding onto mineral surfaces, thus diminishes leaching losses of SOC. Flue gas desulfurization gypsum (FGDG, $CaSO_4 \cdot 2H_2O$), a byproduct of exhaust gas desulfurization in coal-fired power plants, is an inexpensive source of calcium. The effects of $CaSO_4$ addition are being tested in laboratory soil columns with and without calcium sulfate-amended layers, and in greenhouse soil columns planted with switchgrass, a biofuel crop. The distributions of carbon in columns have been monitored in gaseous, aqueous and solid phases to understand the effect of adding Ca^{2+} on C distribution in soils. A relatively high fraction of ^{13}C-labeled bicarbonate has been injected in one column to differentiate the newly precipitated calcite from native soil calcite.

Accomplishments

Our main accomplishments have been (1) the identification of conditions in which inorganic and organic carbon sequestration is practical in semi-arid and arid soils, (2) development of a method for measuring the total carbon balance in unsaturated soil columns, and (3) the quantification of different pathways for soil C sequestration in response to $CaSO_4$ amendments. Suppression microbial respiration rates constituted the most significant C sequestration impact of $CaSO_4$ addition to soils, amounting to about 100 to 600 g C per m^2 soil per m of infiltrated water. Calcite precipitation is a relatively slow process (about 60 to 90 g C per m^2 soil per m of infiltrated water), but was measurably accelerated in response to $CaSO_4$ treatments. These results demonstrate the feasibility of promoting soil C sequestration through additions of $CaSO_4$, and also show that rates are relatively slow.

The newer studies conducted in the greenhouse on $CaSO_4$ treatments in soils planted with switchgrass are essential for understanding the C mass balance in more complete systems with soil CO_2 generated through respiration from both plant roots and the soil microbial community. In addition, the impacts of the $CaSO_4$ treatments and water use (irrigation rates) on yields of recoverable biomass are being evaluated. Thus, this work is providing information useful for evaluating the effectiveness of a land management practice for increased soil C sequestration under (semi)arid region biofuel crop production.

LB10022

Biological Carbon Sequestration:
Fundamental Research on Biological Carbon Capture and Soil Carbon Stabilization

Principle Investigator: Margaret Torn. co-PIs: Janet Jansson, Christer Jansson, Eoin Brodie, Caroline Ajo-Franklin, Hoi Ying Holman, Trent Northen, Susannah Tringe

Project Description

The purpose of this project is to study and optimize biological means to capture and sequester CO_2—as biochar stored in soil and cyanobacteria-produced carbonates. Biological capture of CO_2 and stabilization in soils is promising because some forms of soil organic carbon persist for millenia. Our aims were to understand: (1) mechanisms of soil carbon stabilization and how to influence them; (2) how to enhance bacterial capture of CO_2 in ecological and industrial environments; and (3) potential loss of already sequestered terrestrial C.

Accomplishments

Biochar is a carbon-rich product of incomplete plant combustion. Biochar carbon has been proposed as a method for carbon sequestration because it is assumed to be stable in soil, but recent research shows that it is degradable by soil microbes. However, the influence of environmental conditions on microbial transformation of biochar is poorly understood. We performed laboratory incubation experiments to compare biochar decomposition in soils from contrasting ecosystems (tropical forest from Puerto Rico and Mediterranean grassland from California), temperatures (ambient and +6°C) and depths (A and B horizons). Heterotrophic respiration of ^{13}C-enriched wood and char was monitored continuously by Cavity Ringdown Spectrometer. The activity of extracellular enzymes and changes in microbial community composition (via pyrotag sequencing of 16S rRNA and 16S rRNA genes) at early and later phases of the incubation. About 1% of the added biochar was degraded in both soils in one year, about 50 times slower than wood decay. Biochar-amended soils had a decline in cellulose- and hemicellulose-degrading enzyme activity in grassland soils, although not in tropical soils. Both soils harbored different microbial communities as well as having distinct communities at different depths. Interestingly, Actinobacteria were enriched and Actinobacterial activity was increased by biochar addition. In summary, the addition of biochar to soil preferentially enhanced the growth and activity of several microbial groups with little impact on native organic carbon decomposition.

In the cyanobacteria and carbonate mineralization component of this LDRD, we demonstrated that precipitation of Mg-rich carbonates by marine cyanobacteria is facilitated by ultrahigh CO_2 conditions. Using time-of-flight secondary ion mass spectrometry (ToF-SIMS), synchotron radiation Fourier transform infrared (SR-FTIR) spectromicroscopy, energy-dispersive X-ray (EDX) spectroscopy, and high-resolution scanning electron microscopy (SEM), we showed that: high pCO_2 promoted carbonate mineralization by the marine cyanobacterium *Synechococcus* 8806, the increase in Mg:Ca carbonate precipitation correlated positively with enhanced production of exopolysaccharide substances (EPS), and the carbonate composition shifted from aragonites and calcites to the dolomite forerunner huntite with increased pCO_2 and EPS. These results will help scientists predict the effects of changing ambient CO_2 concentration on future ocean carbonate chemistry, and may be used to design microbial carbonate mineralization for biological C capture and storage.

LB11041

Collaboration with China on Geologic Carbon Sequestration: Novel Field Tests to Characterize Heterogeneity for China's First Pilot Test

Principal Investigator(s): Quanlin Zhou

Project Description

Multiscale subsurface heterogeneity has been demonstrated by monitoring CO_2 plumes on different scales to have a fundamental impact on CO_2 migration and trapping. The objective of the proposed research is to (1) design, through numerical experiments and integrated analysis, a set of pumping, tracer, and CO_2 injection tests to capture the multiscale heterogeneity, (2) validate the methodology by revisiting the existing pumping, tracer, and CO_2 injection tests conducted at the Frio site, with model prediction and comparison to the monitored CO_2 plume, (3) apply a systematic methodology of testing, analysis, and prediction to the Tianjin Pilot Test, and (4) promote the collaborations and partnerships between IGGCAS and ESD/LBNL related to GCS.

Accomplishments in FY 2012

In Tasks 1 and 2, we focused on the predictions of pressure, temperature, CO_2 saturation and other primary variables during field injection tests using current status-of-art numerical simulators (e.g., TOUGH2). We also focused on analysis of the monitoring data in existing field tests (Frio I, Cranfield, and In Salah site), and discovered the mismatches between predicted scenarios and field reality. We attributed these mismatches to new, non-equilibrium transport phenomena and the dynamics of two-phase flow in the field, which are never included in the simulators. Our discoveries will significantly improve our understanding of the transport phenomena in the field and help the entire CCS community.

In Task 3, no progress was made in this task for the planned pilot test because our Chinese partner delayed their CO_2 injection and LBNL did not receive any data for the pilot test. Due to this reason, we did not apply for the renewal of the project in FY13.

We collaborated with a different Chinese partner (China University of Geosciences, Beijing) on the discovery of non-equilibrium CO_2 dissolution in brine and dynamic displacement through laboratory experiments, and published one journal paper.

LB12003

Novel Laser-Plasma Storage Ring for Synchrotron Radiation and Particle Physics Applications.

Principal Investigator(s): Carlo Benedetti

Project Description

The purpose of this project is to investigate the possibility of developing a compact storage ring (a few meters in diameter) that exploits the ultrahigh accelerating fields obtained in the laser-plasma interaction. State-of-the-art laser-plasma accelerators (LPAs) can produce high energy electron beams over a short acceleration distance (e.g., E~0.5 GeV in cm-long plasmas) with high peak brightness. However, the average brightness of LPAs is presently limited by the low repetition rate of the laser driver. This limits the present utility of such LPA electron beams as radiation sources (e.g. via Compton scattering). To address this issue the use of a store ring, adapted to the specific characteristics of LPA generated beams, has been considered. The novel characteristic of the laser-plasma storage ring (LPSR) is that, unlike conventional storage rings built to date, has no injection or extraction system. The electron beam is generated through the laser-plasma interaction directly on the axis of the design orbit of the storage ring. Furthermore, the plasma can subsequently serve as a decelerator for controlled dumping of the beam. This is a fundamental difference from conventional storage rings where the orbit is typically disturbed and electron beams are injected via complex septa and kicker magnets. The major features of the LPSR are the plasma cell that generates and accelerates/dumps the electron beam, and an appropriately designed magnetic lattice to define the LPSR orbit. Additional systems that may be present include a radio cavity to compensate for the turn-by-turn electron beam energy loss. Unlike conventional storage rings, where the goal is to develop lifetimes for the beam which are as long as possible, the lifetime of the LPSR would be designed to be on the order of only a few seconds, corresponding to the repetition rate of the driver laser.

Accomplishments

We developed a 2D cylindrical code (INF&RNO) to model the laser-plasma interaction, and to study the LPA generated electron beams. The code solves the full wave equation for the laser envelope evolution coupled to the equation of motion for the plasma (PIC and cold fluid descriptions are available) and to the Maxwell's equation for the electromagnetic field in the plasma. The plasma responds to the laser field via the averaged laser ponderomotive force. The adoption of the cylindrical geometry allows the description of 3D physics (laser evolution, electromagnetic field structure) at 2D computational cost. Simulation of the laser-plasma interaction with standard numerical tools is generally computationally expensive but the features of INF&RNO allowed us to perform detailed modeling of the plasma cell and the LPA beams.

We proposed a design for the lattice of the storage ring (23 meters long, with low momentum compaction factor) and we performed analytic and numerical calculations, using the tracking code ELEGANT, of the beam dynamics of the LPA-generated electron beams as they orbit in the storage ring. Particle distributions, as obtained from the INF&RNO simulations, were used to calculate the energy loss from Coherent Synchrotron Radiation (CSR). For a beam of energy E~0.5 GeV, bunch length σ_z~5 μm, and total charge Q~600 pC, this energy loss is ~80 MeV/turn, compared with a loss of ~5 keV/turn from Incoherent Synchrotron Radiation (ISR), making this ring a source of high-power broad-band CSR radiation. For a beam with E~0.6 GeV, σ_z~1 μm, and Q~30 pC, the CSR and ISR energy losses are, respectively, 50 MeV/turn and 15 keV/turn. In both cases the CSR losses are severe. The beam bunch length remains short after one turn. Further simulation studies of the multi-turn (~10^7) dynamics, where nonlinear and collective effects are taken into account, have to include also the RF acceleration cavities which compensate for the energy loss. With the present ring design the CSR losses prohibit ring-based light sources applications of the LPA beams.

LB11024

From fossil fuel to photovoltaics:
Economic, environmental and health impacts for policy considerations

Principal Investigator: Nancy Brown
Dev Millstein, Pei Zhai, Lucas Bastien and Nancy Brown

Project Description

The goal of this project is to evaluate large-scale deployment of photovoltaics through a comprehensive analysis of environmental, health and economic costs associated with their deployment to better inform and guide US energy related policy options. In order to assess the environmental impacts of substituting PV for coal generation, we investigate tradeoffs that affect both air quality and radiative forcing. The reduction of coal based CO_2 emissions will lead to lower radiative forcing; however, surface albedo changes due to PV adoption and reductions in regional air pollutants, aerosols and particle precursors such as SO_x and NO_x may have the opposite radiative effects that can, in turn, also affect regional weather patterns and air quality. The state-of-the-art numerical model, WRF (Weather Research and Forecasting model), with its fully coupled chemistry module, will be used to predict the effects of changes in land-use and emissions on weather and air quality, including representation of aerosol direct and indirect effects. Emission changes will be modeled with an economic/engineering electricity grid model.

Accomplishments

We have developed and employed, on a national and regional scale, a modeling framework that can evaluate the air quality and regional climate effects of the addition of substantial photovoltaic energy generation into the electricity grid. This effort was a two-step process. First, we evaluated the type of generation and emissions that the use of solar power would displace. Using an economic/engineering energy grid model we found that the type of generation (coal, natural gas, oil) offset by solar power use depended on a region's prior generation resource mix, meteorological factors, and the relative amount of power that would be introduced by the solar resources. Once the type of generation offset by solar power was identified by region, the effect on regional emissions of local pollutants as well as carbon dioxide could be calculated. Emission changes do not translate linearly into changes to complex air pollutants such as tropospheric ozone or secondary particulate matter. In the second part of the study, we used a state-of-the-art meteorological and atmospheric chemistry model (WRF-Chem) to evaluate the effects of specified emission changes on air quality. We evaluated a suite of pollutants that is readily translated to health and economic burdens. We also examined highly localized changes in meteorology at high spatial resolution that might occur when large scale solar plants were introduced, and found that the changes were small and affected boundary layer heights and temperature fields. Each of these increases ozone pollution, but this may be offset by changes in precursor emissions.

In addition to multiple peer-reviewed journal publications and conference presentations, specific accomplishments include building software capacity to evaluate and model the effects on air quality of national energy policies and technological change. Specifically, a set of software tools has been created that can generate, with a fine spatial resolution, historical and future emission scenarios based on user specified data about emissions from various economic sectors for direct input in to the WRF-Chem model.

LB12039

Low-Energy, Low-Cost Refrigerators for Vaccine Delivery

Principal Investigator: Shashi Buluswar

Project Description

The purpose of this project is early prototype development for a low-cost/low-energy refrigerator to be used for vaccine delivery. After careful field analysis of the gaps in current vaccine cold chain, this project was selected in order to provide concrete results by the end of FY2012 and also provide LIGTT with early momentum towards further development and refinement of the refrigerator. The approach included-

- Identification of specific components of the refrigerator that can be deployed in the short-term: insulation, phase-change materials, chassis and temperature control mechanisms.
- Analysis of cost and performance of components
- Completion of an early prototype design and technical specs, and review with external partners and funders

Accomplishments

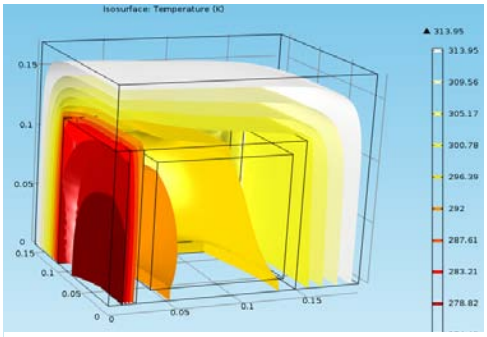


Figure 1: A series of thermal modeling was conducted ahead of prototype engineering to assure validity of the geometry, insulation, phase change materials and thermoelectric cooling engines.

In FY2012, LIGTT developed the early concept of a solar-powered vaccine refrigerator. The team weighed several design options, worked closely with two external partners: Sheetak, Inc., on design and configuration of thermal diodes, thermoelectrics, insulation and chassis design; and with PATH, a leading NGO on global health technologies, on understanding performance parameters required by the World Health Organization (WHO). The LIGTT team then conducted simulations to select and improve the best technical design options for meeting WHO's performance specifications. The most significant outcome of the project was a set of robust design specifications and an early prototype that have laid the foundation for a technology that promises to solve a major problem in delivery of life-saving vaccines. Follow-up funding has been achieved through the LDRD FY'13 cycle. This is being currently utilized for further development and testing of the prototype, in-field demonstrations and further refinements.

LB11023

Mapping Genes and Acres: Engineering Switchgrass Lines for Large-scale Biofuel Production on Marginal Lands

Principal Investigator(s): Larry Dale, James McMahon, Gary Fitts, Sarah Lewis

Project Description

The purpose of this proposal was to evaluate the potential to grow drought and salt tolerant switchgrass varieties on marginal lands in the United States. The proposal combined a genetic research effort at JBEI with GIS mapping and economic analysis at UC Berkeley and Lawrence Berkeley National Laboratory. The genetic component of the research identified candidate genes conferring drought tolerance to rice and switch grass and validated their usefulness for engineering drought and salt tolerant perennial grass varieties.

The geographical component of the analysis included a GIS mapping study of the Midwest that identified land available for cultivation of drought tolerant switch grass lines. The GIS analysis identified the acreage of land suitable for cultivation with drought tolerant (and in some cases) salt tolerant switchgrass. The economic modeling component was designed to provide information about the market viability of the switch grass lines developed by the geneticists. The economic modeling analysis determined the cost of producing bio fuels from existing switch grass lines, the cost of producing biofuels from the switch grass lines developed in this project, and the feasibility of cultivating the new switch grass lines.

Accomplishments

We mapped land use variables in California and the Kansas linked to suitability for growing switchgrass. These include crop and land use data, topography, soil texture, climate variables, and switchgrass target variables. We experimented with different model formats for linking these variables to switchgrass success, including both a regression model and a and fuzzy spacial suitability model. We identified rice (and by extension switchgrass) genes thought to respond to drought and salinity, and made a preliminary assessment of the tolerance of plant strains with these genes to drought. Finally, we projected and mapped regions in the US most suitable for growing drought tolerant switchgrass.

We calculate that approximately 80% of the suitable land area in Kansas falls within a dryness index equivalent to about four 22-day long dry stretches, or one 45-day long dry stretch. By identifying the dryness threshold where land area is maximized, the results of this analysis both inform the development of drought-tolerant varieties of switchgrass as well as identify marginal areas where efforts to plant such a species may prosper.

LB12026

Sodium Ion Batteries for Grid Storage Applications
Principal Investigator: Marca M. Doeff

Project Description

The goals of this project are 1) to develop a dual intercalation battery based on sodium using aqueous electrolytes and 2) to investigate titanates as potential anode materials for sodium ion batteries with either aqueous or organic electrolytes. These goals were chosen with the specific purpose of enabling devices intended for cost and resource-sensitive applications such as large-scale energy storage (grid applications). Other benefits include the potential development of alternatives to lithium ion batteries for vehicular applications in case of lithium supply insecurity, a matter of increasing concern to the battery community.

Sodium ion batteries operate on a similar principle as that of the better-known lithium ion analogs; alkali metal cations shuttle between two host electrodes, which undergo reductive insertion at differing potentials. Sodium does not, however, insert into graphite, the most common negative electrode used for lithium ion systems; therefore, a suitable anode material must be found. Ternary titanates often exhibit ion exchange properties that imply high mobility for univalent cations including sodium, and can be synthesized from cheap and abundant precursor materials, making them attractive as anode materials for sodium ion batteries. Because many structures are available and the structure affects the voltage profile, it should also be possible to tailor the electrode to the type of battery (aqueous or organic electrolyte).

The lowest cost variant of the sodium ion battery employs an aqueous electrolyte with inexpensive salts such as Na_2SO_4 or Na_3PO_4. The reductive and oxidative stability limits of water are pH dependent, with a total voltage stability window of about 1.2V. Because oxygen and hydrogen evolution tend to be slow, in principle, the operating window can be extended somewhat in practical devices. In addition, gas recombination techniques can be used in systems employing electrodes that operate slightly outside the voltage stability window to ensure safety and long cycle life. By selecting electrode materials that intercalate sodium within or slightly outside this window, it should be possible to develop a sodium ion cell that cycles stably. Although the energy density will be lower than that of devices designed for use with organic electrolytes because of the narrower voltage window, the system should be rugged and very low cost.

Accomplishments

We have successfully demonstrated an aqueous sodium ion cell using $NaTi_2(PO_4)_3$ as an anode, Na_2FePO_4F as the cathode, and 1M Na_2SO_4 as the electrolyte and have shown that it can be cycled. In addition, we have surveyed several ternary titanate anode materials and have identified promising candidates. A record of invention has been filed for a material with a theoretical capacity of over 280 mAh/g, which discharges much of its capacity below 0.5V vs. Na/Na^+, and can be cycled. A second structure we have identified can readily be modified by substitution and ion exchange processes, allowing tailoring of the discharge properties. The theoretical capacities range from about 160-280 mAh/g. One compound discharges at an average potential of 1V vs. Na/Na^+ with good reversibility. These materials, as well as the first one described above also undergo lithium insertion reversibly, with initial capacities as high as 200 mAh/g. A record of invention is being prepared for this concept.

LB10044

Toward a US Greenhouse Gas Information System
Principal Investigator: Marc L. Fischer

Project Description

We are conducting research and development of methods to quantify anthropogenic greenhouse gas emissions at local, regional, and eventually continental and global scales. The immediate goals of this work are to develop techniques for measurement and inverse model estimation of GHG emissions supporting State compliance with California's Global Warming Solutions Act (AB-32). The longer-term goal of this work is to support international control of anthropogenic greenhouse gas emissions, which will require systematic estimation of emissions and independent verification. In the present work, we are expanding on the LBNL California Greenhouse Gas Emissions Measurement (see CALGEM.lbl.gov) project, which we started for the California Energy Commission.

Accomplishments

Our primary research has focused on improving both data and modeling capabilities to make California a uniquely powerful test-bed for measurements of GHG emissions. As proposed, we participated in a multi-agency CalNex2010 campaign, updated our atmospheric transport model simulations for summer 2010 to present, and combined LBNL, NOAA, and CARB measurements to produce several important results. In 2012, we completed several papers and found extramural research support for two new projects. First, we published a paper showing that N_2O emissions from central California are significantly higher than expected and, when scaled to the State level, are 2-3 times greater reported in the existing State inventory (Jeong et al., 2012). Second, we participated in two papers examining CH_4 emissions from rice in the Central Valley (Peischl et al., 2012) and urban activities in the South Coast Air Basin (Wennberg et al., 2012). The airborne measurements demonstrated that the CH_4 from rice agriculture are strong vary with time, supporting our earlier work on the seasonality of total emissions from the Central Valley. The work in Sourthern California show that CH_4 emissions from the urban area may include significant emissions from petroleum and natural gas infrastructure, emphasizing potential for emissions mitigation in that sector. Finally, this LDRD project enabled focused activity on proposals, leading to two new research projects The first will investigate promising economic and technical solutions to mitigate CH_4 emissions from natural California's gas production and processing infrastructure will, one for the California Energy Commission. The second will expand the CALGEM project to measure GHG emissions from new sites and with new instruments for the California Air Resources Board.

LB11021

The Emerging Technologies Analysis Team: Developing analytical and communications frameworks to enable breakthrough low-carbon technologies

Principal Investigator: Jeffery Greenblatt

Project Description

The purpose of this project was to develop and apply new analytical capabilities and collaboration frameworks to bridge gaps between basic, applied, and analysis research at LBNL, helping to achieve the Carbon Cycle 2.0 vision. Together with several complementary, cross-divisional LDRDs, the LDRD aimed to analyze the environmental (especially carbon cycle), human health and other impacts of various emerging energy technologies, and where possible, to improve the net benefits and viability of these technologies in the marketplace. Core capabilities included a suite of analytic tools for life-cycle assessment (LCA), air quality modeling, human health impact assessment, geographic information system (GIS)-based analysis, scenario analysis and economic modeling. The five core areas of work were: dynamic window technologies, drought-tolerant biomass, CO_2 capture and sequestration, solar energy, and exergy analysis.

Accomplishments

Windows: 1. We applied LBNL-developed tools to evaluate potential heating/cooling savings from dynamic electrochromic nanocrystal window films for a range of near-infrared transmittance levels across 16 U.S. climate regions, and identified a range of transmittance performance targets necessary to realize significant savings in building energy demand and ensure market success. This collaboration with the Molecular Foundry is partly responsible for a recent $3.1 M ARPA-e grant to further develop this technology. 2. We also investigated window coatings containing dynamic prismatic optical elements to enhance daylighting energy savings.

Biomass: We identified marginal lands for drought-tolerant biomass in the Midwest through an analysis of localized precipitation constraints. Our work contributed a technology and economic model of second-generation biofuel production supply chain and LCA, and estimated the implications of "droughtiness" on Kansas biofuel supply-chain costs.

CO_2 Capture and Sequestration (CCS): 1. We examined the economic uses of brine produced as a CCS byproduct. We built the capacity to map and evaluate brine production in all regions of the U.S., compiled a range of brine management options, and applied LCA to evaluate overall costs and feasibility. 2. We examined time-dependent radiative forcing benefits of large-scale CCS deployment. We developed three analytical elements—energy supply models, life-cycle emissions inventories, and radiative forcing calculations—to find that retrofitting existing power plants yields significant radiative forcing reductions, but at a higher energy cost.

Solar energy: 1. We quantified meteorological, albedo and air quality impacts of large-scale solar photovoltaic (PV) use. We updated national air pollutant emission inventories and developed software tools to forecast national emissions scenarios to 2030, and refined an economic- and engineering-based electricity grid model to estimate pollutant and carbon emissions changes from high levels of PV in different U.S. regions. 2. We also developed a materials and manufacturing process LCA of an artificial photosynthesis-based hydrogen system.

Exergy: We published a paper on identifying loss mechanisms and areas of improvement for homogeneous charge compression ignition engines using detailed exergy analysis.

The Lab also recently received a five-year, $1.9 M DOE grant on advanced hydrogen fuel cells, awarded in part because of LDRD-initiated efforts to include LCA costs, human health benefits, carbon offsets, and displacement of competing technologies.

LB12008

A Balloon-Borne Platform for Measuring Vertically Resolved Concentrations of Black Carbon in the Troposphere

Principal Investigator(s): Odelle Hadley and Thomas Kirchstetter

Project Description

The purpose of this project is to increase our understanding about how aerosol particles are vertically distributed in the atmosphere, which in turn will clarify how air pollution influences climate. The project initially focuses on measuring sunlight-absorbing black carbon particles. Black carbon particles are emitted during combustion of fossil and biomass fuels. A recent comprehensive study concludes that black carbon emissions warm the climate and are the second most important human emissions in terms of climate forcing in the present-day atmosphere. Only the greenhouse gas carbon dioxide is estimated to have a greater climate forcing. The climate effects of black carbon particles depend on their vertical distribution in the atmosphere. However, vertically resolved BC concentrations have scarcely been measured.

This project will develop a balloon-borne platform for routine vertical profiling of black carbon, akin to the wide deployment of radiosondes and ozone sondes that routinely measure the vertical distributions of meteorological variables and ozone. It will test, modify, and integrate several technologies into a payload to be lifted through the atmosphere by a balloon. The payload will include a) radio communication, data logging, telemetry, and tracking capabilities for payload retrieval, b) instruments that measure black carbon concentration, particle number concentration, and aerosol light scattering, and c) relative humidity, temperature, and altitude sensors. Once developed, instrumented balloons will be launched routinely in California to quantify temporal variation in the vertical distribution of black carbon in the atmosphere. The data will be useful in distinguishing between locally emitted air pollution aerosols and aerosols transported long distances over the Pacific Ocean. Opportunities will be sought to include balloon-borne vertical profiling of black carbon in collaborative scientific campaigns where a variety of ground, aircraft, and satellite measurements are integrated to better understand atmospheric processes related to climate change.

Accomplishments

The most significant accomplishment has been five successful launch and recovery missions of an instrumented payload. The payload included a new instrument that, in collaboration with its manufacturer, was modified for increased stability and measurement sensitivity required for this project. At a predetermined altitude, the payload's onboard computer releases the balloon, a parachute deploys, and the payload descends back to the Earth's surface. Transmitters incorporated into the instrument payload relay its location to a ground operator's laptop throughout the flight, allowing the payload to be recovered after each mission. We have repeatedly demonstrated the ability to predict the rise rate, flight path, and recovery location of the instrumented payload.

We are in the process of integrating a second black carbon sensor and an optical particle counter to increase our confidence in measured black carbon concentrations.

LB11022

Life-Cycle Analysis of Geologic Carbon Sequestration
Principal Investigator: Thomas E. McKone

Project Description

The goal of this study is to evaluate the regional variability of economics, environmental impacts, and societal risks of a pressure management technique involving brine extraction for carbon sequestration in saline formations following carbon capture. One of the challenges of the global climate-energy crisis is the vast scale of the problem. This challenge should be met with a variety of responses, including geologic carbon sequestration (GCS). We use Life-Cycle Assessment (LCA) of GCS to analyze different options for implementing GCS. Key targets for GCS in North America are brine-filled aquifers in large sedimentary basins. If GCS is to play a major role in reducing CO_2 emissions to the atmosphere in the next few decades, there is a compelling need to evaluate ways of disposing of brine produced to reduce pressure in geologic carbon sequestration storage reservoirs.

The particular focus of this effort is compiling the options, costs, risks, and benefits from the production of large amounts of brine and saline water. Options we consider include hot brine energy recover, evaporation pounds and/or desalination plants with staged mineral recovery, reverse osmosis treatment, saline aquaculture and algae ponds for producing biofuels, surface discharge (to rivers or oceans), and reinjection. We selected three saline aquifers targeted for carbon sequestration from different geographic regions in the United States to assess brine extraction and disposal scenarios. GIS databases are queried for data from these three regions to perform network analysis. Initial calculations were performed assuming ten GW-size coal fired power plants are injecting 90% of their CO_2 emissions into a saline aquifer with an annual injection of nearly 90 million tonnes of CO_2 and an annual brine extraction of nearly 750 million liters.

Accomplishments

The CO_2 sequestered from a 1-GW coal-fired power plant can displace as much as 20 million m^3 brine annually. We have compiled map-based information on location and CO_2 production magnitude for both industrial facilities and electrical-power-production facilities that produce significant quantities of CO_2. Previous studies have determined that the management of large volumes of brine would require flexible options for brine treatment and disposal in different regions of the country, but portrayed brine management was as a costly waste management issue of GCS. Our work has confronted the question of whether and how site-specific sequencing of treatment, use, and disposal stages could provide a source of energy, water, or capital to the power plant, or significantly reduce the cost of brine management. We approached this question by performing a technical and economic assessment to determine the feasible and net present value (NPV) of brine use sequences (BUS) in different regions of the country. Low and high values were used in calculations of NPV to generate bounding results for brine management scenarios. Our results reveal that the feasibility of a BUS is highly sensitive to spatial parameters including—(a) the temperature and chemistry of the brine; (b) markets values for energy, water, minerals, and land; (c) the cost of disposal options; (d) available transportation; and (e) disposal infrastructure.

This project has produced one LBNL report, five conference presentations, and one peer-reviewed journal paper.

LB11027

Accelerated Materials Design through First-Principles Calculations and Data Mining
Principal Investigator(s): Kristin Persson

Project Description
Materials innovation today is largely done by intuition and based on the experience of single investigators. One of the foremost reasons for the long process time in materials discovery is the lack of comprehensive knowledge about materials, organized for easy analysis and rational design. First-principles calculations have reached the point of accuracy and speed where many materials properties, relevant for photovoltaics, batteries, and thermoelectrics can be reliably predicted in a reasonable amount of time. The goal of the proposed work is to leverage the computing age to accelerate the way materials discovery is done by creating a high-throughput computing environment together with a searchable, interactive database of computed materials properties powered by a user-friendly web-based access. In our vision, both experimentalists and theorists will have materials properties of all known inorganic compounds and beyond at their fingertips to scan, analyze and provide inspiration for novel materials development. We are envisioning a dynamic 'Google' of materials properties, continually increasing and changing as more users come onboard to analyze the results, verify against experiments, increase their knowledge, and ultimately, lead the way towards accelerated materials design in the scientific community.

Accomplishments
During 2011 we built an integrated software infrastructure handling automated high-throughput first-principles calculations across different computing facilities, a flexible document-based database and analysis software and a web-based access portal. Together with our co-founders at MIT, we successfully launched the freely available Materials Project web site: www.materialsproject.org in October 2011, which was recognized at DOE as a 'First-Of-Its- Kind Search Engine' for materials research and a groundbreaking project within the recent Materials Genome Initiative announcement. Today, the site contains close to 16,000 computed compounds and we are continuously adding more. To supply new computed materials and properties, the project has been granted computer time at NERSC in the excess of 4 Million CPU-hrs and we are testing Teragrid as well as resources at the Computational Center of the University of Kentucky. At MaterialsProject.org, the currently available compounds and properties can be searched and investigated using several functionality applications ('apps') such as 1) the 'Materials Explorer' where the user can search for materials with general materials properties, 2) the 'Li-ion Battery Explorer' containing known and new compounds for Li-ion battery electrode materials, 3) the 'Structure Predictor' where the user can predict crystal structures for any target ionic compound, 4) the PD app, which displays computed phase diagrams for any chemical system and 5) the 'Reaction Calculator' which calculates the reaction enthalpy for any set of compounds available in the database. Only a month after launch, The Materials Project already has over 500 registered users, whereof many are from industry. Our team at LBNL spans multiple divisions; CRD, NERSC and EETD which reflects the project's need for multi-disciplinary expertise encompassing computer science, professional web design and deployment and computational materials science. We are also exploring collaborations with other researchers who can add complementary data management and materials science expertise. We are moving forward with several ideas for improvement both in terms of increasing the number of compounds, increasing the materials properties to span more applications areas, improving the data management, implementing new schemes for data privacy, etc. To expand and fund the future directions of the Materials Project we have written several multi-disciplinary proposals to incorporate statistical methods for materials predictions, data provenance tools and expanded materials property data and algorithms.

LB11032

Dynamic Light Redirection by Optical Metamaterial Coatings
Principal Investigator(s): Stephen Selkowitz, Delia Milliron,
Research Collaborators: B. Helms, S. Cabrini, A. McNeil, E. Lee, J. Jonsson, A. Anders

Project Description

Static diffractive holographic optical elements (HOE) and prismatic optical elements (POE) provide effective redirection at only limited incident angles and wavelengths. Metamaterials whose properties can be dynamically tuned in response to angle and wavelength will be developed based on an electroactuated inverse polymer opal. The optical characteristics of inverse opals made from soft materials have recently been shown to be tunable over a broad range through mechanical deformation. A parallel effort will explore a dynamic POE with a controllable microstructure that can be switched from a POE to a flat coating permitting view. The design of the coatings will be informed by extensive simulation over hourly/seasonal solar changes, and changing sun/sky conditions. Full optical characterization of the transmittance and scattering behavior of laboratory scale prototypes will be carried out using a scanning gonio-radiometer and other optical assessment methods. Numerical models of the optical metamaterials will be developed to understand the interaction between the electromechanical response and changes in refractive index that create the overall optical response.

Simulation will define required performance attributes, how various coating options might be incorporated into multi-layer windows and explore new automated control systems to dynamically adjust coating properties. Lab based coating R&D would provide proof of concept demonstration that one or more optical metamaterials systems shows promise to meet redirection requirements.

Accomplishments

A dynamic POE prototype was successfully fabricated. Applying a broadly used curing protocol in silicone industry known as room temperature vulcanization (RTV), an area of 2.5×2.5 in^2 was coated with a stimuli-responsive polymer. This process enabled curing in total confinement with virtually no shrinkage and is compatible with low cost industrial manufacturing processes.
The prototype was used to collect data from goniophotometry at 10 and 40 degree angle of incident light and compared with results from theoretical simulation. The structure was simulated using Fullwave at several discrete wavelengths for different angles of incidence. All simulations were in a 2D plane corresponding to the scattering plane. The main diffraction peaks line up well between experiment and simulation. However, the experiments indicate that the produced grating is less efficient than the simulated one. Most likely this is due to higher order diffraction seen in the simulation where the coherence length is longer than in the experiment.

The grating structures were and the goniometry data collected again. On the basis of the normalized values of the specular peak, the diffraction is significantly lower altering the structures. This represents a significant data point in proving that the concept of a stimuli-responsive grating is able to modulate the fraction of incident light which is redirected. Both chemo- and electro- actuations pose significant difficulties in uniform changes throughout the entire grating structure and fully recovering into pristine state. These issues will need to be addressed with additional R&D.

LB11030

Highly Parallelized, Low-Cost Synthesis of Microbial Genes Using High-Density Oligonucleotide Arrays

Principal Investigator(s): Sam Deutsch

Project Description

The purpose of this project is to develop a high-throughput pipeline for DNA synthesis that will enable the functional characterization of large sets of genes and pathways predicted from next generation sequencing data. Deep sequencing of genomes, metagenomes and single cells, coupled with bioinformatics annotation pipelines, is revealing millions of novel genes, many with potentially useful applications in 'clean technologies'. Translating sequencing data (digital information) into biochemical molecules that can be tested for function is challenging. Synthetic biology methods can bridge the gap between digital and biological information, but these have not been implemented for large-scale functional characterization efforts due to its high cost.

We aimed to explore a number of new technologies including array oligonucleotides, Ultramer oligonucleotides, new cloning enzymologies, use of next generation sequencing for clone validation and advanced robotics, to develop a robust and low cost synthesis pipeline to enable sequence-driven gene and pathway characterization at large scale. As a proof of principle, we will apply this technology for the synthesis and characterization of genes involved in biomass degradation (200 GH1 cellulases) and bio-based chemical and fuel production (30 polyketide synthase modules) as part of the Carbon Cycle 2.0 initiative.

Accomplishments

With support from this LDRD, we have developed a fully automated, and lower cost DNA synthesis pipeline that incorporates a number of technical advances such as the use of Ultramer oligos, automated gene assembly protocols, high-throughput robotics for cloning and screening, and clone validation using a commercial sequencing platform.

We have synthesized 190 GH1 cellulases (300 Kb of synthetic sequence in total) identified from protein databases as well as from internal metagenomics sequence data, with over 65 % showing soluble expression.

Full biochemical characterization of these enzymes has been completed using using a combination of traditional and novel high-throughput assays leading to the identification of a number of robust enzymes that will be tested in an industrial setting. We have also synthesized 25 novel 8 kb modules for the biological production of biofuels, and have developed technology for generating these modules in a combinatorial fashion. Strains expressing these modules are currently being tested for alkene production.

LB10010

Predictive High-Throughput Assembly of Synthetic Biological Systems: From Gene Expression to Carbon Sequestration

Principal Investigators: Cheryl Kerfeld, Adam Arkin, Chris Anderson, Eddy Rubin

Project Description

The goal of the project is to develop methods for the design and assembly of a type of bacterial organelle, the carboxysome, with increased CO_2 fixation activity. The project is divided into two research components: the Arkin group will design and characterize controllers for gene expression, while the Kerfeld group will assemble and test various combinations of carboxysome structural components for assembly and function in cyanobacteria. The results of these studies will be combined to enable a predictive approach to design of functionally enhanced carboxysomes for specific environmental conditions. The carboxysome is the best characterized example of a bacterial microcompartment; these are naturally occurring, self-assembling organelles composed entirely of protein that confer distinctive functions on the organisms that encode them. Bacterial microcompartments are anticipated to have widespread use in synthetic biology-based approaches to engineering bacteria for the production of useful compounds. Accordingly, the methods developed for and the results of this project will be useful in the design and characterization of other types of bacterial microcompartments that can be used as metabolic modules.

Accomplishments

In the third year we have continued to obtain cyanobacterial carboxysome mutants, characterized their ultrastructure and physiology and refined methods for their genetic manipulation, including fluorescently labeling all components. These efforts were supported in part by an NSF grant (EF1105897) that was funded based on foundational studies supported by this LDRD award. One of the mutants is particularly of note in that we have shown that this previously uncharacterized carboxysome component is essential to the organelle. We identified a peptide from this protein as essential to carboxysome formation and localization. Moreover, we were able to identify specific functional regions in the protein including a domain for organizing other CO_2 fixation enzymes and a domain for adherence to the shell. These data are summarized in Kinney et al., JBC 2012. Collectively, the continued development of strains and tools will substantially enhance the genetic toolbox available for use in carboxysome engineering in cyanobacteria, thus facilitating future synthetic biology experiments aimed at expanding metabolic capabilities within this important bacterial phylum.

We have leveraged knowledge gained from this and a large scale cyanobacterial genome project led by our group (Shih et al., PNAS in press) to select 150 carboxysome genes drawn from diverse cyanobacterial genomes to obtain a JGI CSP award for DNA synthesis and synthetic operon assembly for large-scale analysis of carboxysome function. Finally, an industry collaborative research project will begin shortly that makes use of the findings and tools resulting from this project.

LB12015

Revolutionizing genome sequencing of unculturable microorganisms: Development of a high-throughput pipeline for targeted single-cell genome amplification
PI: Rex Malmstrom

Project Description: Microbial communities represent one of the largest reservoirs of genetic and biochemical diversity on the planet, and genome sequencing represents one of the most powerful tools for accessing this reservoir. However, the vast majority of microbes cannot be cultured in the laboratory, making genome sequencing impossible using traditional approaches. Single-cell whole genome amplification (WGA) allows us to bypass the culturing bottleneck by generating large quantities of DNA from only one cell. Our goal is to develop a high-throughput pipeline for generating high-quality sequencing libraries from single cells. The pipeline will also enable rapid pre-screening for cells encoding genes of interest. Briefly, the system will encapsulate individual cells into droplets and allow single-cell WGA. Droplets containing genes (and thus genomes) of interest will be rapidly identified and separated prior to full genome sequencing. Realization of this technology requires the transition of bench top chemistries to the nanoliter scale, with a primary focus on developing an effective cocktail compatible with microdroplet generation. This single-cell genomics pipeline will represent a major advancement in our ability sequence microbial genomes. The system will be integrated into the Joint Genome Institute's operational portfolio where it will be available as a unique resource for DOE researchers as well as the broader scientific community.

Accomplishments: For several years there has been a strong desire in the scientific community to improve genome amplification from individual cells using microdroplets, yet technological limitations have prevented realization of this desire. During the first stage of LDRD funding we have developed new strategies that overcome key technological hurdles. For example, we have:

- Designed and assembled a custom device for generating microdroplets
- Developed novel reaction chemistry for droplets
- Upgraded FACS hardware and operation procedures for screening and sorting microdroplets

With solutions to key challenges now in hand, we are moving forward with single-cell WGA in droplets. Over the next several months we will be optimizing procedures and assessing improvements to genome recovery that the transition to droplets should provide. In addition, we are now exploring techniques that will enable high-throughput screening of droplets.

LB12017

Computational, Data Management and Analysis Methods for the Study of a Rapidly Expanding Genome and Metagenome Sequence Data Space

Principal Investigator: Konstantinos Mavrommatis (Joint Genome Institute)

Project Description

The significant drop in the cost of sequencing with next generation technology platforms, such as Illumina HiSeq, has resulted in an exponential growth of new genome sequence datasets. However, due to the computational cost, performing comparative analysis involving a rapidly growing number of genomes and metagenomes is becoming an increasingly complex challenge. The computational, data management, and analytical challenges can be addressed by applying the pangenome construct on groups of genomes. A pangenome consists of the core part of a species (i.e. the genes present in all of the sequenced strains or of all samples of a microbial community) and the variable part (the genes present in some but not all of the strains or samples). From a data management perspective, pangenomes offer an efficient framework for handling the rapidly growing number of sequenced genomes while their analysis will help reveal genotypic and phenotypic properties across species, and track the evolution of member genomes in.

Accomplishments

The focus of our work this fiscal year has been on the determination of methods for the selection of genomes to compile pangenomes and the development of high throughput methods to generate and mine the pangenomes.

In order for a pangenome to provide biologically meaningful results, a careful selection of organisms is needed based on objective metrics that can define the similarity between the members of the aggregate group. We have developed a method and index to allow us to define groups of genomes that are close together. Following this definition we have generated more than 200 groups comprised by more than 1400 genomes that are having an index greater than 96, a value that agrees largely with the current taxonomy, however exposes some discrepancies. This allowed us to quantify the distance of genomes and correlate with the results of pangenome analysis.

The concept of the pangenome involves the identification of common (non-redundant) genes between members. We developed a method to construct gene families, which in addition splits paralogous families. Furthermore, we track the information of gene family order on the pangenome, based on their order on the individual chromosomes allowing the exploration of their spatial relationships (e.g. operons, genome rearrangements between species).

For this purpose a new representation of an organism is needed, whereby instead of the linear chromosome a genome is represented as a network of connections between gene families. The functional content, functional diversity and evolutionary history of the species can be accessed through the pangenome since it contains information about the sequences of genes and other genomic features as well as the structure of the chromosome, i.e., the order of the genes on it as well as the information about the genome and chromosome of origin. Such information can be used in a drill down operation, that will allow the identification of sequence polymorphisms using the protein and nucleotide sequence of the individual genes and chromosomal rearrangements (insertions, deletions, inversions, duplications, etc) and gene transfer between different replicons. Methods for these steps are in various levels of development.

LB11036

Transcriptome Analysis of *Agave*, a Candidate Biofuel Feedstock for Semi-Arid Climates

Principal Investigator: Axel Visel

Project Description

A future with sustainable bioenergy requires efficient biomass production from a diverse collection of bioenergy plants capable of growing in marginal environments not otherwise usable for staple food production. Agaves, perennial plants native to hot and arid regions of North America, have recently been proposed as bioenergy feedstocks for their ability to grow in environments too harsh for other bioenergy plants to survive. A principal component of *Agave* endurance of xeric conditions is due to crassulacean acid metabolism (CAM), a form of photosynthesis with low water usage and bioenergetic optimization for hot environments. While the ecology and physiology of some *Agave* species have been studied extensively, no sizeable sequence resources for *Agave* exist, hindering modern methodologies such as massively-parallel RNA sequencing (RNA-seq) to evaluate gene expression on a global scale. A comprehensive sequence dataset for *Agave* would not only enable RNA-seq for detailed understanding of *Agave* molecular and cellular biology, but also facilitate downstream applications such as marker-assisted breeding for bioenergy-optimized agaves.

The *Agave* genome is substantial (approximately 4–7 billion base pairs) and even with modern sequencing technology completing a draft *Agave* genome is a technical and financial challenge. A more rapid alternative is *de novo* transcriptome assembly, where deep sequence data from expressed genes, or transcripts, is used to build a comprehensive resource of protein-coding genes.

Accomplishments

Using RNA-seq data, we have assembled *de novo* transcriptomes for two *Agave* species: *A. tequilana*, an agave grown extensively in Mexico for tequila production, and *A. deserti*, native to mountainous regions of the California desert. Together, these two species comprise a synergistic platform for molecular studies of *Agave* and more rapid deployment of bioenergy-optimized agave cultivars. *A. tequilana* is a leading candidate for agave bioenergy, having both rapid growth and established protocols for planting, harvesting, and ethanol production; yet *A. deserti* survives extremely long periods of drought and displays remarkable thermotolerance to both cold and hot temperatures lethal to *A. tequilana*. Pursuing transcriptomics in both species allows comparative analyses potentially enabling deployment of *Agave*-based bioenergy production in a broad range of environments in the United States and beyond. Along these lines, we have teamed with LBNL scientists in EETD to explore the bioenergy potential of agaves in the United States and identify potential biological limitations of *Agave* that may be solvable through further transcriptomic and molecular investigations.

Final annotations of the *Agave* transcriptomes have been made and a manuscript documenting the agave sequence resources is nearing completion. With quality reference *Agave* transcriptomes now on hand, we have initiated a more through investigation of *Agave* transcriptome responses over time to heat and drought conditions. From these experiments, we will obtain insights into the adaptations of *Agave* to prolonged heat and drought and identify critical genes and genetic pathways responsible for responses to abiotic stress. These genes will identify potential targets for selection and improvement through standard plant breeding or genetic modification to further improve *Agave* as a reliable, domesticated bioenergy resource.

LB12023

Buchner: A Homology Independent, Computationally Efficient Method for New Enzyme Discovery.

Principal Investigator(s): Zhong Wang

Project Description

The rapid pace in microbial genome sequencing, especially deep metagenome sequencing, has enabled rapid identification of millions of genes without cultivation, thereby providing a large pool for identifying new enzymes with desirable biochemical traits. Homology based gene discovery (BLAST or HMM) with millions of genes against a rapid growing database, however, is becoming increasingly impractical due to its computational complexity.

To overcome the limitation, we developed a homology independent and computational efficient approach for gene function prediction. This approach takes the assumption that discriminative sequence features can be exploited for protein family assignment without expensive multiple alignments procedures required by BLAST or HMM. The resulting software, "Buchner", achieves not only comparable sensitivity to homology based methods, but also near linear computational performance with the growth in both queries and databases.

Accomplishments

We systematically tested Buchner for the computing efficiency and accuracy in assigning proteins to existing protein families and the ability to identify novel protein families. Starting from a subset of 1000 families having at least 1000 members from the Pfam-A database, we divided 20% of families as "new" and 80% as known protein families, and used 80% samples of known families as the training set and the rest 20% as the testing set. Frequencies of amino acid dimers with distance 0-5 were used as feature vectors. We adapted and optimized a learning algorithm based a logistic regression using a library to reduce memory consumption and maximize parallel processing.

In collaboration with NERSC (National Energy Research Scientific Computing Center), we could successfully learn 1.5 billion elements of training data in 20 minutes with less than 5GB memory requirement per process (average 480MB) using 800 processes. The average prediction accuracy among 800 families tested was 97.33%, and the time elapsed to calculate 160K records of the testing set were less than 3 minutes. For the specificity test, we examined 200K "new" sequences using learned classifiers and found that they are not likely—less than 5% chance—to be assigned into wrong families even with a liberal threshold that assigns a sequence to a family if it has 50% or greater membership probability to the family, suggesting that our method is robust to false positives while maintaining high sensitivity. Lastly, we applied genetic k-means algorithm to the sequences from "new" families and successfully assigned 70% of them correctly to the families they come from.

In conclusion, Buchner represents a computationally efficient and accurate protein function prediction method scalable to millions of genes.

LB11015

Identification and Analysis of Proteins that Regulate the Dynamic Response of Heterochromatin to Radiation

Principal Investigator: Gary Karpen

Project Description

In eukaryotes, most repeated DNA sequences are contained within heterochromatin. Due to its repetitive nature, improper repair of repeats in heterochromatin can lead to genome instability, such as aneuploidy. Our lab discovered that the initial phases of homologous recombination (HR) repair in heterochromatin are different from euchromatin; specifically, early HR events occur in the heterochromatin domain, whereas completion of HR repair requires relocalization of double strand breaks (DSBs) to the euchromatin domain. These dynamic responses are required to maintain genome stability by avoiding aberrant HR with other repeats.

The purpose of this LDRD project is to use *Drosophila melanogaster* tissue culture cells to perform an immuno-fluorescence-based genome-wide RNA interference (RNAi) screen to identify, and subsequently confirm, proteins that regulate the dynamic responses of the heterochromatin domain and heterochromatic repair foci to X-rays. The impact of RNAi depletion on heterochromatin expansion and repair foci relocalization is determined by staining fixed cells for HP1a (heterochromatin), γH2Av (general repair foci), and DAPI (DNA). We have developed custom software to analyze and interpret the images generated from this screen using the correlation between the HP1a and γH2Av signals on a pixel by pixel basis per nucleus to identify defects in the relocalization of γH2Av from the HP1a domain to the euchromatin.

Accomplishments

We have successfully screened all Drosophila genes (>15,000) and identified candidate novel regulators of the heterochromatic DNA damage response (hDDR). We have identified both known and novel genes involved in the hDDR and the proper localization, recruitment and/or maintenance of heterochromatin and repair foci. Another important accomplishment has been development of computational tools necessary to extract data from this image-based screen, which will facilitate analysis of future genome-wide screens performed by our lab and the community. Our software is now able to characterize 39 unique imaging features on a per nucleus basis, and to use this information to identify the most promising candidates.

We have focused on further characterization of select candidate genes in order to gain a deeper understanding of the molecular mechanisms that regulate the formation of heterochromatin and the response of this domain and DSBs to radiation. For example, we have shown that a previously uncharacterized protein regulates heterochromatin formation in a dose-dependent manner: too little CG8108 results in abnormal increases in the amount of heterochromatin in the nucleus, whereas the consequence of excess protein is reduced heterochromatin. Interestingly, this protein physically interacts with a key heterochromatin component, and preliminary studies suggest an association with both the nuclear matrix and RNA. These findings have revealed an unexpected connection between nuclear architecture, heterochromatin formation, and the hDDR. We expect to submit a manuscript describing the screen, and the characterization of the previously uncharacterized protein and other identified regulators, by early 2014. Meanwhile, we have used the findings from this LDRD project, combined with other results, to obtain an NIH R01 grant that will support continuation of this project for 4 years.

LB11016

Effects of low dose radiation on communities of epithelial cells as a function of age
Principal Investigator(s): Mark LaBarge

Project Description

The purpose of this project is to determine how gamma radiation exposure impacts the cell fate decision process and rudimentary tissue-level organization in a normal human bilayered epithelium. This was a continuation of my FY2011 start-up/proposal, in which we were developing the functional cell screening technology platforms to study cell-radiation interactions in the contexts of microenvironment and tissue-level organization. Specifically we are developing assays to determine the functional effects of low dose radiation (LDR) on normal human mammary epithelial cell (HMEC) physiology as a function of patient age. To do so we are utilizing a unique and well-characterized resource of over 47 finite-life span HMEC strains, derived from women aged 16 to 91 years, together with three cutting-edge functional assay platforms, which enable measurement of responses to combinatorial microenvironments, to elastic modulus, and measurement of the ability to self-organize into epithelial bilayered tissues. It is particularly important to understand the effects of LDR (defined as ≤10cGy at a rate of ≤0.1cGy/day) on patients already in higher-risk categories for diseases, and age is the greatest risk factor for all solid cancers; 75% of new breast cancer diagnoses are made in women over 50 years old.

Accomplishments

We significantly changed our understanding of the processes and mechanisms by which human mammary epithelia maintain normal organization, and we have established a putative screening system for identifying environmental toxins (e.g. chemicals, radiation) and pharmaceuticals that can alter tissue-level organization. Prior to this work, our entire understanding of how different types of cells organize into a cohesive tissue was based on experiments with pond-dwelling organisms and engineered cell lines not reflective of in vivo. Manipulation of surface chemistry of the microwell assay and modulation of the polymer stiffness revealed that normal self-organization of mammary epithelia not only requires cell-cell contact via E-cadherin, but that associations between the myoepithelial (outer layer) cells and ECM through integrins also is required. We demonstrated that by altering the microenvironment allows exquisite control of tissue organization. Conversely pharmacologically controlling a cell's perception of the environment also can control tissue organization. Commercially, this assay system represents a robust method for quantifying the effects of different agents on tissue-level organization, which is important as loss of tissue organization can unleash pre-malignant cells into a fully malignant state. Scientifically, this work expands our understanding of basic mechanisms that tissues use to form asymmetry and to organize.

LB10013

Identification of genetic networks controlling susceptibility to radiation-induced carcinogenesis
Principle Investigator: Jian-Hua Mao

Project Description

Biological responses to radiation exposure – DNA damage and tumor development - are controlled by a multiplicity of genetic factors, most of which remain unknown. The overall goal of this project is to exploit the power of mouse genetics, together with novel developments in genomics to identify genetic networks that confer resistance or susceptibility to radiation-induced DNA damage and tumor development. The identification of human homologues of these predisposition genes and discovery of their roles in carcinogenesis will ultimately be important for the development of methods for prediction of risk and prevention for human cancers after relatively high doses of radiation used to treat diseases in the clinic.

We will use a Systems Genetics approach to identify the main features of the genetic architecture of gene expression in the normal thymus, and to characterize the changes in this architecture that take place during perturbation by radiation or tumor induction in mouse inter-species crosses. We will use a genetic approach that exploits the genetic and phenotypic diversity in mouse inter-species crosses, to examine the effects of radiation in different genetic backgrounds. We will characterize gene expression in normal thymus from interspecific backcross animals to identify genetic variants that control gene expression in the normal unperturbed thymus. These gene expression networks will provide the basis for investigation of the changes induced in mouse thymus by treatment with radiation, and of the relationship of these changes to lymphoma susceptibility. These data will be integrated with QTL analysis of susceptibility to radiation-induced genomic instability and lymphoma. In addition to these analyses of the relationship between germline polymorphisms, gene expression, and lymphoma susceptibility, we will identify allele-specific somatic changes in radiation-induced lymphomas from a population of interspecific backcross mice using a combination of array CGH and genotyping. Linkage to specific genetic changes, or preferential gains or losses of parental alleles will identify candidate susceptibility genes. These data will provide a comprehensive picture of both the somatic genetic events and the genetic susceptibility factors that contribute to the genesis of lymphomas induced by radiation.

Accomplishments

Our most significant accomplishment is that we have completed F1Bx mice that have been subjected to a single dose of 4Gy whole body x-radiation and are being monitored for tumor development. Most of them have developed thymic lymphomas. So far we have collected about 150 thymic lymphomas and some other tissues including tail, lung, liver, kidney and spleen, and have stored them in a tissue bank. Less than 20 mice are being still monitored for tumor development that will end at the beginning of 2013. The tail DNAs from all F1Bx mice have been made. All of them have been proceeded for SNP genotyping by Illumina Mouse LD Linkage panel that contain an optimized of 377 loci in mouse genome. In addition, the total RNAs have been made from thymuses for gene expression analysis using Affymetrix platform. We anticipate being awarded new funding to continue the analysis of gene expression networks for the normal unperturbed thymus and to characterize the changes in gene expression networks that take place during perturbation by radiation and to support the analysis of thymic lymphomas LOH, CGH, gene expression micorarray. I have resubmitted one R01 grant to NCI in November, 2012 and hope to get this fund to support and continue the study.

LB11045

Modeling Desert Soil Crust Microbial Community Responses To Pulsed Climate Events.
Principal Investigator(s). Trent Northen

Project Description

Our overall goal is to provide fundamental insights into the synchronization between pulsed activity events (e.g. precipitation) and soil microbial community activities. This will contribute significantly to unraveling key mechanistic aspects of biogeochemical carbon (C) cycling in soils utilizing a tractable environmental system, desert biological soil crusts (BSCs), and will explore for the first time the relationship between altered environmental factors and the "system" metabolic response. This comparatively simple soil system will allow us to evaluate if the "system" responses of natural communities can be recapitulated in minimal microbial consortia, thus helping to define the *minimal level of microbial interactions* that are required to explain carbon cycling behavior, and by extension the critical, sufficient, redundant and expendable components in the biogeochemical machinery of a biological soil crust system.

We are applying integrated biogeochemical, microbiological, genomic and metabolomic approaches to define alterations in carbon cycling and community structure in response to climate changes. Field samples are utilized for laboratory experiments to study the community response to a simulated rainfall event. Here, light (bacterial dominated) crust samples are monitored for liquid and gas composition and samples are collected before and over the course of a three day time-course following a simulated pulsed wetting event. The resulting samples are analyzed for biogeochemical composition, metabolomics, (meta)transcriptomics and (meta)genomics to address the critical question of how the BSC 'poises' its metabolic state such that it can be activated by a wetting event following prolonged dormancy.

Accomplishments:

To elucidate the key events involved in soil carbon cycling in response to pulsed activity events we performed a wetting experiment of a BSC and followed the response of the communities primary producer, the cyanobacterium, *Microcoleus vaginatus, in situ* using a whole-genome transcriptional time-course that included two diel cycles. Immediate upon wetting of the dried soil we observed a transient induction of DNA repair and regulatory genes signaled the pulsed activity event. Recovery of photosynthesis occurred within one hour, accompanied by up-regulation of anabolic pathways. Well-characterized processes were observed during hydration that reflected concurrent biogeochemical measurements. Onset of desiccation was characterized by the induction of genes for oxidative and photo-oxidative stress responses, osmotic stress response and the synthesis of C and N storage polymers. Interestingly, many genes were found to follow a 'desiccation cycle' with increase upon drying and decrease upon wetting. Many of these are consistent with what would be required to anticipate wetting. Overall, these data highlight the synchronization between this cyanobacterium and its environment, and provides key mechanistic insights into its metabolism *in situ* that may be used to predict changes in soil carbon cycling in response to climate perturbations.

We have now isolated dozens of other bacteria from this community and plan to use these to investigate tropic interactions with *Microcoleus vaginatus* as informed by meta-transcriptomic samples collected over a wetting event and being sequenced at JGI.

LB11033

Enabling structural systems biology at ngls
Principle Investigator: John Tainer

Project Description

After decades of synchrotron biology and accelerating genomics (major DOE accomplishments), the next decade will increasingly harness the power of 3 billion years of evolution knowledge written in gene sequences that will require structures to understand. The next generation light source (NGLS) in planning phase at LBNL, should be a major part of this process. NGLS is predicted to deliver 36 trillion pulses per hour. A human cell contains approximately 4 trillion proteins and microbial cells far fewer. Thus the scales are complimentary. We propose to develop technologies to improve the tractability of the NGLS as a probe of all macromolecular structures within cells by both 1) extending the heterogeneity tolerated by experiments and 2) improving native purification strategies. Several analysis strategies have been proposed which reconstruct macromolecular structure from snapshots of a small number copy of the macromolecule. We will utilize these evolving analysis tools and develop an expanded experimental and analysis framework for the characterization of individual structures from a heterogeneous population. We will also innovate fractionation and nanofabrication methods that move towards tractable homogeneity from small quantities of cells. By pushing these limits on complexity and sample preparation from both ends, we will attract the attention of the biological community and develop revolutionary biological capabilities for the NGLS.

Accomplishments

Small angle X-ray scattering (SAXS) in the planned next generation light source will provide data from sub-microliter volumes of sub-microgram quantities on sub-second data collection times. These qualities are transformative in structural biology as current SAXS is sample limited and structural results are far outpaced by the rate at which new targets are being identified through genomics. At NGLS biological sample size will decrease sharply while throughput will increase. Capitalizing on these capabilities requires high-throughput and comprehensive structure evaluation methods. We have developed a Structural Comparison Map (SCM) which objectively assesses similarity among macromolecular states from SAXS signals. Through our maps built with SAXS data we provide a comprehensive perspective on the functional conformations connecting structures to biological outcomes. Our SCM approach is currently under review at the journal Nature Methods.

A primary system of interest in our laboratory has been gold nanocrystal end-labeled DNA molecules. The manipulation of DNA is of critical importance for cellular function. The gold nanocrystal scatter 1000 times greater than proteins of similar size. At the NGLS the molecules may be used to report on much smaller populations informing on conformations adopted by individuals. The higher fluxes will enable very precise time resolved measurements. The anomalous effects will enable the identification of signals from the gold labels in quite complex environments like those within a cell. The analysis tools developed will be applicable to the other elements. A particular target is distinguishing the structural distribution of Nitrogen from Phosphor in membrane protein imbedded in a phospholipid membrane.

Over the course of the last several years we have improved upon the synthesis, data collection and analysis of SAXS data from the gold labeled systems. We have provided novel insights on the mechanism of the repair of mismatched bases in duplex DNA. DNA base pair mismatch errors are common in DNA replication and must be repaired for genomic maintenance. The first enzyme to recognize a mismatch (MutS) has been shown to bend DNA at mismatch sites. The mechanistic influence of such bending has been shrouded in controversy with multiple techniques providing conflicting evidence. Our work has been prepared for submission in the Proceedings of the National Academy of Sciences. Because of our systems importance to human health, its scattering power advantage over typical biological material and our detailed understanding from conventional SAXS we expect to be competitive for a free electron laser proposal wherein we will test our developed analysis tools.

LB10035

Multinozzle Arrays for Single Cell Metabolomics

Principal Investigator(s): Daojing Wang

Project Description

The purpose of this project is to develop breakthrough multinozzle array-based nanoelectrospray ionization mass spectrometry for single cell analysis particularly metabolomics and proteomics. Cellular heterogeneity arising from stochastic expression of genes, proteins, and metabolites is a fundamental principle of cell biology, but single cell analysis has been beyond the capabilities of 'Omics' technologies. This is rapidly changing with the recent examples of single cell genomics, transcriptomics, proteomics, and metabolomics. The rate of change is expected to accelerate owing to emerging technologies that range from micro/nanofluidics to microfabricated interfaces for mass spectrometry to third- and fourth-generation automated DNA sequencers. Single cell analysis is the new frontier in Omics, and single cell Omics has the potential to transform systems biology through new discoveries derived from cellular heterogeneity.

However, single cell proteomics and metabolomics present unprecedented challenges. There is a great need for further improvement in miniaturization, integration, and detection sensitivity. There is also a great need for automation, throughput, and bioinformatics to study multiple individual cells to achieve statistical significance.

We propose to develop silicon-based multinozzle arrays and demonstrate their proof-of-principle applications in single cell analysis using mass spectrometry. Specifically, we will fabricate prototype multinozzle arrays, measure their physical characteristics, perform surface derivatization, and demonstrate their proof-of-principle applications in mass spectrometry analysis of small amounts of biological samples.

Accomplishments

We have made important progress for the project this year. This was built upon our breakthroughs in the last two years. Among them is a major publication in 2011: Mao P., Wang H.T., Yang P., and Wang D.*, "Multinozzle Emitter Arrays for Nanoelectrospray Mass Spectrometry," (2011) *Analytical Chemistry,* 83(15), 6282-6289. PMCID: PMC3146565. The MEA technology reported in the paper has won the prestigious 2012 R&D 100 Award. In 2012, our most significant accomplishment has been to have another major paper accepted in December 2012: Mao P., Gomez-Sjoberg R., and Wang D.*, "Multinozzle Emitter Array Chips for Small-Volume Proteomics" (2013) *Analytical Chemistry,* ac3032965, published online as Just Accepted Manuscript on 12/19/12. In this paper, we report a novel silicon-based microfluidic device, multinozzle emitter array chip (MEA chip), as a new platform for small-volume proteomics using liquid chromatography-nanoelectrospray ionization mass spectrometry (LC-nanoESI-MS). We demonstrate parallel, on-chip, and on-line LC-MS analysis of hemoglobin and its tryptic digests directly from microliters of blood, achieving a detection limit of less than 5 red blood cells. Our MEA chip will enable clinical proteomics of small-volume samples. Berkeley Lab has filed patent applications for the above-mentioned technologies. In summary, we have made significant achievements in this LDRD program. We have developed breakthrough and commercially-relevant technologies, namely, the robust silicon-based MEA chips for nanoelectrospray mass spectrometry, which open up the possibility of a fully-integrated microfluidic system for ultrahigh-sensitivity and ultrahigh-throughput proteomics and metabolomics of small-volume biological samples down to single cells.

LB12025

Project Title: Self-Assembled Battery Electrodes

PI: Nitash Balsara; Co-PIs: Miquel Salmeron, David Prendergast, Jordi Cabana

Project Description

This project is aimed at determining the molecular structure of species at electrified electrode interfaces. This is an important and poorly known aspect of materials science, relevant to electrochemistry, batteries, photocatalysis, and solar synthesis of chemical fuels. We aim to study adsorption, structure, intercalation and diffusion reactions of species near electrode interfaces. We have focused on S_x^{2-} (x=2, 4, 6, 8) and Li^+ in solid electrolytes. Experimentally determined X-ray absorption measurements are compared with theoretical spectra based on a combination of molecular dynamics and quantum mechanics. This combination of approaches provides fundamental insight into the underpinnings of the redox chemistry of lithium-sulfur cells. This chemistry is of considerable importance because the theoretical energy density of lithium-sulfur cells is greater than that of current lithium-ion cells by a factor of about four.

Accomplishments

Computer simulations successfully showed the correspondence between coordination of the ions of interest with electrolyte molecules and X-ray absorption. In particular, interactions between the lithium ions and the ether oxygens in the electrolyte result in a simulated XAS spectrum that exhibits significant broadening of the main-edge and pre-edge features induced by broken octahedral symmetry at finite temperature. Experiments have confirmed the presence of these features in the measured spectra. Computer simulations have also provided surprising insight into the reason for the increased solubility of the S_x^{2-} polysulfide anions with increasing *x*. We have shown that solubility is enabled by entropic reasons. This is surprising because the entropy of uncharged chains decreases with increasing chain length. It appears that the opposite is true of the charged S_x^{2-} chain.

We have made significant progress on instrumentation for studying electrified sulfur electrodes. Methods for depositing thin and uniform S films on Au and Si by solution casting and by electrolytic decomposition of Ag_2S have been established. The electrochemical cell for *in situ* X-ray absorption studies has been built and tested. An electronic filter/chopper combination for separating the modulated electron current from the much larger Faradaic current due to electrochemical reactions has been built and tested. X-ray Absorption experiments have been conducted that show the evolution of the spectral signature in the S K-edge due to different content of S in Li2Sx, with the appearance of a low energy satellite that increases in intensity as x decreases from 8 to 2, both in SEO and PEO polymer electrolytes. Our calculation show that this is due to the changing charge distribution along the chain. Corresponding changes in the spectral signature of the O and C K-edges was observed in SEO and PEO. These results are providing an understanding of the chemical evolution of the electrolyte when polysulfides are dissolved into it as it occurs during the charging cycles.

Partial funding for the work on the redox chemistry of sulfur was obtained from the BATT Program of the DOE. Funding from the recently approved Battery Hub (JCESR), while unconfirmed yet, is expected in the coming years.

LB12032

Ultrafast Spin and Magnetization Dynamics in Nanoscale Magnetic Structures
Principal Investigator: Jeffrey Bokor

Project Description

One purpose of this project is the creation of new capabilities at the PEEM3 beamline at the ALS for time-resolved studies of magnetization dynamics on the ~100 ps time scale, with a view towards laying the foundation for sub-ps time scale study of spin dynamics at the NGLS. There are a number of experiments envisioned for this capability. One goal is to study the dynamics of closely coupled, interacting nanomagnets following full switching to the hard axis. This fundamental study lays the groundwork for a new way of processing information at ultra-low energy dissipation. A second goal will be to characterize the switching dynamics of the multiferroic material bismuth ferrite in order to understand the detailed nature of the origin of electric field control of magnetism in this complex oxide material. More generally, the dynamics of magnetoelectric composites and their potential for voltage control of magnetism for energy applications will be studied. Finally, the phenomenon of ultrafast magnetization dynamics triggered by femtosecond laser excitation will be generalized to investigate the creation of nonequilibrium electron distributions in magnetic materials by purely electrical hot electron injection across Schottky barriers. This overall effort, in turn, is intended to lead to a program at NGLS to study fascinating open questions in ultrafast magnetization dynamics in magnetic and ferroelectric materials triggered by excitation of nonequilibrium electronic states using both laser and direct electrical excitation.

Accomplishments

The initial effort in this project was devoted to the design, construction, and testing of the high speed circuit to be incorporated into the PEEM-3 sample holder, and the laser system and electronics that are used to trigger and synchronize the current pulse to the synchrotron x-ray pulse. Technical constraints imposed by the design of the PEEM-3 chamber and sample transfer system lead to the inevitable conclusion that the circuit must be electrically isolated and optically triggered. A low power, high-speed laser diode is mounted to the outside of one of the PEEM vacuum chamber windows. The laser pulse is aligned and focused onto a high-speed photodiode on the sample holder that then triggers the circuit which delivers the current pulse to the sample.

Work proceeded at a fast pace in order to get ready for scheduled beam time during 2-bunch mode operation at the ALS in mid-March 2012. We succeeded in building this sample holder and fabricating nanomagnet samples in time for the run in March. Our first samples were linear chains of interacting rectangular single-domain nanomagnets fabricated on top of the copper line carrying the current pulse to trigger the magnetization dynamics. The goal was to observe the magnetization rotate by 90º to the shape hard axis of the magnets during the current pulse, and then observe the dynamics of the magnetic relaxation of the interacting magnets after the current pulse terminated.

During the March run, we succeeded to get all key elements of the experiment to work. That is, we could align the sample for magnetic contrast imaging in the PEEM, align the laser beam onto the photodiode detector, find the “time zero” delay when the electrical pulse and the x-ray pulse were perfectly synchronized on the sample, and then take magnetic contrast images as the electrical delay between the x-ray pulse and the electrical pulse was varied. Unfortunately, outgassing from our complex sample holder led to rapid carbon buildup on our sample during x-ray exposure, leading to poor quality images. An improved version with better materials has been built and is ready for use during our next 2-bunch run in Spring 2013.

LB12033

Template Assisted Assembly of Monodisperse Discotic Phases as Highly Tunable Electronic Materials

Principal Investigator(s): Felix Fischer

Project Description

The increasing importance of functional materials based on organic molecules for applications in electronics/computing, miniaturization of sensory devices, and energy production is well recognized. While the structure of these materials can conveniently be fine tuned at the molecular level many of the relevant electronic properties such as the charge carrier mobility, the absorption profile, and the exciton diffusion length directly depend on quantum-mechanical boundary conditions imposed by the random assembly of nanometer scale domains. A central challenge in the field of organic electronic materials is the control of the structure of nanometer size domains with atomic precision. We herein explore the potential of using template assisted self-assembly to control the formation of unambiguously defined monodisperse discotic phases. From the study of these supramolecular model systems both in solution and in OPVs/OFETs we seek to uncover structure-performance relationships and new assembly strategies that improve the performance of bulk organic electronic devices.

The use of template assisted self-assembly of discotic materials will allow for an unprecedented control of stacking order in all three special dimensions. The resulting functional materials are essentially monodisperse, providing for a highly reproducible performance and sensitivity. We seek to explore structure-function relationships that will provide the tools to rationally design desired photo– and electrophysical properties into organic materials. The highly modular solution-based synthesis provides for the facile introduction of diversity and meets the requirements for swift scale-up of the production of promising materials.

Accomplishments

Our most significant accomplishment has been the development of a synthetic strategy that can be used to direct the self-assembly of discotic chromophores into columnar arrays ranging in length between 1-3 nm. Our approach takes advantage of π-π stacking interactions to assemble the discotic materials inside a covalently linked molecular cage. This strategy allows for the asymmetric functionalization of both ends of the discotic stack required for the highly ordered assembly into larger well-defined hierarchical structures. We are confident that our synthetic methods can be expanded to the assembly of larger discotic building blocks.

We have also been able to introduce anchoring groups into the periphery of the host structure that direct the deposition of the discotic columns onto solid supports. Preliminary results of monolayers on atomically flat surfaces have been studied using atomic force microscopy (AFM).

We are currently using this newly developed system to explore the influence of stacking length and order on the charge transport in monodisperse discotic phases.

LB11013

Attosecond XUV Condensed-Matter Science: Electronic Wavefunction Coherence and Correlated Dynamics

Principal Investigator(s): Robert A. Kaindl, Predrag Ranitovic, and Zahid Hussain

Project Description

The purpose of this project is to directly probe coherent electron dynamics in solids on the attosecond time scale for the first time. On such extremely short times, the effect of light waves on the material can be directly observed with sub-cycle resolution, yielding a measure of the time-dependent perturbation and evolving coherence. Using XUV attosecond pulses, we can apply photoelectron spectroscopy to access the dynamics of transient electronic states. Such studies can provide insight into a host of condensed matter processes, including charge transfer dynamics, quantum kinetics, high-field transport, and correlation timescales. In this way, this work will help establish a new experimental technique to investigate condensed-matter processes on the shortest timescales.

In solids, the eV-scale electronic excitations are fundamentally linked to an ultrafast dynamics of the electron wave functions that evolves on the attosecond time scale. Our approach to study this physics employs a customized scheme that combines few-cycle optical light fields, attosecond XUV pulses, and momentum-resolved photoelectron spectroscopy. In this project we take advantage of a laser-based source of attosecond XUV pulses to develop a unique attosecond condensed-matter UHV chamber and associated timing interferometer. We aim to apply this instrumentation to novel types of experiments that can access the attosecond and few-fs coherent dynamics of electronic wavefunctions, non-equilibrium electronic structure, or field-induced carrier acceleration.

Accomplishments

Up to now, we have completed the construction and optical alignment of the complex condensed-matter attosecond instrument, which combines tunable IR streak-fields and attosecond XUV pulses for time-resolved studies of solids. In our approach, a customized ultra-high vacuum chamber delivers the sample environment necessary to study intrinsic condensed-matter processes on clean surfaces, while attosecond timing between the infrared streak field and isolated XUV attosecond pulses is provided in a separate vacuum chamber. In particular, we overcame the large pressure gradient ranging from 100 Torr at the laser-generated XUV source down to 10^{-10} Torr at the sample location via multi-stage differential pumping in four separate regions. Moreover, precise time delay was implemented and demonstrated with an external piezo-controlled optical interferometer based on the Pancharatnam-phase design.

Optical alignment of the complex setup has been performed, resulting in the successful delivery of attosecond XUV pulses onto a solid-state target in the UHV chamber. For this purpose, the broad spectrum of the attosecond pulses was measured with a XUV spectrometer that we custom built. The spectral width, energy position, and XUV harmonics structure was optimized by varying the stabilized carrier-envelope phase of the intense few-cycle driving pulses. Importantly, photoemisson using the attosecond XUV pulses was successfully demonstrated with both a time-of-flight analyzer and hemispherical analyzer. The latter allows for energy and momentum resolved studies, which together with the XUV attosecond source provides for a unique combination for resolving condensed-matter attosecond dynamics. Having completed the alignment and also prepared nano-structured samples for initial studies, we are now working towards first experiments of attosecond coherent electron dynamics in solids.

LB11014

Ultrafast 2D Fourier-Transform Spectroscopy of Electronic Dynamics in Photovoltaic Nanomaterials

Principal Investigator(s): Robert A. Kaindl, Jeff Urban, Emory Chan, Robert W. Schoenlein, Lin-Wang Wang

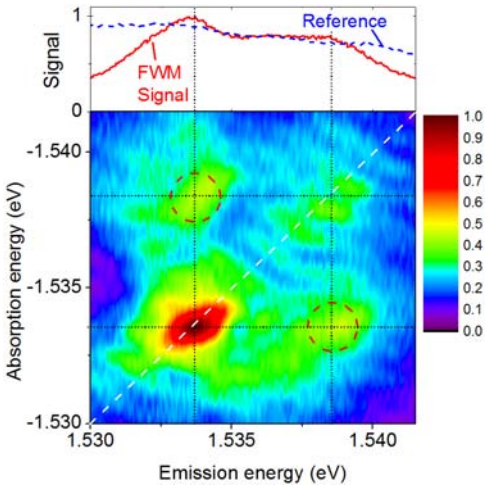
Project Description

This project aims to study the ultrafast dynamics of complex semiconductor nanostructures relevant for photovoltaics using broadband 2D Fourier-transform spectroscopy (2D-FTS). While nanoscale heterostructures offer important new routes to exciton creation, coupling, and rapid charge separation as essential components of efficient photovoltaics, their dynamics is presently only poorly understood. Conventional pump-probe studies are hampered by broad optical features, making it difficult to isolate specific energy eigenstates and couplings. In contrast, we pursue broadband 2D-FTS that can reveal coherent and incoherent dynamics in multi-component optical spectra, for insight into exciton creation, energy transfer and directed charge separation.

Our approach is based on an ultrafast laser source with broad tunability in the visible and near-IR combined with a customized 2D-FTS interferometer developed in the project. This is closely coupled with advanced synthesis and ab-initio theory to calculate exciton states, exciton-exciton interactions and wavefunctions. We intend to first demonstrate our method using type-I and type-II multi-component semiconductor structures. These initial experiments can provide insight into charge separation dynamics, and will be expanded to a larger set of nanoscale materials and physics, to study e.g. high-energy carrier relaxation in nanorods, coherent exciton coupling in superlattices, or electron transfer in photocatalytic structures.

Accomplishments

We have completed construction and alignment of the 2D-FTS instrument for coherent multi-dimensional spectroscopy and verified its applicability in first ultrafast studies. The complex setup incorporates four interleaved interferometers with precise time delays, which we successfully stabilized. Using a new digital feedback scheme, reproducible motion over many thousands of optical cycles was demonstrated along with precise manipulation of the optical phase using a phase-cycling technique. We also developed computer algorithms for constructing two-dimensional 2D-FTS spectrograms from the collected time-domain data.



Mutual exciton level couplings (off-diagonal) in our 2D-FTS setup

First ultrafast studies to demonstrate 2D-FTS with this setup were carried out on photogenerated electron-hole pairs in 14-nm wide GaAs quantum wells. An example rephasing spectrogram (see figure) clearly indicates the couplings between light- and heavy-hole excitons, and separates homogeneous from inhomogeneous broadening of the resonance features. From the dynamics of such spectrograms, we can track coherent and incoherent exciton dynamics on the femtosecond timescale. This novel capability is now ready to be applied to study electronic dynamics in nanoscale heterostructures, where initial work can focus on charge separation in core-shell nanocrystals and electron transfer in seeded rods.

LB11026

Probing and Controlling Spin and Charge in Strong Spin-Orbit Materials

Principal Investigators: J. Orenstein, J.E. Moore, A. Vishwanath, R. Ramesh, A. Lamzara

Project description

Purpose/Goals: The recent discovery of "topological insulators" creates the opportunity to design and synthesize new materials with highly desirable properties. Topological insulators (TI's) are a new class of materials whose electronic states are distinct from the states that are accessible to free electrons, much as a donut is topologically distinct from a sphere. The incompatibility of states inside and outside the material leads to a topologically protected two-dimensional metal at the interface.

Approach/Methods: The TI's that have been identified and synthesized to date are very simple materials with very weak electronic correlations. As such, they do not support other phases, such as magnetism and superconductivity. On the other hand, the theoretical work on this subject indicates that the potential for novel device structures can only be realized if TI's can either exhibit such phases, or be interfaced with other superconducting and/or magnetic materials. The approach taken in this project is to focus on materials that are based on oxides of iridium. These materials are predicted to be TI's with strong magnetic interactions.

Accomplishments/Theory

Strongly coupled spin orbit systems were studied, in particular novel phases that might arise in iridium oxides, where strong spin orbit coupling coexists with electronic correlations. These include Weyl semimetals, which are predicted to be realized in pyrochlore iridates and exhibit unusual phenomena like Fermi arc surface states as well as unique transport properties. Unusual types of topological superconductivity are also predicted on doping Mott insulators with strong spin orbit coupling. In addition, a theory was developed that showed how the unusual topological surface states of the topological insulators bismuth selenide and bismuth telluride, which are widely used as thermoelectrics, might be used to improve thermoelectric performance, particularly at low temperatures.

Accomplishments/Experiment

Work has proceeded on the synthesis of iridates in thin film and crystalline form. To date, thin films of Sr_2IrO_4 and $SrRuO_3$ have been synthesized and characterized by transport and magnetic measurements. A remarkably strong modulation of the conductivity of $SrRuO_3$ films with lattice strain imposed by the substrate has been observed. In collaboration with a team at the Advanced Light Source, infrared transmission has been performed on b and the spectra thus obtained show clear evidence of the large spin-orbit interactions that are needed for TI materials.

LB12019

Electron Microscopy With Vortex Beams Carrying Orbital Angular Momentum

Ben McMorran, Peter Ercius, Martin Linck, Stefano Cabrini, Andreas Schmid

Project Description

Materials directly involved in the Earth's carbon energy cycle are predominantly composed of light elements – "soft matter" such as biological tissue, macromolecules and polymers. Soft matter is difficult to analyze by transmission electron microscopy (TEM) because light elements do not efficiently scatter electrons and none of the conventional methods is capable of producing atomic resolution images for detailed studies of soft matter. A novel class of electron beams with quantized orbital angular momentum (OAM) have recently been demonstrated by several groups. These beams, composed of free electrons with helical wavefunctions, are analogous to widely used optical vortices in beams of light. Utilizing recent advancements in nanofabrication methods, we are creating special diffraction gratings for electrons, which enable us to adopt coherent wavefront engineering techniques from light optics to prepare electron OAM beams. In an electron microscope, these beams can be focused and scanned over a sample, revealing new dichroism and phase contrast signals that can provide more information about the sample's structure or magnetic properties. This development of spiral phase electron microscopy (SPEM) allows us to enhance capabilities for (a) imaging atomic magnetic moments and (b) enhancing contrast and resolution in soft matter imaging.

Accomplishments

In Year 1 of this LDRD we developed the fabrication of electron diffractive optical elements (holograms) and we implemented these diffraction elements in our electron microscope equipment. Successful demonstration of electron beams with orbital angular momentum lays the foundation for establishing novel imaging techniques. Prototype apertures were produced at the MF and Oregon, and helical probe beams have been demonstrated in a conventional TEM. We have used our instrumentation and infrastructure to fabricate the largest holograms (80 μm diameter area) with the smallest features (50 nm) to date. A custom condenser aperture assembly has been produced and equipped with several diffraction gratings. Our proof-of-principle experiments and simulations demonstrate the potential capabilities of . Fig. 2 shows how spiral phase contrast can be used to measure the simple distortion of curved wavefronts in a diverging electron beam. Fig. 3 shows a simulation of different imaging methods of a biological object: the phase shift of a bacterium model in vitrified ice has been calculated and propagated through the TEM using different contrast mechanisms. Evidently, the spiral phase contrast method offers superior contrast over existing phase plates. (Note: this LDRD continues for a second year.)

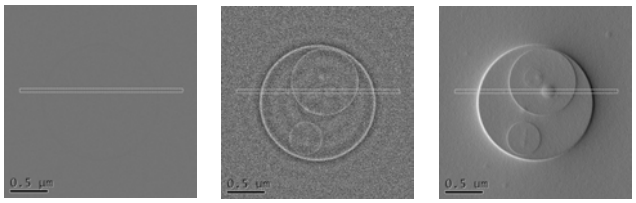


Figure: Simulated phase contrast imaging of a *Spirochaeta coccoides* bacterium in vitrified ice. (left) The in-focus TEM image is blind for the electron phase shift. Instead contrast is dominated by inelastic scattering, which is very weak due to the light elements. (center) Modern phase imaging techniques such as the Boersch phase plate reveal some phase structure, however the contrast is very limited. (right) The spiral phase contrast technique boosts edge contrast and allows imaging of weakly scattering objects with unprecedented quality. Even the smallest object features, not seen with the Boersch phase plate, appear with reasonable contrast.

LB12028

Exploiting Nanowire Surface States for Solar-Spectrum-Matched Plasmon-Enhanced Water Splitting

Principal Investigator(s): P. James Schuck, J. B. Neaton, J. J. Urban, A. Schwartzberg, S. Aloni

Project Description

Photogenerated fuels are an essential part of our nation's future energy portfolio. Within this context, direct photo-electrochemical water splitting is being widely pursued through various technologies, all searching for novel materials with optoelectronic properties that both match the solar spectrum and provide appropriate over-potentials for driving electrochemical processes. These contradictory requirements make the search incredibly challenging, and so far there are no clear winning technologies. Current methods of water splitting mostly utilize large bandgap materials that absorb a fraction of the solar spectrum, rendering them inefficient for large-scale solar fuel production. This work describes a completely new approach based on semiconductor mid-gap surface (and defect) states, which provide greater solar spectrum overlap, efficient voltage offsets, and play a vital role in charge transfer at the liquid interface. Here, we propose the integration of plasmonic nanoparticles and III-Nitride nanowire cavity structures to enhance mid-gap state absorption and overcome many of the current difficulties in water splitting. These device structures make use of an abundant, easy to mass-produce, inert semiconductor (GaN) possessing desired bulk surface, optical and electronic properties. This solution, if successful, will significantly advance and alter the solar fuel generation landscape by greatly enhancing the rate and efficiency of direct photon-to-fuel conversion.

Accomplishments

In the first year of this project, we have taken a systematic approach, concentrating on the theoretical investigation of GaN surface states and on growth of NW substrates with controllable surfaces. On the theory front, we have had significant success in understanding the origin and properties of GaN surface states as a function of specific crystalline face, surface termination, and surface adsorbates. We have successfully calculated the energetics of the GaN (11-22) surface. Of particular note, the calculations showed that a significant density of mid-gap states (i.e. those with energies that best match the solar spectrum) are *associated with the (11-22) surface*. Next, (11-22) surface energies were calculated as a function of Au coverage, which led to the important finding that the metal-GaN interface is sharp, i.e. - the GaN surface is not corrugated by the presence of Au, and the nature of the surface state does not change with Au coverage. Together, these pieces of information have led us to initially concentrate on the (11-22) face in our growth and experiments, as they suggest that this surface may be well-suited to plasmon-enhanced absorption and PEC activity at the relevant wavelengths.

To this end, our growth and structural characterization efforts have yielded GaN NWs and thin film substartes with a variety of crystal faces, surface terminations and doping. We have demonstrated reliable growth of NWs with triangular crossections. These wires' surfaces are the (0001), and (11-22) or (10-11) faces, depending on the catalyst used for their growth. Moreover the wires are supported by a few 100's of nm thick thin GaN film providing an easy way to contact the monolithic nanowire array. We are currently preparing a manuscript describing these results.

LB12031

Electrically Created Fuels

Principal Investigator: Eli Yablonovitch
Other Participants: Prof. John Newman and Mr. Joseph Thurakal

Project Description

There has been tremendous progress in photovoltaics. The real cost per Watt has dropped by 30× in the past 30 years, and the efficiency for a single-junction, thin-film, cells is now approaching 30%. A learning curve analysis suggests that costs will continue to drop over the next 10 years. The issue then arises, what we will do with the excess solar electricity that will be generated at mid-day in the summer months?

In this LDRD project, we recognized that storage of the electrical energy would ultimately have to be seasonal as well as day/night. Seasonal storage of fuels is a well-developed, low cost, industry. The challenge then becomes how to convert solar electricity to storable fuels.

We did a bottoms-up analysis, of fuel production options from solar electricity, to identify which weak link in the process, does require research. Hydrogen, as a fuel, does not store well or transport well. The desirable high value fuels are the liquid hydrocarbons, diesel fuel and jet fuel, which have a high price, and are of immediate usefulness in society.

In the progression from solar electricity → fuel, the gas to fuel portion has experienced significant industrial development in the past 10 years. Methane feedstock, as in Qatar, makes the Fischer-Tropsch process economically viable. However, the first step of the process is the creation of syngas H_2+CO from the methane. The cost of the Fischer-Tropsch process would drop further if the syngas were supplied by water electrolysis to produce H_2, and the CO supplied by the inverse water gas shift reaction from CO_2.

Accomplishments

We identified the weak link in the progression from solar electricity → fuel. The H_2 electrolyzers need to follow the daily power curve of sunlight, just as the photovoltaic panels cycle up and down. The duty factor of sunlight is 25%. Therefore the capital cost of the H_2 electrolyzers is 4 times higher than expected. From our analysis, new research should focus on reducing the electrolyzer capital cost, so that the cost per Watt is less than the solar cell cost per Watt.

There is reason for optimism. The electrolyzer is a thick film device, about 100μm thick, with opposite electrodes on either side, somewhat similar to the profile of a c-Si solar 30 years ago. They can be made of materials that are much cheaper than Silicon. Just as Si solar cells have come down in price, we should expect that elctrolyzers, which are much more compact, can also come down in price. Catalysts are optional, be even if precious metals are used, they would only contribute $0.005 to the cost.

LB10036

Surface-Selective Synthesis of Graphene Nanoribbons on Nanowire Templates
Principal Investigator(s): Yuegang Zhang

Project Description

Graphene has a great potential for future high-speed and low-power electronics due to its unique transport properties. Quantum confinement effect in quasi-1D graphene nanoribbons (GNR) could open a bandgap that is inversely proportional to the GNR width and strongly dependent on the atomic geometry of its edges (crystallographic orientation). However, a method to pattern GNRs with precise control over their width, edges, alignment, and registry is still needed for large-scale device fabrication.

This project aims at developing new methods to grow GNRs on a selected surface of a nanowire (NW) template.

Accomplishments

Based on the surface-catalytic-selectivity of the materials for graphene growth in a chemical vapor deposition process (CVD), a method that enables the growth of GNRs directly on silicon oxide (SiO_2) substrates with accurate control over their width, length, and position has been developed. Based on this approach, a process for the fabrication of back-gated GNR field effect transistor (FET) test structures has been designed.

The process has been applied to the fabrication of die-scale FET arrays hosting hundreds of devices and these devices have been tested. Scanning electron microscopy (SEM) and Raman spectroscopy have determined that the growth of the graphene occurs only at the surface that had been defined by the catalyst cross section thus, validating the method and confirming the growth of the GNRs. The electrical characteristics of the GNR-FETs have confirmed the opening of a bandgap and are in agreement with those of previously reported, similar width GNRs. The FET mobility from our GNR-FETs has been estimated to be higher than that from previous devices fabricated on SiO_2 substrates. This is related to the transfer-free and contaminant-free direct GNR growth characteristic of our process. After the electrical testing, the device fabrication yield was calculated to be higher than 60% for the 3 μm long GNR devices. Thus, if devices based on GNR lengths smaller than 3 μm were fabricated, a device fabrication yield higher than 60% shall be envisioned.

This GNR patterning method has many advantages over the previous ones. First, it enables the tunable width growth of GNRs since the nanotemplates are controlled after the thickness of the catalytic material layer. If the layer was scaled down to an only few angstroms thickness, GNRs with band gaps larger than 0.5 eV or even 1 eV are expected, thus, enabling room temperature GNR-FET based applications. Furthermore, the morphology of these nanotemplates defines the length and the position of the GNRs. Last, the method is compatible with the standard fabrication techniques.

In conclusion, our method overcomes the practical limitations for the patterning of GNRs with precise control over their width and position, and for the scalability of the process. Therefore, it may pave the way to the successful integration of GNRs into nanoelectronics.

LB11040

Development of An Environmental Cell with Local Temperature Control
Principal Investigator: Haimei Zheng

Project Description

The goal of this project is to develop environmental cells with local temperature control for imaging through liquids using transmission electron microscopy (TEM). This development will advance environmental cell TEM and assist its applications in the study of nanocrystal growth, electrochemical processes of materials, etc. by real time observation with high spatial resolution.

The approaches are two-fold. First, we will fabricate an environmental cell by exploring the different membrane thickness, patterning of gold pads and/or a heater inside a cell, different cell geometries, etc. to fit the requirements of various experiments. The environmental cells will be used for imaging nanocrystal growth in real time, electrochemical processes and other materials transformation dynamics in fluids. Second, since the local environment of a TEM sample is often strongly modified by the electron beam especially when fluids are present, one key component of this project is the study of electron beam interaction with the matter inside an environmental cell.

Accomplishments

We have been able to fabricate environmental liquid cells with ultra silicon nitride membranes. Those cells have been used for the in situ TEM study of platinum iron nanowire growth in solution. The key importance of using ultra thin membranes (i.e. 10 nm low stress silicon nitride membranes) in an environmental cell has been demonstrated by the improved resolution for TEM imaging. We were able to reveal for the first time the dynamics of one-dimensional growth by shape directed nanocrystal nanoparticle attachment, self-correction of crystal structure and shape, mass transport at atomic level during growth, etc. This work opens many opportunities for the in situ TEM study of materials transformation dynamics in fluids.

It is a great challenge to fabricate liquid environmental cells by lithography and patterning in whole wafer scale when there are free-standing ultra thin membranes. We have overcome the challenge and achieved liquid environmental cells with patterned electrical pads where an electric current/bias can be applied. This success is not only critical for making a local heater inside a cell but also important for further developing electrochemical cells to study electrochemical processes in situ using TEM. We have also been able to make liquid cells with smaller windows, thinner liquid gaps, etc., which makes them more robust for various experiments. So far, liquid cells with the controlled local environment by applying an electric potential have been achieved. These technical advances have enabled the success of scientific studies on the observation of dynamic processes if materials in liquids.

We have also made significant progress in the understanding of electron beam-matter interaction inside an environmental cell. We have been able to use electron beam to manipulate nanoparticles and directly measure the forces from electron beam trapping a nanoparticle. This success has demonstrated for the first time the quantification of the electron beam interaction with nanomaterials. It also opens the opportunity to develop new manipulating tools for nano-device fabrication.

LB10005

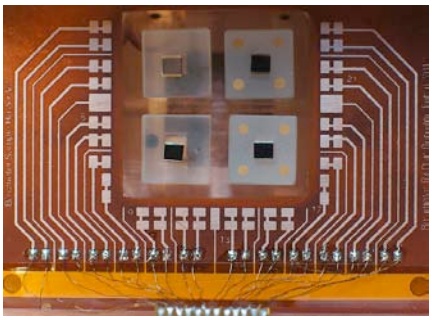
Bolometric Detectors for the Neutrino-less Double-Beta Decay Experiments

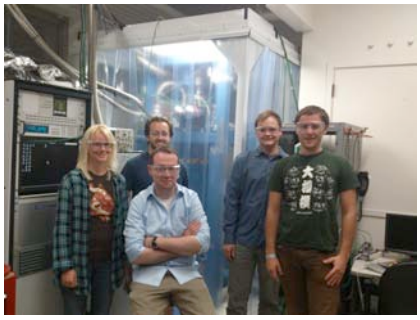
Principal Investigators: Stuart Freedman and Yury Kolomensky

Project Description

This LDRD project is aimed at developing advanced bolometric detectors for underground experiments searching for neutrinoless double-beta decay (DBD) and dark matter. The project plan includes constructing a cryogen-free ^{3}He-^{4}He dilution refrigerator and associated hardware that can enough to allow for the possibility of using other detection methods (scintillation detection, ionization detection, etc.) in coincidence with the phonon signal from the bolometer. The plan accommodates moving the complete system, including an associated facility for ultra-clean sample preparation, to an appropriate underground site. The system must be compact, self-contained, and portable.

Accomplishments





In the third year of the LDRD we have demonstrated routine remote operations of the Triton-400 cryogen-free dilution refrigerator from Oxford Instruments, with base temperature routinely reaching below 10 mK. Remote monitoring and control capabilities and protocols have been developed, necessary for operations at a distant underground facility. We completed the fabrication of a lead shield, which encapsulates the sample volume, providing reduction of the environmental background radioactivity. The shielding system includes a mechanism to safely move the shield when access to the sample volume is necessary. We have also installed a clean module around the cryostat to reduce the contamination of the experimental volume (picture on the right, bottom).

We have designed and constructed a versatile experimental plate, instrumented with a RuO_2 thermometer, calibrated against a ^{60}Co nuclear-orientation thermometer, and a dedicated sample holder, optimized for thermal balance and ease of wiring. The capability to make appropriate temperature measurements below a few hundred mK has been implemented and refined by graduate student Jon Ouellet and postdoc Ke Han, using a commercial resistance bridge from Lakeshore Cryotronics. A set of CUORE-style electronics for reading out bolometric detectors has been assembled by postdoc Tommy O'Donnell and graduate student Melanie Veale in preparation for the first measurements of small bolometric detectors. In addition we have assembled the equipment and developed procedures necessary to characterize NTD thermistors of the type used in CUORE and we are making comparisons of our characterizations with those of our CUORE colleagues in Europe. Investigating NTD characteristics is becoming an important part of the program.

The first system of small bolometers has been prepared (picture on the right, top) by Ke Han. We have taken advantage of synergies offered by the Berkeley environment to do this work. The mechanical parts of the apparatus are designed by our group members and machined by students and postdocs in the student machine shop in the Physics Department. We use the precision wire bonders at the NanoLab in the College of Engineering and at LBNL to bond the NTD thermistors; we also use NanoLab and LBNL facilities for surface depositions (gold and tungsten). We now have the capability of running small bolometric detectors at Berkeley; larger, CUORE size detectors require operation in an underground environment because of unacceptably high cosmic ray backgrounds.

LB11010

Lattice QCD Codes by Discretizing Time and Space: FY2012

Investigators: Wick Haxton (lead), Volker Koch, Sergey Syritsyn, Andre Walker-Loud NSD

Project Description: This LDRD project is focused on developing a lattice QCD capability in the Nuclear Science Division, with particular emphasis on Standard-Model problems connected with weak interactions, fundamental symmetries, and astrophysics. Our program includes strategies for utilizing lattice QCD output as input into effective theory treatments of light nuclei, so that properties of light nuclei can be predicted from lattice results for two-nucleon systems, with known systematic errors. Our initiative is based on the "CalLat" partnership with Lawrence Livermore National Laboratory and Nvidia. Project goals include

- Solving problems important to our understanding of weak interactions, including Standard Model sources and hadronic parity and time-reversal violation.
- Advancing lattice QCD methods for petascale machines, including LLNL's Sequoia;
- Positioning our LBNL group to compete in SciDAC3 and other new funding initiatives.

LDRD funding has allowed us to support two outstanding young researchers in lattice QCD, Andre Walker-Loud, a key member of the NPLQCD group that is leading efforts to calculate properties of two-nucleon systems, and Sergey Syritsyn, who previously helped lead the MIT group's efforts on computing nucleon properties and form factors.

Accomplishments: Walker-Loud and collaborators developed methods for determining the isovector nucleon electromagnetic self-energy, valid to leading order in QED. This is part of an envisioned program to better understand the apparent extraordinary fine-tuning of the Standard Model, and the significance of that fine-tuning for critical astrophysics problems, including the synthesis of He in the Big Bang and hydrogen fusion in the Sun. This fine tuning can be appreciated by comparing the resonance energy of the two-proton system, which is unbound by 66 keV, with the natural scale of the strong interaction, $\Lambda_{\rm QCD} \sim 0.25$ GeV. The group is currently exploring whether a more accurate estimate of the up-down quark mass difference can be extracted from the known Big Bang He/H ratio.

Another accomplishment has been the further development of lattice QCD methods for estimating parity-nonconserving (PNC) meson-nucleon couplings. Our group performed the first such calculation, determining the PNC pion-nucleon coupling. This work provides important guidance for the $\vec{n} + p \to D + \gamma$ PNC experiment now underway at ORNL's SNS. Current work includes efforts to calculate the disconnected contributions to this coupling and to perform calculations that will bring us closer to physical pion masses. We also have embarked on an effort to calculate the isotensor contribution to PNC associated with rho exchange. Knowledge of this coupling is crucial to the interpretation of the most precise experimental results available in this field, the asymmetries for polarized proton-proton scattering at low and intermediate energies. As the isotensor rho coupling has only connected contributions, our lattice QCD calculations should yield very reliable results, with minimal systematic uncertainties.

LB12012

Explosive Astrophysics Using High Performance Computing

Principle Investigator: Daniel Kasen

Project Description

The purpose of this LDRD is to better understand the conditions leading to the creation of the elements in extreme astrophysical environments. Our approach is to use advanced simulation codes on high performance computing systems to model the dynamics, nucleosynthesis, and the radiative transport of supernova explosions. Our end-to-end calculations will allow us to predict the composition, velocity and geometry of the ejecta, and thereby derive spectral signatures that are directly comparable to observational data. In this way, we will test our understanding of the conditions in explosive astrophysical environments and identify the important observable indicators of the nuclear physics occurring within.

We model the dynamics and radiation transport of explosions using a variety of codes. Postdoc Cody Raskin is an expert in smooth particle hydrodynamics code and uses the SNSPH to model compact object mergers. In addition, we use the grid based adaptive mesh refinement hydrodynamics code CASTRO to model explosions. The radiation transport problems is addressed primarily using the SEDONA code, an implicit Monte Carlo (IMC) transport code which includes modern acceleration and variation reduction techniques.

Accomplishments

We have studied aspects of three different classes of astrophysical explosions: (1) supernovae (SNe) from massive star disruptions, (2) thermonuclear SNe from white dwarf (WD) explosions, and (3) radioactive transients from the merger of two neutron stars. Our studies of (1) have focused on extreme events which produce very luminous SNe. In particular, very massive (> 100 solar masses) stars may undergo a pair production instability and explode entirely, synthesizing a large amount of radioisotopes. We showed that such events lead to very bright and long duration SNe that could be seen out to very large distances (Pan et al., 2012a,b). We also modeled lower mass (< 100 solar mass) stars which collapsed to form a central black hole. We found that the subsequent fallback and accretion of stellar material onto the black hole could likewise power very luminous events (Quataert and Kasen 2012, Dexter and Kasen, 2013).

Our studies of WD explosions allowed us to use observations of the nearby Type~Ia event SN~2011fe to provide some of the tightest constraints on the radius of the star (Nugent et al., 2011, Bloom et al., 2012). This confirmed that the progenitor did indeed include a compact WD. We have been working on models to distinguish whether the explosion consisted of a single WD, or rather the merger of two WDs (Shen 2012, Raskin and Kasen in prep). Our studies of neutron star mergers have focused on the observable properties of the radioactive material ejected from these events. We found that if the ejecta includes heavy r-process elements, the opacity is increased and the resulting spectra were significantly redder (Kasen et al.~in prep, Barnes and Kasen in prep). This provides a means of distinguishing these transients from other sorts of explosions, and suggests an important means of directly observing newly formed r-process nuclei.

LB11019

Probing the Partonic Structure of Protons and Nuclei
with Isolated Photons at the LHC
Principle Investigator(s): Constantin Loizides

Project Description

The goal of this LDRD is to formulate and carry out a systematic program for precise photon measurements with the ALICE detector at the LHC with sufficient precision to impact PDF measurements in an interesting kinematic regime. In proton–proton collisions at center-of-mass energies at 7 TeV, cross section measurements of isolated photons will allow one to constrain the gluon distribution at small x ($< 10^{-3}$) with large leverage in Q^2 in the proton. In lead–lead collisions at center-of-mass energies of 2.76 TeV per nucleon, the yield of isolated photons will provide a reference for the quantification of hot nuclear matter effects.

In particular, the following points will be addressed: a) Simulation of the physics capabilities of ALICE' setup for 2011; b) Development of the reconstruction code for photons using the shower shape in the kinematic range of about $10-30$ GeV/c, where the main background, two-photon decays from neutral mesons, can still be distinguished in the calorimeter; c) Development of alternative reconstruction algorithms outside of or complementary to the applicable region of the shower shape method; d) Investigation of new isolation strategies using modern jet finders; e) Investigation if further theoretical development for competitive results on PDFs is needed.

Accomplishments

The most significant accomplishments are the measurements of the raw isolated photon spectra, and their purity and efficiency, in proton–proton collisions at 7 TeV, using the shower shape approach. The isolation criteria have been obtained with a data-driven method using a template derived from neutral meson production in jets. These results have been shown at 3 conferences in 2012.

We have further improved the understanding of the response of the EMCal to incident photons and electrons, and carried out realistic simulations of the physics performance of ALICE for proton–proton collisions at 7 TeV in the 2011 runs. The simulations have been obtained separately for generated events containing only the signal, and for events containing only background. For the latter a strategy has been developed that allowed to run the detailed detector simulation only in case a particle from the background (high momentum hadron or decay photon) points to the calorimeter.

Currently, we are working on the evaluation of the systematic uncertainty on the isolated photon cross section. In particular, the comparison of the data-driven method, and a method which fully relies on Monte Carlo simulations, does not give consistent results. We are trying to understand the discrepencies, but the remaining differences between the results obtained in the two ways will probably make up a large part of the total systematic uncertainty on the measurement. We expect the results to be published by the middle of 2013.

LB11001

Direct Determination of Electrostatic Interactions Through Advanced Analysis of High-resolution Macromolecular Crystal Data

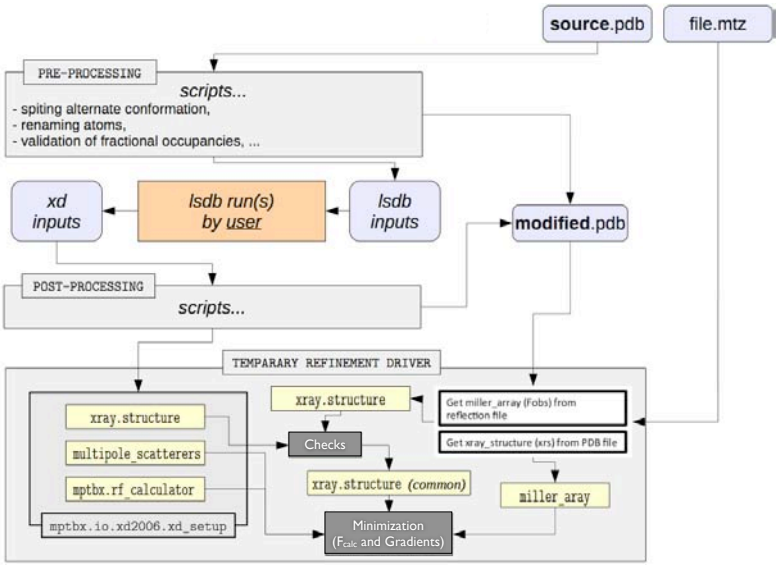
Principal Investigator(s): Paul Adams, Philip Coppens (U. Buffalo)

Project Description

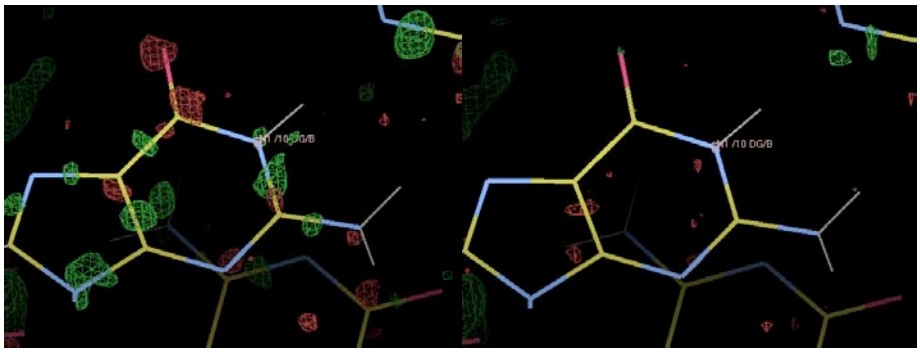
The electronic structure of an atomic system defines its conformation. Additionally, in complex macromolecules such as enzymes, it is the detailed distribution of electrostatic charges that confer catalytic activity and often specificity. Direct experimental determination of electrostatics in macromolecules will dramatically improve our ability to elucidate and manipulate the catalytic mechanism of enzymes relevant to bioenergy and biofuels applications, and develop targeted therapeutics for human health. High-resolution macromolecular crystallography is the basis for our proposed methodological advance. This technique has made dramatic progress in the last decade and an increasing number of high-resolution structures are becoming available. However, current analyses continue to be based on an approximate scattering model that ignores the effects of chemical bonding on the electron density. Our improved methods for analysis will allow for the evaluation of electrostatic interactions directly from X-ray crystallographic results.

Accomplishments

In the first year of the project we identified the components of the XD program that are relevant to the calculation of aspherical scattering factors. In this last year of funding we used a combination of automated translation of the XD code to C++, and new code generation to create a working system for aspherical atom scattering calculation in the Phenix software. This requires that the aspherical densities are described using spherical harmonic terms that closely approximate the underlying electrostatic multipoles. Currently the databank of aspherical atoms (University of Buffalo Pseudoatom databank; UBDB databank) is used.



The flow of control and data in the current implementation is shown in the figure above. This implementation has made it possible to test the impact of using aspherical scattering factors for small macromolecular test cases. The results show that standard crystallographic statistics (e.g. R-factor) are improved. Initial results also suggest that the electron density maps are improved, with a reduction of residual noise arising from aspherical density distributions (see figure) and increased signal for atomic features.



Left: bonding difference density (green). Right: after multipolar refinement

LB11009

Assembly and Function of Organelles for Carbon Fixation

Principal Investigators: Daniel A Fletcher, Cheryl Kerfeld, Phillip Geissler

Project Description

Biological systems greatly enhance the diversity, selectivity, and efficiency of biomolecular reactivity through spatial organization at the nanometer-to-micron scale. Bacterial microcompartments are an example of such specialized structures that appear to be constructed to enhance specific reactions. In cyanobacteria, carbon fixation occurs inside a self-assembling microcompartment called the carboxysome, whose recent study has generated a wealth of interest and information. However, there exists a lack of understanding of how carboxysomes are assembled and what factors during assembly affect their function, limiting efforts to understand carboxysome function and to construct synthetic organelles with enhanced biochemical activity.

This project brings together the biology, imaging, and simulations necessary to understand the process by which carboxysomes assemble into functional organelles. By producing a fundamental understanding of how carboxysomes are assembled into functional organelles, we expect to develop insights that can be used to construct functional nanosystems constituted of both synthetic materials and biological molecules to advance carbon sequestration efforts.

Accomplishments

In the second year of this project, our group has advanced understanding of carboxysome assembly. We have devised a pentamer-hexamer fusion that, when combined with additional hexameric proteins, assembles into empty shells in E. coli or in vitro. These assemblies were characterized with dynamic light scattering and transmission electron microscopy. We have also developed combined optical and force microscopy methods that can be used to obtain simultaneous topographical and fluorescence information from purified carboxysomes as well as in vitro assembled carboxysomes. Data from the combined optical and force microscopy will be used to compare carboxysomes purified from bacteria with protein shells assembled from purified proteins in vitro.

Finally, we have developed new methods for simulating self-assembly of carboxysomes. Coarse-grained models have been developed for the two main components of the carboxysome shell and Monte Carlo and molecular dynamics results using these models have successfully replicated the crystal packing of the shell components into molecular layers. Future work on carboxysome assembly will be aimed at understanding the key structural questions of the carboxysome shell.

LB10006

Metafluxomics of a phosphorus removing microbial community

Principal Investigators: Héctor García Martín and Aindrila Mukhopadhyay

Project description

We proposed to develop a method to measure intracellular metabolic fluxes for a complete microbial community. Whereas measurement of intracellular fluxes (i.e. the rate at which molecules proceed through a reaction per unit of time) for all metabolic reactions in an organism has been so far limited to pure cultures (fluxomics), measurement of metabolic fluxes for a full microbial community (metafluxomics) would be a first in scientific literature and a logical progression in the advent of metagenomics, metatranscriptomics and metaproteomics technologies.

We developed proteomic methods to measure and assign intracellular metabolic fluxes to each of the species in a microbial community. We will use this information as a stepping stone to produce quantitative predictive models of microbial community metabolism and its impact on its environment. The study of internal metabolic fluxes is the optimal basis for community modeling since they include knowledge of growth rates (which are just fluxes to biomass) and the biochemical impact on the environment (which is just the incoming and outgoing metabolite fluxes into/to the environment).

The project unfolded in two different phases of ascending complexity: the first step involved computationally testing that the same results are obtained with the proteomic method and the standard amino-acid based method. The second one involved the experimental check that, for *E. coli*, the same results are obtained using both methods.

Accomplishments

In the first two years we were able to compare the new proteomic-based method with the traditional amino acid-based approach and show that similar flux profiles are obtained. We also developed an information content measure and used it to understand how much information loss is incurred by using the peptide-based method instead of the standard amino acid-based approach. We determined that for peptides containing five amino acids, the information loss incurred by using peptide labeling can be countered by using a large quantity of random peptides, of the order of 60-80. We also found that for longer peptides (10 amino acids) increasing the number of peptides counters the loss of information and it can help produce the same amount of information content as the amino-acid based.

In our last year of funding we have gone beyond the computational test to use realistic *E. coli* genome peptides (as opposed to randomly generated) to show the validity of the method. We have also performed ^{13}C labeling experiments to obtain fluxes from peptide labeling patterns and troubleshot problems in peptide detection. We have the draft for the paper based on the computational method and are analyzing the data to write the paper on the experimental test.

LB12027

DNA DIVA (Design, Implementation, Verification Automation) Pipeline
Principal Investigator(s): Nathan J. Hillson, Vivek K. Mutalik

Project Description

Although DNA construction has been practiced for decades across bioscience labs, from crystallographers and microbial engineers to plant and cancer biologists, the process remains an inefficient diversion from the core research aims under investigation. Each researcher is currently responsible for: 1) designing the DNA to be constructed; 2) designing the corresponding DNA construction protocol(s); 3) ordering the requisite reagents (e.g., DNA oligos), constructing the DNA, transforming the DNA, isolating clones, and validating clonal sequences; and 4) putting all of the annotated sequence information and experimental metadata in a repository database. This current paradigm does not benefit from processes of scale, and implementing and verifying DNA sequences distracts researchers from their core comparative advantages in design and functional assessment. Furthermore, the process precludes the systematic capture of success/failure rate data which would prove extremely valuable for the further refinement of DNA construction practices.

We are developing an alternate process in which researchers design their DNA with a web-based graphical user interface, submit their designs to a central queue, and a few weeks later receive their sequence-verified clonal constructs through a central DNA repository. Researchers have web-based access to their DNA design queues, and can track the progress of their submitted designs as they progress from “evaluation”, to “waiting for reagents”, to “in progress”, to “complete”. Along the way, all DNA construction success/failure rates will be captured.

Accomplishments

Technology stack specifications, researcher use-cases/workflow schematics, and wireframe mockups have been developed for the DIVA graphical user interface (GUI). After evaluating several technologies including Adobe Flex and Sencha Architect, it was determined that HTML5/javascript/jQuery, leveraging Twitter Bootstrap, would aptly serve as the web technology platform for the DIVA. Multiple use cases (*e.g.*, a researcher creates a new DNA design and saves a draft copy for later revision) along with their corresponding workflow diagram schematics (*i.e.*, conditional flow-charts that model the work processes invoked by each use case) have been developed. Wireframe mockups for the DIVA interface have been rapidly prototyped and iteratively refined using OmniGraffle and Adobe Illustrator. These mockups will serve as templates for subsequent HTML5/javascript/Bootstrap instantiation of the DIVA GUI.

In addition to software development efforts, we have successfully applied the experimental methodologies and computer-aided design/manufacture technologies that underpin the DIVA to the construction of a variety of DNA designs. Specifically, we have: 1) designed and constructed a 36 bp leader-sequence codon variant library for a difficult to express biofuel pathway enzyme, and identified multiple leader sequences that significantly increase expression; 2) designed and constructed combinatorial libraries of tandem bi-cistronic design expression systems for two fluorescent proteins and for two difficult to express biofuel pathway enzymes; 3) designed and bench-scale validated a DNA assembly test bed consisting of type IIs endonuclease or flanking homology-mediated isothermal assembly of 4 DNA assembly pieces, along with the development of qPCR probe sets spanning each of the 4 DNA assembly junctions. These construction efforts serve as real-world use-cases and validations of the DIVA platform.

LB11017

Piezoelectric Biomaterials for Novel Energy Conversion
Principal Investigator(s): Seung-Wuk Lee and Ramamoorthy Ramesh

Project Description

The purpose of this project is to develop novel, scalable energy converting biomaterials using genetically engineered M13 bacteriophages (viruses). The M13 virus possesses features that make it very attractive as a building block for energy generating materials. These features include its piezoelectric, nanofiber-like structure, and its abilities to self-replicate, self-assemble, and evolve. M13's unique material properties come from its physical and biological structure. M13 is a long-rod shaped bacterial virus composed of a single-stranded DNA that is encapsulated by 2700 copies of the major coat protein, pVIII. pVIII has an alpha helical structure with a dipole in the carboxy- to amino-terminal direction; and it covers the viral surfaces periodically with 5-fold helical symmetry and no inversion center. This structural arrangement enables M13 to act as a piezoelectric nanofiber that can convert mechanical energy to electric energy and *vice versa*. In addition, M13 can replicate in large quantities through amplification in bacteria. Due to its monodisperse long-rod shape, M13 can self-assemble into periodically ordered two- and three-dimensional structures. By genetically engineering various components of the M13 and screening them through a directed evolution process, we can quickly select for M13 viruses that have desired or enhanced piezoelectric functions. In order to achieve our goal, we will characterize the piezoelectric properties of the M13 virus using piezoresponse force microscopy. We will then enhance the piezoelectric properties of M13 through genetic engineering. Finally, we will fabricate M13 virus-based piezoelectric devices. The success of the proposed research will result in the development of novel biomaterials that can self-replicate, self-assemble, and evolve to fabricate electric energy converting materials and devices using ubiquitous mechanical energy. The proposed approaches will significantly help to secure a predictable energy future.

Accomplishments

We have successfully developed a piezoelectric energy-converting biomaterial from a bacterial virus, M13 phage. First, we fabricated a novel self-assembled phage film structures using a self-templating phage assembly processes. In this process, the liquid crystalline property of the M13 phages enabled the spontaneous-ordering of piezoelectric phage films in a cost-effective manner. We also verified chemical and physical structure-dependent piezoelectric properties of M13 phage thin film using piezoresponse force microscopy techniques in single phage level. We tuned the piezoelectric properties of the phage through modulating dipole strength by addition or reduction of negatively charged amino acids in the major coat protein using genetic engineering. In addition, we controlled physical structures to enhance piezoelectric strength up to 7.8 pm/V through formation of multi-layered phage films. We also developed enhanced phage-based electrical generator with periodic piezoelectric micropatterns producing 80-100 nA and 800-900 mV.

LB12013

4D Biology and Optogenetics of Microbial Biofilms

Principal Investigator(s): Jan Liphardt

Project Description

In their natural environment, microbes organize into communities held together by an extracellular matrix composed of polysaccharides and proteins. Compared to free-living planktonic cells, cells within communities are significantly more resistant to extremes of pH and salinity. Moreover, unlike typical planktonic cells, microbial communities can efficiently perform chemical transformations of central importance to the DOE mission, such as remediation of heavy metal contaminated soils and conversion of plant matter into transportation fuels.

This project seeks to learn how DOE-relevant microbes such as *Desulfovibrio*, *Pseudomonas*, and *Shewanella* form biofilms and how extracellular matrix proteins and sugars influence that process. We have recently developed technologies for superresolution imagining of the biofilm formation process and the resulting structures (Berk *et al*., ***Science* 337**, 2012) but these technologies were not immediately suitable for DOE-relevant microbes.

The specific goals of this LDRD were to

(**a**) develop microfluidic technologies for reliably growing DOE-relevant microbes inside flow chambers that are compatible with conventional and super-resolution imaging

(**b**) determine if the labeling strategies reported in Berk *et al*. can be applied to DOE-relevant microbes

(**c**) develop genetically encoded fluorophores for multimodal optical imaging of extracellular microbial protein complexes

(**d**) develop strategies for optically controlling the expression of biofilm-relevant genes in *Shewanella*, in the first instance.

Accomplishments

Our most significant accomplishment has been to develop reproducible protocols for growing *Shewanella* and *Desulfovibrio* directly inside temperature controlled microfluidic flow chambers. In the latter case, all reagent flow is controlled to preserve the anaerobic conditions needed by *Desulfovibrio.* The major technical difficulties we encountered (and ultimately solved) were the slow growth of the *Desulfovibrio* biofilms (~many days) compared to the standard model species and the experiment-to-experiment variability in the growth rates of *Desulfovibrio* biofilms.

We also made progress in aim (**c**), with the development of mMaple, the first genetically encoded photoswitchable tag that can be used in (1) conventional fluorescence and confocal microscopy, (2) structured illumination microscopy, and (3) photoactivation light microscopy (PALM). Our progress is described in McEvoy, AL, et al., "mMaple: a photoconvertible fluorescent protein for use in multiple imaging modalities," PLoS One 2012; 7(12), Epub 2012 Dec 11.

Since we are now able to reliably culture DOE-relevant microbes directly on various microscopes, inside controlled microfluidic flow, we are now in a position to test optogenetic strategies for controlling gene expression in various microbes and directly observe how those changes influence biofilm organization.

LB12014

Engineering of Plant to Improve Epicuticular Wax Deposition and Water Use Efficiency
Principal Investigator(s): Dominique Loqué

Project Description:

In 2000 it was estimated that more than 40% of the freshwater in the US was utilized for irrigation. In general, water limitation reduces photosynthesis and consequently plant growth and biomass yield. Developing renewable energy based on large-scale productions of energy crops will unfortunately further increase water needs.

The purpose of this project is the development of strategies to improve crop drought stress tolerance and water use efficiency by reducing uncontrolled water losses without reducing biomass yield. The approach is to enhance the deposition of epicuticular waxes and cutins, which are known to reduce water permeability of epidermis from leaves and stems, without altering plant growth and development. Several transcription factors have been identified to control genes involved in the biosynthesis and deposition of epicuticular waxes and cutins. Unfortunately, constitutive overexpression of some of these transcription factors is accompanied with plant growth deficiencies. An alternative approach to alleviate negative phenotypes related the overexpression would be to increase expression of the same transcription factors only in native (epidermal) cell layers. Recently, we developed a new technology at JBEI to boost secondary cell wall transcription factor expression in native tissues, which is based on the design of an Artificial Positive Feedback Loop (APFL). This technology allows overexpressing master transcription factors specifically in native tissues in contrast to most common practices that use constitutive promoters, which often cause undesired side-effects because of the absence of tissue specificity. Therefore, our strategy is to apply this APFL technology for drought stress tolerance and water-use efficiency. In order to test rapidly this approach we applied it in the model plant specie *Arabidopsis* and implemented it with the used of transcription factors which belong to distant plants species to test the transferability of this approach across multiple plant species using only one model plant.

Accomplishments:

We could successfully build 12 synthetic genes and generate several independent transgenic *Arabidopsis* plants, which overexpressed different transcription factors of interests. Most of the synthetic constructs resulted in an overexpression of key genes involved in wax biosynthesis. More interestingly, the ability to induce genes involved in wax biosynthesis using monocot transcription factors in *Arabidopsis* supports that this approach should be transferable into other plant species including crops. Some of the engineered plants also exhibited increased epidermal wax deposition and improved drought stress tolerance. Unfortunately for some of the constructs we were unsuccessful to increase drought stress tolerance since the overexpression was so strong that it caused silencing of the synthetic gene.

Because of the limited time of the LDRD (12 months) and the time required to generate stable transgenic lines, none of the lines could be fully characterized. However, generated data allowed us to apply for additional funding to continue this work and to develop new technologies to accumulate hydrocabons (potential biofuels) in specific tissues. Finally, the obtained results were used to reinforce the patent application on the APFL technology and they further support that this technology opens a new horizon for plant engineering since it could be used to boost different metabolic pathways and associated bioproducts.

LB12016

Genetically-Encoded Optical Sensors And Actuators Of Protein Complexes And Machines

PI: Gerard Marriott
Co-PI: Paul Adams

Project Description:

The goal for the 1-year study was to initiate development on multiscale, multiplexed opto-genetic approaches for (**A**), sensing and mapping of protein complexes and assembly of protein machines inside of living cells; (**B**), to bring about reversible control of protein activity and protein signaling pathways that lead to directed motility of endosomes within a living cell. Given the limited period of funding, we focused our attention on section (**A**) of the proposed work, i.e. on the generation of new genetically-encoded protein probes for Foerster resonance enrgy transfer (FRET) and fluorescence anisotropy (FA) measurements to detect and image target proteins and their complexes in living systems. We used high-resolution structural analysis to optimize the FA probe. The FA-sensors were evaluated using fluorescence anisotropy measurements conducted in an SLM fluorometer.

Accomplishments:

We engineered the blue-light sensor to serve as a genetically-encoded probe to quantify protein hydrodynamics and protein complexes. We generated a brilliantly fluorescent mutant that has a remarkably long ~4.5ns lifetime, yet with only 75% of the mass of GFP. The small size makes this probe useful for FRET measurements and superior to CFP since by the distance between the donor and YFP is decreased in a complex Ro compared to CFP. Future studies will advance this property for FRET based imaging of sensor-CFP fusions. Because of its small hydrodynamic volume and long fluorescence lifetime, our sensor is well-suited for FA measurements of the size and shape of proteins and their complexes. For example, the steady state FA value is only 0.22 at 20c in buffer compared to 0.35 for GFP under the same condition. In fact our sensor has the longest lifetime and lowest FA value of any genetically encoded fluorescence protein. With the limiting FA value being 0.4,we can safely say that it has a much larger dynamic range for FA studies compared to GFP. The addition of an 17 amino acid tag from MLCK onto our sensor is being used to target calmodulin, an important signaling protein in living cells. The additional sequence on our sensor increases the FA value to 0.25, which is still low and suitable for FA measurements and imaging of calmodulin, which on binding should increase the FA to >0.32. We are continuing to work on these studies and anticipate submitting a manuscript this year. Towards the end of the project we also discovered a new candidate protein for FA measurements, a fluorophore derived from a bacterial binding protein. The fluorophore has the longest fluorescence lifetime of any cofactor in the cell (15 ns) and given the small mass of the protein, the FA value of the original protein harboring an amino acid tag for actin is only 0.16 and this increases to as high as 0.25 on binding to F-actin. Modeling studies suggest that the mass of the fluorophore could be reduced to 10kD without impacting the binding of the protein. Studies directed towards this goal are underway and should result in a mini probe that is highly optimized for both FA and FRET measurements. A provisional patent filing is being prepared by LBNL for the probes detailed in this report

LB12034

Computational Methods for Photosystem Structure Probed by X-ray Free-Electron Laser Studies

Principal Investigator(s): Nicholas Sauter, Ralf Grosse-Kunstleve,
Vittal Yachandra, Junko Yano, Paul Adams, Petrus Zwart

Project Description

The purpose of this project is to understand light-induced water splitting in green plants, algae and cyanobacteria; organisms that are responsible for producing most of the oxygen in the atmosphere. An important application of this knowledge will be in the design of future fuel production schemes based on artificial photosynthesis. The splitting of water, creating oxygen and hydrogen, is accomplished by the protein complex photosystem II, which contains a catalytic center containing four manganese atoms. To drive the reaction to completion, four sunlight photons sequentially oxidize the Mn atoms after which the catalyst returns to the reduced state. Traditional methods for studying structure and function, such as X-ray crystallography, have been hampered by the high sensitivity of the Mn center to probing X-rays, which reduce the metal atoms.

We have an unprecedented opportunity to map out the detailed reaction mechanism using X-ray free-electron laser experiments at the Linac Coherent Light Source (LCLS). In the experimental design, photosystem II crystals will be driven through the redox cycle with an optical laser. X-ray probe pulses at LCLS are short enough (50 fs) that all observations can be made before reduction and other damage processes occur. As the probe pulses are extremely intense, the sample becomes fully ionized after the observations are recorded; therefore, a continuous stream of new crystals must be delivered to complete the full data set. Atomic structure of the protein will be determined by X-ray diffraction, and the electronic state of the Mn atoms will be measured by X-ray emission spectroscopy. The experimental team is a collaboration between many groups at different institutions. This LDRD is specifically targeted at developing the requisite computational methods to interpret the data. Main challenges are the data size (~100 TB) along with novel detector and optical designs.

Accomplishments

The project was awarded three LCLS X-ray beamtime allocations for FY2012 and additional experimental time for FY2013. The team demonstrated that small photosystem II crystals can be delivered to the interaction region using a novel liquid-jet design. A new X-ray emission spectrometer was developed and tested, and both emission spectra and diffraction images were collected on new-design pixel array detectors that image at 120 Hz, the LCLS X-ray pulse repetition rate. We developed computational techniques for processing both the emission and diffraction data. Notably, our implementation gives an immediate view of the emission spectra and Bragg spots, so experiments can be adjusted in real time. Massive parallel computation was required for full processing, and additional computational methods are still under development.

We demonstrated that as expected, the 50 fs X-ray pulse is short enough to observe X-ray diffraction from both photosystem II crystals and a control protein (thermolysin) before damage processes affect the signal. Unfortunately, the small crystal size required for liquid-jet delivery (~10 μm) degrades the resolution of photosystem diffraction, which was an unexpected result. We are attempting to find different crystallization conditions and/or a different protein construct that improves the resolution. We proved that the X-ray probe does not reduce or damage Mn atoms, and collected initial excited-state data using the optical pump approach.

LB11042

Feasibility and development of fluctuation X-ray scattering at the NGLS
Principle investigator: Peter H. Zwart

Project Description

X-ray solution scattering is a routine biophysical technique used to determine structure and dynamics of macromolecules in solution. When solution scattering data is interpreted, often with the aid of known atomic models, an improved understanding of the macromolecule's biological function and properties emerges. The main challenge associated with solution scattering data is the intrinsic lack of information that can be obtained from solution scattering curves. By performing the solution scattering experiment at the femtosecond time scale by using a free-electron laser, a technique known as fluctuation X-ray scattering, the information content of the data can be significantly enhanced, leading to fewer ambiguities in derived structural models and a better understanding of the associated biology. Whereas the development of fluctuation scattering at free electron lasers has been targeted primarily to obtain the shape of macromolecules, its scope and uses should be seen as an extension of classic solution scattering.

Accomplishments

Over the last year, a number of important advances have been made. First and foremost, a novel efficient computational route for the calculation of model fluctuation scattering data has been developed [1]. This technique, which is an extension of earlier development methodology for the computation of small angle scattering profiles and utilizes 3D Zernike polynomials, shows an increase in performance as compared to the standard spherical harmonic based calculations.

The second major accomplishment is the design and implementation of an *ab initio* structure solution method for fluctuation scattering data [2]. Whereas earlier attempt by others in the field have attempted to accomplish this by solving a double phase problem, our method is the first method that has been demonstrated to work in absence of symmetry constraints. The current implementation furthermore utilizes only a fraction of the information that is contained in the data and can thus be improved upon further.

The third accomplishment of this research program is an experimental demonstration of this method on metallic nanoparticles with data collected at the Advanced Light Source. Our results have indicated that this technique can be used to perform structure determination of metallic nanoparticles using existing synchrotron light sources.

The later research has furthermore provided highly relevant insights for the fourth accomplishment of this project: proof of principle experiments of fluctuation X-ray scattering of biological molecules at the LCLS. This data was collected in a multi-institutional collaboration and has resulted in the further development of data reduction algorithms and data validation routines. Further analyses and structure determination of these samples is currently under way.

In conclusions, we have made significant advances in the development of theoretical and experimental methods for fluctuation scattering.

LB11003

Fiber System Development for Surveys of Baryon Acoustic Oscillations (BAO) Applicable to the Future BigBOSS Experiment

Principal Investigators: Chris Bebek, Jerry Edelstein, David Schlegel

Project Description

For the next generation ground-based dark energy experiments using the baryon acoustic oscillations technique, the BigBOSS collaboration is proposing to construct a 5000 fiber-fed, multi-object spectrograph for the prime focus of the Mayall telescope. Issues that need to be understood are: fiber termination, bonding, and polishing at the telescope end; fiber termination, assembly, and positioning at the spectrograph end; intermediate connectorization; and the effects of repetitive fiber bending on focal ratio degradation and fiber transmission.

Accomplishments

FRD measurements. Light incident at a single angle on a fiber will exit the fiber with a distribution of angles. This effect is called focal ratio degradation (FRD). We developed facilities to measure FRD of terminated fibers to demonstrate fiber process and mechanical strain relief methods and fiber performance survival.

Mechanical Connections: We tested the FRD of fibers terminated with mechanical connectors of various types. We found that while uncoupled mechanically terminated fibers have FRD comparable to the high-quality standard fiber, the coupled mechanical connectors did not deliver the FRD performance needed to meet our requirements.

Spliced Connections: As an alternative to mechanically coupled connectors, we explored the performance of fiber fusion splice connections. Our conclusion is that fusion splicing is a viable scheme for high throughput, low FRD fiber connections.

Bending Survival: An apparatus was built to subject fibers to repetitive bends at the recommended minimum bend radius. Our results showed no significant FRD degradation following 90,000 bending cycles.

Fibers & Ferrules: We conducted extensive converging beam FRD tests on polished end fibers to characterize key optical tolerances. Our collaborators at Durham University provided polished ceramic ferrules that we found in tests to provide superior baseline FRD and the required axis alignment.

Slit Array: The spectrograph slit array, a group 500 fibers terminated into a polished block, was designed. Vendor contacts were made to proceed with test slit array fabrication testing.

AR Coatings: Fiber antireflective coatings are needed to reduce light loss at the fiber ends. We worked with vendors to develop AR coating designs and costing.

Cable Management: Extensive design and simulation activities were accomplished regarding fiber and cable management schemes including telescope declination and polar axis pivots, fiber stress relief junction boxes, and fiber focal plane individual fiber support.

LB12040

New Monolithic CMOS Sensors on a Fully Isolated Substrate
Principal Investigator(s): Maurice Garcia-Sciveres

Project Description:

15 Years ago all digital cameras used CCD image sensors. Today they all use CMOS image sensors. This led to widespread interest in the potential for scientific applications. But development of an “ideal” monolithic device, where the sensing function places no restrictions on the electronic circuits and the fill factor is 100%, has so far proven elusive. This LDRD is to design and fabricate a proof of principle, radiation tolerant demonstrator for particle physics and x-ray detection that may finally realize this ambition. This project received end-of-year finding in FY12, which was requested in order to begin design work before FY13, and by doing so be able to target a fabrication run in calendar year 2012. As integrated circuit fabrications have significant lead time and only occur a few times per year, it was important to be able to have submission in calendar year 2012 in order to have a chance to make significant progress in FY13 (said another way, the fiscal year calendar is not ideally matched to the proposed integrated circuit fabrication schedule).

FY12 Accomplishments:

Thanks to the LDRD funding received in FY12, we started design work in August 2012. This allowed us to target an meet an integrated fabrication run in November 2012. A demonstrator chips has been designed with a total area of almost 12 square millimeters in 130nm feature size CMOS. This chip contains an active pixel matrix with 64 rows by 20 columns. Several different variants have been implemented. Full coverage active pixels (100% fill factor) contain synthesized digital logic in addition to a complex analog front end. Partial coverage pixels contain a collection electrode in the analog section only, with isolated digital circuitry separated form the collection electrode. Fully isolated collection electrodes (with no circuitry at all over the electrode) have been included to use as a reference. All circuits in this test chip, including periphery and pads, have been isolated from the substrate by making extensive use of the deep N-well feature of this process. This will permit applying a bias voltage of up to 10V to the substrate in order to reverse bias the collection electrodes and collect charge by drift. The expected delivery date for this submitted chips is March 30, 2013. There were no publications in FY2012.

LB11038

High Voltage Up and Down Converters for Low Power Low Density Detector Instrumentation

Principal Investigator: Henrik von der Lippe

Project Description

This project pursues the development and prototyping of integrated DC-DC converters for use in fully-integrated detector readout ICs. Two distinct design tracks are targeted to different detector applications. One is the development of medium power density DC-DC down converters for use in next generation, fully integrated HEP read-out ICs (i.e. ATLAS upgrade at CERN). The integration of a DC-DC down-converter in this application could significantly lower the overall detector mass by reducing the wire mass, thereby achieving the required low detector cross-section required for future experiments. Second, the development of high voltage (i.e. 40V) DC-DC up-converters could allow for monolithic avalanche photo diode (APD) detectors for medical imaging and other applications (i.e. SSPMs).

The design of fully integrated, high power density down-converters in standard CMOS processes is a relatively new area of research, made possible by the smaller feature sizes and increased capacitance density available with modern processes. We have been specifically following the applicable research of the Berkeley Wireless Research Center (BWRC), with the intent to extend conversion ratios beyond 2:1 for our application area. Many technology-specific parameters must be optimized to successfully implement high efficiency, high power density converters. The development of high voltage up-converters is less demanding with regard to the required power density (low), but has more complex design requirements for maintaining all devices at specified safe operating voltages with reasonable efficiency.

Accomplishments

CMOS DC-DC converter design offers a nearly unlimited combination of topologies, conversion ratios, transistor voltages, process feature sizes, etc. To reduce this huge design space, we have developed a methodology that allows us to analytically select good design candidate topologies and conversion ratios, and only then move to schematic implementation, optimization, and evaluation of the select designs. From these results, we will select the best design for complete implementation in physical layout, detailed simulation, and prototype IC fabrication.

This methodology has already been used to produce the first prototype IC, a 4:1 down-converter fabricated in 65 nm CMOS. This test-bed will allow for different modes of operation (addition of external capacitance, multi-phased converter using daisy-chained devices, load switching, etc.). The design will be tested in early 2013. It achieves a relatively low power density, but will be an important analysis tool and stepping-stone to our next prototype.

Preliminary work on the design selection has already begun for the second prototype. We are focusing now on only a few design types and transistor options. It is clear that more work will be needed on process optimization to achieve the desired efficiency (beyond 70%). We ultimately hope to achieve power density in the range of 100 mW/mm^2, at a ratio 4:1 or better.

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