LBNL-5435E

Laboratory Directed Research and Development Program FY 2011

May 2012

Report on
Ernest Orlando Lawrence
Berkeley National Laboratory

Laboratory Directed Research and Development Program

FY 2011

BERKELEY LAB

Ernest Orlando Lawrence
Berkeley National Laboratory
Berkeley, CA 94720

MAY, 2012

Prepared for the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

Table of Contents

Introduction ix

Accelerator and Fusion Research Division 1

André Anders	Plasma-Assisted High Rate Deposition Concept for Energy Applications	1
John Byrd, Russell Wilcox	Attosecond Synchronization for Future Light Sources	2
Paolo Ferracin	Fourth Generation ECR Ion Sources	3
Derun Li	Experimental Accelerator R&D Towards a Future Source at LBNL	4
David Robin	Novel Accelerator and Engineering Strategies for Ion Beam Cancer Therapy	5
Peter Seidl	Ion Beam Driven Fusion and Fusion-Fission Hybrids	6
Jeroen van Tilborg	Experimental Realization of a High-Harmonics-Seeded, Laser-Plasma-Accelerator Driven Free-Electron Laser	7
Jonathan Wurtele	Linac Driver and Coherent Soft X-ray Sources	8

Advanced Light Source Division 9

Alexander Hexemer, Howard Padmore, Ting Xu, Thomas Russell	Long-Range Ordering of Block Copolymers on Faceted Silicon	9
David Kilcoyne	Search for a Permanent Electron Electric Dipole Moment (EDM)	10
Martin Kunz, Nobumichi Tamura	Structure Solution of Inorganic Materials Using Energy Resolved Laue Microdiffraction	11
Alastair MacDowell, et al.	X-ray Fluorecence Tomography – 3D Elemental Mapping	12
Stefano Marchesini	Nanoscale Surveyor	13
Howard Padmore	High Quantum Yield Multi-Alkali Cathodes for psec Pulsed Electron Sources	14
Hendrik Bluhm, Zahid Hussain, Tolek Tyliszczak	Ambient Pressure Photoemission Spectromicroscopy	15
Tony Warwick	Test Monochromator/Spectrometer Systems with Prototype High Density Gratings for High Resolution X-ray Scattering	16
Wanli Yang, et al.	Soft X-Ray Spectroscopy of Lithium and Conductive Polymers for Li-Ion Batteries	17
Kenneth Goldberg, Valeriy Yashcuk	X-Ray Optical Metrology for Coherence-Preserving Adaptive Optics	18

Chemical Sciences Division **19**

Ali Belkacem, et al.	Scientific Tools in Multi-Dimensional X-ray Spectroscopy and Coherent Diffractive Imaging	19
Dmitry Budker, Holger Mueller	Direct Comb Spectroscopy of Lithium in the Vacuum Ultraviolet and Beyond	20
Mary Gilles	Development of *In Situ* Cells for Reactive Spectroscopic and Microscopic Studies	21
Charles Harris	Dynamics of Homogeneous Catalysis Reactions Investigated with Transient Two-Dimensional Infrared Spectroscopy	22
Wayne Lukens	Investigating f-Electron Exchange in Actinide and Lanthanide Complexes	23
Thorsten Weber	Double-Auger Emission of Small Molecules Following Core-Excitation and Ionization	24

Computing Sciences (National Energy Research Scientific Computing Center, and Computational Research Divisions) .. **25**

Deb Agarwal, Keith Jackson	Enabling HPC Workflows on Clouds	25
Shane Canon	Defining an Ecosystem to Support Data-Intensive Science	26
Xiaoye Li	Next Generation Computing for X-ray Science	27
Peter Nugent	*Nyx*: The Lyman Alpha Forest Cosmology Simulator	28
Chao Yang, Stafano Marchesini	Computational Techniques for Non-crystalline X-ray Diffraction Imaging	29

Earth Sciences Division **30**

Eoin Brodie	Uncovering the Mechanistic Basis for Soil Microbial Community Response to Altered Precipitation Patterns	30
Michael Commer	Enhanced Subsurface Fluid Characterization Using Joint Hydrological and Geophysical Imaging	31
James Davis	Effect of Mineral Coatings on Biogeochemical Processes	32
Christer Jansson	CyanoAlkenes: Engineering Cyanobacteria for Phototrophic Production of Advanced Biofuels	33
Curtis Oldenburg	CO2 as Cushion Gas for Compressed Air Energy Storage in Subsurface Reservoirs	34
David Romps	Interactions Among Cloud Processes, Convection, and Climate Change	35
Rohit Salve, William Dietrich, Stefan Finsterle	Identifying and Predicting Climate Change Impacts on the Land-Based Components of the Water Cycle	36
Young-Soo Han, Tetsu Tokunaga	Testing a New Carbon Sequestration Strategy by Accelerating Calcite Precipitation in Soils	37
Margaret Torn	Biological Carbon Sequestration: Fundamental Research on Biological Carbon Capture and Soil Carbon Stabilization	38

Quanlin Zhou	Collaboration with China on Geologic Carbon Sequestration: Novel Field Tests to Characterize Heterogeneity for China's First Pilot Test	39
Engineering Division		**40**
Diego Arbelaez	Investigation of Image Current and Magnetic Field Tolerance Effects on High-Temperature Superconductor Undulators for Soft X-ray FELs	40
Rafael Gómez-Sjöberg	Parallel Microfluidic Synthesizer: A Fully Automated Chemical Evolution Platform for Novel Materials Discovery	41
John Joseph	Real-Time Data Compression for High Speed Imaging X-Ray Detectors for the Next Generation Light Source	42
Soren Prestemon	Development of Variable-Polarization Superconducting Undulators for Soft X-Ray FEL Radiators	43
Soren Prestemon	Development of a Calorimeter for the Measurement of Image-Current Heating on Wakefield-Surfaces for High-Performance Undulator Applications	44
Environmental Energy Technologies Division		**45**
Katie Coughlin, David Fridley	Physical Accounting for Alternative Energy Pathways	45
Marc Fischer	Toward a US Greenhouse Gas Information System (GHGIS)	46
Ashok Gadgil	Developing a Fuel-Efficient Cookstove for Haiti	47
Eric Masanet, Surabi Menon	Developing Analytical and Communications Frameworks to Enable Breakthrough Low-Carbon Technologies	48
Thomas McKone	Life Cycle Analysis of Geologic Carbon Sequestration	49
James McMahon, et al.	Mapping Genes to Salty Acres: Engineering Switchgrass Lines for Large Scale Biofuel Production on Marginal Lands	50
Surabi Menon	From Fossil Fuels to Photovoltaics: Economic, Environmental, and Health Impacts for Policy Considerations	51
Kristin Persson	Accelerated Materials Design Through First-Principles Calculations and Data Mining	52
Stephen Selkowitz, et al.	Dynamic Light Redirection by Optical Metamaterial Coatings	53
Michael Wetter, Wangda Zuo, Alberto Sangiovanni-Vincentelli	Building Systems for Net Zero Energy Buildings	54
Genomics Division		**55**
Sam Deutsch, Eddy Rubin	Highly Parallelized, Low-Cost Synthesis of Microbial Genes Using High-Density Oligonucleotide Arrays	55
Axel Visel, Zhong Wang, Stephen Gross	Transcriptome Analysis of *Agave*, a Candidate for Biofuel Feedstock for Semi-Arid Climates	56

Life Sciences Division **57**

Eleanor Blakely	Synchrotron-Based Microtomography for Functional Analysis of Normal Tissue and Tumor Molecular Markers, and Their Perturbation by Low-Dose Radiation Exposure	57
Gary Karpen	Identification and Analysis of Proteins that Regulate the Dynamic Response of Heterochromatin to Radiation	58
Mark LaBarge	Determination of Impact of the Microenvironment and Tissue-Level Self-Organization on Cell Fate Decisions and Homeostasis in the Mammary Gland, to Ultimately Inform Drug Discovery	59
Jian-Hua Mao	Identification of Genetic Networks Controlling Susceptibility to Radiation-Induced Carcinogenesis	60
Cynthia McMurray	SPARKLE- A Fluorescence Energy Transfer (FRET) Methodology for Visualization of Simultaneous and Reversible Interactions	61
Trent Northen	Modeling Desert Soil Crust Microbial Community Responses to Pulsed Climate Events	62
John Tainer	Enabling Structural Systems Biology at NGLS	63
Daojing Wang	Multinozzle Arrays for Single Cell Metabolomics	64
Claudia Wiese	Functional Characterization of *NUCKS*- a Potential Cancer Susceptibility Locus Required for Recombination	65

Materials Sciences Division **66**

Joel Ager	Induced "Bucket Brigade" Photovoltaic Effect	66
John Clarke, Harmut Haffner	Heating Rates of Planar Ion Traps for Quantum Information	67
Robert Kaindl, Joseph Robinson, Zahid Hussain	Attosecond XUV Condensed-Matter Science: Electronic Wavefunction Coherence and Correlated Dynamics	68
Robert A. Kaindl, Jeff Urban, Emory Chan, Robert Schoenlein, Lin-Wang Wang	Ultrafast 2D Fourier-Transform Spectroscopy of Electronic Dynamics in Photovoltaic Nanomaterials	69
Joseph Orenstein, Joel Moore, Ashvin Vishwanath, Ramamoorthy Ramesh, Alessandra Lanzara	Probing and Controlling Spin and Charge in Strong Spin-Orbit Materials	70
Berend Smit	Tuning the Self-Assembly of Membrane Proteins	71
Matthew Tirrell	Structured Charged Polymers	72
Wladysiaw Walukiewicz, Kin Man You,	Intermediate Band Solar Cell – Proof of Concept and Search for New Materials	73
Feng Wang	Integrated Optoelectonic Devices Based on Graphene	74

Peidong Yang, Ali Javey, Junqiao Wu	Design and Surface Properties of Semiconductor Nanowires	75
Yuegang Zhang	Surface-Selective Synthesis of Graphene Nanoribbons on Nanowire Templates	76
Haimei Zheng	Imaging Through Liquids Using a TEM	77
Nuclear Science Division		**78**
Stuart Freedman, Yury Kolomensky	Bolometric Detectors for the Neutrinoless Double-Beta Decay Experiments	78
Kenneth Gregorich	Heavy Element Mass Analysis and Detector Capabilities	79
Wick Haxton	Lattice QCD Codes by Discretizing Time and Space	80
Constantin Loizides	Probing the Partonic Structure of Protons and Nuclei with Isolated Photons at the LHC	81
Physical Biosciences Division		**82**
Paul Adams, Philip Coppens	Direct Determination of Electrostatic Interactions Through Advanced Analysis of High-Resolution Macromolecular Crystal Data	82
Daniel Fletcher, Cheryl Kerfeld, Philip Geissler,	Assembly and Function of Organelles for Carbon Fixation	83
Héctor García Martín, Aindrila Mukhopadhyay	Metafluxomics of a Phosphorus Removing Microbial Community	84
Nathan Hillson	Advances in Standardized, Scar-less, Sequence-Independent Cloning Methods	85
Seung-Wuk Lee, Ramamoorthy Ramesh	Pizoelectric Biomaterials for Novel Energy Conversion	86
Henrik Scheller	Engineering of Drought and Heat Tolerance in Bioenergy Crops	87
Christopher Voigt	Engineering Thermophilic Bacteria for Converting Hydrocarbon to Valuable Chemicals, Methyl Halides	88
Petrus Zwart	Development of Reusable Software Modules for the Analyses of bioSAXS Data	89
Petrus Zwart	Feasibility and Development of Fluctuation X-ray Scattering for the NGLS	90
Physics Division		**91**
Chris Bebek, Jerry Edelstein, David Schlegel,	Fiber System Development for Surveys of Baryon Acoustic Oscillations (BAO) Applicable to the Future BigBoss Experiment	91
Richard Muller	Gathering and Analysis of Worldwide Land Temperature Data	92
Yasnori Nomura	Theoretical Studies of Dark Matter Beyond the Standard Model	93
Henrik von der Lippe	High Voltage Up- and Down-Converters for Low Power, Low Density Detector Instrumentation	94

Cross-Divisional **95**

Cheryl Kerfeld, Adam Arkin, Eddy Rubin	Predictive High-Throughput Assembly of Synthetic Biological Systems: From Gene Expression to Carbon Sequestration	95
Delia Milliron, Jeffrey Urban, Yuegang Zhang, André Anders, Thomas Richardson	Multifunctional Window Coatings for High-Performance Buildings	96

Publications List **97**

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) 2011 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 2012, 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 FY2011* 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 (dated April 19, 2006). 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 FY2011, Berkeley Lab was authorized by DOE to establish a funding ceiling for the LDRD program of \$23.1M including General & Administrative (G&A) overhead, which equated to ~3.3% of Berkeley Lab's FY2011 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 \$20.4M was expended for operating expenses (2.85% of actual Berkeley Lab FY2011 operating and equipment costs excluding ARRA funding).

In FY2011, scientists submitted 209 proposals, requesting about \$44.1M in funding prior to assessing laboratory overhead. Ninety six projects were funded, with awards ranging from \$65K to \$960K. These projects are identified in the Table of Contents.

Accelerator and Fusion Research Division

LB10032

Plasma-Assisted High Rate Deposition Concept for Energy Applications
Principal Investigator: André Anders

Project Description

The purpose of this project was to significantly enhance (by a factor 2 or greater) the deposition rate of coatings used in energy-related devices such as solar panels, solar concentrators, photo-catalytic surfaces, and energy-efficient windows. Specially, we consider low-cost (indium-free) high quality transparent conducting oxide films. Such films are currently produced by reactive sputtering, a well established but slow and costly process.

It is straight-forward to increase the absolute deposition rate by simply increasing the power to the sputtering system, however, this approach runs into serious limitations such as overheating of the apparatus, followed by melting of the target and damage to the magnets, and switching to the undesired arcing mode. In this project we explored innovative ways of enhancing the absolute and relative (power-normalized) deposition rates while maintaining the features of plasma assistance to film growth. We investigated hot target sputtering, high power impulse magnetron sputtering, and filtered arc deposition, and considered the issues of too energetic negative ion bombardment, which is detrimental to the quality of crystalline films.

Accomplishments

We picked aluminum doped zinc oxide (AZO) as a sample material of special interest since it has the potential to replace the much more expensive and less abundant indium tin oxide. Hot target sputtering turned out to deliver excessive zinc vapor fluxes. We therefore focused on particle-filtered arc deposition and negative-ion-filtered high power impulse magnetron sputtering. We showed that especially the arc method delivered excellent material at very high rate, namely about factor 4 greater than conventional techniques. After optimizing substrate temperature and partial gas pressures, AZO films could be made from abundant, very low cost ($40/kg) zinc stock material with superior optical and electrical properties. Specifically, the electron mobility could be pushed up to 60 cm^2/Vs, compared to the typical 20-40 cm^2/Vs obtained in sputtered AZO. This enabled us to limit the carrier concentration, thereby making the films transparent in both the visible and infrared part of the solar spectrum. The material can be applied to multi-junction solar cells and electrochromic windows. Follow-up work is ongoing funded by DOE-EERE.

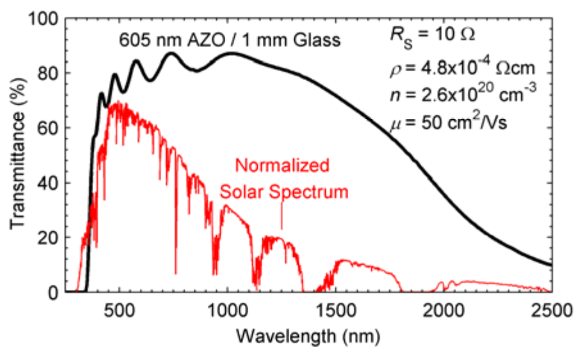


Figure: Transmittance of aluminum doped oxide made at very high rate; note the high mobility and match to the solar spectrum. The corresponding publication [R. J. Mendelsberg, et al., J. Phys D: Appl. Phys. 44, 232003 (2011)] was downloaded over 500 times in the first 90 days after publication.

LB11006

Attosecond Synchronization For Future Light Sources
Principle Investigators: John Byrd, Russell Wilcox

Project Description

Optical pump/x-ray probe experiments at ultrafast light sources require a precise synchronization between the x-ray and optical pulse. Our present generation timing system with resolution of ~10 fsec is in use now at LCLS and Fermi@Elettra. We are developing a novel approach for synchronization of remote lasers by locking corresponding lines in the mode-locked optical spectrum. This new technique holds the promise of reaching fsec and sub-fsec levels of synchronization. This will become a critical enabling technology for future ultrafast free electron lasers.

Our approach to reach sub-fsec stability uses stabilized optical fiber links to lock the optical carrier to a comb line in a carrier/envelope/phase (CEP) stabilized mode-locked laser. Locking the optical carrier at the other end of the link to the same harmonic in a second CEP-stabilized laser should allow sub-fsec level synchronization of the two lasers over separation distances of several hundred meters.

Accomplishments

We have achieved three important results towards experimental demonstration of sub-fsec synchronization. The first is publication of journal paper in which many of the details of the approach are described. The second is the formation of a collaboration with a leading German company in order to test the approach on CEP-stabilized laser systems. The third result is that some initial tests were completed at LBNL to test subsystems part of this approach.

Our corporate partner manufactures CEP-stabilized fiber and titanium sapphire lasers, a spinoff from the original CEP stabilization work done at Max Planck Institute for Quantum Optics. As part of this collaboration, we were able to assemble two CEP-stabilized fiber laser comb systems, a cavity-stabilized CW diode laser, other equipment to test a version of the proposed synchronization concept where two lasers are synchronized to a CW laser master clock. This involved improved laser controls that could eliminate more of traditional high frequency jitter. We were able to show that this type of comb laser can be locked to a CW source, using a new high-speed intracavity EO crystal offered by our collaborator.

We completed two laboratory demonstrations of parts of the synchronization system. The first experiment selected a spectral line from a modelocked laser, phase locked a CW laser with this line, transmitted the CW signal through an interferometer and then compared the transmitted signal with the original spectral line using optical interference. We were able to lock the CW laser to the spectral line to less than 1fs, and transmit the line with an additional 0.4fs jitter, showing that these techniques are adequate for the proposed sync system. This experiment locked a CW fiber laser to the spectral line using a phase-locked loop. In a second experiment, we tried an alternative technique where a CW diode laser is injection locked to the spectral line of a modelocked laser. We were able to characterize the locking range of the diode laser and seed it with a few spectral lines, but we lacked a narrow bandpass filter to select a single line, so the laser output was not sufficiently stable.

LB11008

4th Generation ECR Ion Sources
Principal Investigator: Paolo Ferracin

Project description

Next-generation heavy ion beam accelerators such as a proposed radioactive ion beam accelerator (Facility for Rare Isotope Beams, FRIB) in the US, the Radioactive Ion Beam Factory at RIKEN, the GSI upgrade project, and the LHC-upgrade require a great variety of high charge state ion beams with unprecedented high currents. ECR (Electron Cyclotron Resonance) ion sources are ideal injectors for these heavy ion facilities because of their versatility and reliability. ECR sources are therefore widely used for the production of high quality multiply charged ion beams.

Increases in the magnetic confinement fields in combination with higher microwave frequencies are directly linked to increases in the plasma density, the confinement time and reducing the neutral gas density in the plasma. The relationship between performance and ion source design parameters was recognized early on in the development of ECR ion sources, and summarized in Geller's famous ECR scaling laws, which predict that the extractable ion current scales roughly with the square of the microwave heating frequency if the magnetic confinement field is scaled appropriately. The development of the VENUS magnet combined with its advanced source and beam line design has pioneered the field of high field superconducting ECR ion sources.

The scope of this LDRD is to develop a conceptual design of a magnetic design and structure capable of reaching the fields required for optimized operation of a 56 GHz ECR ion source as a first step in the development of such a novel ECR ion source. Preliminary analysis indicates that the magnet requirements are achievable with state-of-the-art Nb3Sn superconductors. The proposed effort includes a review of possible solenoid-sextupole configurations, review of conductor options and their impact on system operation and cryogenics, developing a concept for the clamping structure, and optimizing the structure for building an ECR into the warm bore. The study will include a preliminary estimate for the cost range of such a magnet structure and the ECR ion source. The goal by the end of this year is to have a feasible concept for the magnetic field structure that will allow us to submit a proposal to DOE for further funding for a detail engineering design.

Accomplishments

A 3D modeling of the Gen IV-ECR magnet and support structure has been successfully completed. The model provides an excellent basis to proceed with the design and fabrication of a prototype magnet. The analysis includes a full 3D calculation of the magnetic fields, the Lorentz forces and methods to assemble and prestress the structure. The calculations indicate that it is essential to use a full 3D model because of the interactions between the coils, which are much more complex than in the case of a simple solenoid, dipole or quadrupole. The design, assembly and testing of the magnet cold mass appear to be the most challenging aspects of building a fourth generation ECR ion source and this will require a team with the appropriate expertise. The conceptual design of the cryostat shows that there are a number of improvements that can be made to extend the cryostat used on VENUS to work with the GenIV-ECR. Finally, it appears that using a RF delivery system tailored to the short wavelength of the high frequency gyrotrons could improve the RF coupling and provide further gains in the performance.

The work funded by this LDRD has been presented at the 14th Int. Conf. on Ion Sources (ICIS11), held on September 12th-16th, 2011 in Giardini Naxos, Italy, and reported on a paper accepted for publication in Rev. Sci. Instrum. The proposal has been selected for an Early Career Research Program award (2.5 M$).

LB09007

Experimental accelerator R&D toward a future light source at LBNL

Principal Investigator(s): Derun Li

Project Description

There is a scientific research need for a facility capable of generating high repetition rate and high brightness photon pulses, with full coherence and ultrafast time duration. In response to this need, LBNL has proposed the construction of a next-generation light sources (NGLS) based on a high repetition rate Free Electron Laser (FEL). The purpose of this proposal is to support experimental accelerator R&D toward the NGLS at LBNL. In order to build such a machine, several key questions must be answered first. This proposal basically addresses some of those questions and proposes the design and the construction of critical parts and the study and analysis of several issues that may significantly affect the construction and the cost of the NGLS. The R&D activities in this proposal include: (1) Design and testing of a fast kicker and pulser for ~ns rise/fall time, 10 ns pulse, 3 mrad deflection, with high stability and reliability, which is required for beam spreading of the NGLS; (2) Evaluation of superconducting linac RF parameter choices for NGLS; (3) Analysis of design challenges for CW harmonic cavities for NGLS.

Accomplishments

A MOSFET switch with the necessary drive electronics has been prototyped and tested to the full peak power of the system. The circuit has demonstrated it can deliver the peak power with <5 ns rise and fall time. Four of these circuits have been connected in a transmission line adder configuration, and the concept of voltage addition was demonstrated. A prototype magnet was designed, built, and some preliminary testing was done to show that the magnet impedance agrees with the 50 Ω design goal.

A parameterized top-level design and cost model for NGLS has been established to illuminate choice of SRF gradient, bath temperature, cryogenic infrastructure, etc. We have required a survey of current state-of-the-art of SRF gradients and Qs, and investigated likely Higher Order Mode (HOM) beam losses for NGLS, researching dependence on cavity shape, frequency spectrum (extends to the THz regime after the bunch compression steps), and amount of heat to be absorbed by 2K bath. We also developed a conceptual design for a wideband waveguide HOM absorber with fundamental frequency rejection via symmetry. The absorber design includes features to make it nearly perfect in the optical limit (short bunch, high gamma).

A simulation model has been established to study a multi-cell superconducting harmonic RF cavity, wakefield and impedance. Preliminary simulation results are achieved and will be used to guide, and explore design challenges in order to meet the required performance for NGLS.

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 Bevatron 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. Critical to the new 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 magnetic fields strong enough to bend the ion beam.

To precisely guide the stream of accelerating, heavy carbon ions around the curve through the toroid, we used intensive computer modeling to simulate the required magnetic fields, and further to determine the optimal placement for the opposing coils as they wrapped around the toroid. To precisely guide the stream of accelerating, heavy carbon ions around the curve through the toroid, we found the magnetic field requirements. To determine how to precisely guide the stream of accelerating, heavy carbon ions around the curve through the toroid, we used intensive computer modeling to simulate the required magnetic fields and to ascertain the optimal placement for the opposing coils as they wrapped around the toroid.

We are now in the process of understanding the feasibility of constructing such a winding and with the goal of building a prototype coil.

LB10012

Ion Beam Driven Fusion and Fusion-Fission Hybrids
Principal Investigator: Peter Seidl

Project Description

We assess 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, radially-zoned liquid-salt cooled pebble bed and other subcritical fission blankets were performed in the first year of this LDRD series. 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 this second year of the LDRD, we focused a greater fraction of our effort on heavy ion fusion (HIF). We explored new accelerator driver systems to increase our confidence in HIF. Novel accelerator designs and beam manipulations were explored, with an emphasis on seeking breakthrough techniques that would enable a high-reliability driver at reduced cost.

Accomplishments

We studied the beam physics for the creation of high-charge state beams for high-current heavy-ion accelerators to drive inertial fusion energy targets. To date, most accelerator designs assume singly ionized heavy ions of atomic mass A>100, which have been proven to be feasible for high current and low emittance. Heavy-ion inertial fusion (HIF) would benefit from low-emittance, high current ion beams with charge state >1. For average accelerator gradients of a few MV/m, the total accelerator length is several km. Higher charge state ions with suitable beam parameters would enable shorter accelerators. We explored the space charge, multiple scattering and straggling implications of stripping a singly ionized beam (q=1) to a higher charge state (q=12) shortly after injection. Our models were based on beam parameters that have recently been considered for heavy ion fusion, and analytical models for straggling and multiple scattering. To capture the nonlinear space charge forces between groups of ions with different charge states as they separate, we modeled a chicane (a series of four dipoles) using the particle-in-cell accelerator code Warp, to follow the charge state separation for a nearly monochromatic input beam. We concluded that energy spread in the stripper would increase the longitudinal emittance. Transverse emittance growth due to space charge is significant, but magnetic separation of charge states after the stripper can lower the emittance growth. The results, presented at the Particle Accelerator Conference, suggest that further study is of interest.

The National Ignition Facility campaign of ignition experiments are underway and generating much excitement in the fusion community. These are stimulating interest in various inertial fusion energy systems, including Heavy Ion Fusion (HIF). To that end, we engaged the interest and expertise of a wide range of accelerator physicists before and during workshop at LBNL on Accelerators for Heavy Ion Fusion. The participants expressed interest in a follow-up collaboration to address key issues in greater detail. Finally, we contributed to presentations and reports to the National Academies of Sciences and Engineering review of "Prospects for Inertial Confinement Fusion Energy Systems."

LB11035

Experimental Realization of a High-Harmonics-Seeded,
Laser-Plasma-Accelerator Driven Free-Electron Laser
Principle Investigator(s): 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 proposed system will benefit the non-linear X-ray community and serve as a test-bed for seeded FEL's.

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. 5% of the 2-Joule, 35-fs T-Rex laser pulses will be split off and this portion will be reflected off an overcritical plasma mirror for HHG production. Through an estimated conversion efficiency of $\sim 5 \cdot 10^{-6}$ per harmonic order, and considering soft X-ray losses in subsequent optics, it is expected that approximately $>1 \times 10^{11}$ seed photons are delivered to the undulator. Such a strong flux is expected to sufficiently compensate for the large seed beam divergence. The remaining 95% of the laser pulse will be used to produce femtosecond 0.5-GeV-class electron beams in a capillary-based LPA.

Accomplishments

We have developed two designs for HHG production, namely HHG in a gas-cell (gas-based HHG) and HHG from a plasma mirror through coherent wake emission (CWE HHG). Based on several considerations (practical implementation, e-beam & seed combining, and photon flux) we have selected CWE HHG as our primary approach. The plasma mirror used for CWE production will also serve as the combining optic, whereas the large divergence of the seed beam is compensated by the absence of transport optics losses. Our design integrates a CWE line with the already existing LPA, undulator, and soft-X-ray spectrometer. Temporal synchronization will be intrinsically guaranteed.

We have performed simulations with the code THUNDER to confirm that coherent build-up of undulator radiation is achievable for our parameters. The coherent gain is sufficiently large to study seeding concepts such as timing, overlap, divergence matching, and gain. With the gain potentially up to 3 orders of magnitude, this compact LPA-based FEL could have great scientific potential.

We have designed and built a CWE HHG test setup, allowing us to diagnose the soft X-ray seed production. A plasma mirror based on a circulating solid-density VHS tape is in place, with good shot-to-shot reproducibility and surface uniformity. An ultra-thin aluminum foil will block remnant laser light, after which a transmission grating spectrally disperses the soft X-rays. A large area micro-channel plate (with phosphor screen on the back) and an imaging CCD camera will measure the single-shot spectral profile. With all components in place, the seed source characterization will commence soon.

LB10024

Linac Driver and Coherent Soft X-ray Sources

Lead Investigator: Jonathan Wurtele; Other Investigators: J. Corlett, G. Penn, D. Prosnitz, J. Qiang, M. Reinsch, M. Venturini (AFRD), B. Austin (NERSC)

Project Description:

Key performance metrics for soft x-ray FEL facilities include the capability to deliver high peak and average radiation power to a large number of simultaneous users, generation of pulses with high degree of transverse and longitudinal coherence and adjustable pulse length down to the attosecond scale and capability to produce pairs of radiation pulses with adjustable time delay for pump-probe experiments. The development of an integrated multi-beamline FEL facility that satisfy these users requires the production and acceleration of high brightness electron bunches and finding a workable scheme for seeding high repetition rate FELS. A variety of options for seeding are under active investigation (i.e., EEHG, direct seeding, self-seeding) and new concepts for ultra-high repetition rates are being pursued at a lower level (e.g., use of FEL oscillators to produce seed radiation). New numerical modeling capabilities are needed to study the potential beam-physics limitations to the manipulations required in such FELs, while checking for consistency with the best electron bunch quality that can be delivered by the accelerator. Integrated analysis tools will be developed to study the limits and performance tradeoffs for a wide range of sub-system design choices. The tool will allow us to quantify how parameter choice impact X-ray FEL performance and to develop a risk-balanced facility with an optimal performance/cost ratio. The main objective is to develop integrated modeling of high-brightness beam creation, acceleration, and coherent x-ray production and to be able to optimize performance of the FEL as sub-systems are varied (due to cost or risk) and to find robust risk balanced designs.

Accomplishments:

We have developed an integrated modeling tool, the STAFF (System Trade Analysis for an FEL Facility) code. This unique code allows for rapid analysis of system sensitivity and risk balance, and to optimize the integrated system in terms of performance metrics such as photons/pulse, photons/sec and tunability range. STAFF is a MATLAB program that enables the user to rapidly explore a large range of Linac and FEL design options to meet science requirements. STAFF's modular design simplifies the inclusion of new physics models for FEL harmonics, wake fields, cavity higher-order modes and aspects of linac design such as the optimization of a laser heater, harmonic linearizer, and one or more bunch compressors. Microbunching instability and multiple undulator technologies were included in the STAFF code. Initial optimization of the integrated system in terms of performance metrics such as harmonic generation, photons/pulse, photons/sec and tunability range were performed. We evaluate the jittering effects on the proposed modulation compression scheme for generating short wave length seeding and applications to the generation of atto-second coherent X-ray radiation. We developed lattice designs for a moderate-energy linac driver of a high-repetition rate FEL and by numerical modeling of the main collective effects we demonstrated its capability to deliver beams with the required brightness. We performed analysis and simulation studies of EEHG seeding scheme down up to 1 keV photon energy, including the effect of ISR and characterized requirements on laser and electron beam quality for EEHG to be effective. We generated models for harmonic output from FELs driven by nonlinear bunching from the fundamental near saturation and quantified the minimum requirements for the use of HHG laser sources as a seed for a FEL, including a subsequent jump in the FEL to an even higher photon energy.

Advanced Light Source Division

LB10009

Long-range Ordering of Block Copolymers on Faceted Silicon

Principal Investigators: Alexander Hexemer, Howard Padmore, Ting Xu, Thomas P. Russell

Project Description

The purpose of this project is 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, tens of 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 route to generate highly oriented and highly ordered arrays of BCP microdomains on inexpensive, flexible polymeric substrates where the lateral ordering is as good as that seen on hard surfaces. The use of polymer substrates enables the use of both SFM and transmission SAXS to characterize the lateral ordering and orientation of the microdomains. The well-developed arrays of BCP microdomains in thin films can be used as templates for pattern transfer or scaffolds for the deposition of a wide range of materials for the fabrication of inexpensive, flexible devices.

We have also succeeded to produce unidirectionally aligned line patterns from the directed self-assembly (DSA) of BCPs on reconstructed faceted single crystal surfaces or on flexible, inexpensive polymeric replicas over arbitrarily large areas. A high fidelity pattern transfer to an imprint mold, i.e. a secondary master, was realized. These films are ideal platforms for the fabrication of magnetic storage media, polarizing devices, and arrays of nanowires.

We have also accomplished to fabricate ultradense circular nanolines over macroscopic areas by the DSA of BCPs on topographically patterned substrates. BCPs on the topographically patterned substrates undergo a DSA with solvent annealing, resulting in a flat BCP film with an areal density multiplication of the circular patterns over large areas. This methodology may provide an easy approach to high densities of circularly shaped nanopatterns that can be used to generate a topographic pattern to orient BCP microdomains normal to the surface, as seen with faceted surfaces, which is of interest for data storage device manufacturing.

LB10034

Search for a Permanent Electron Electric Dipole Moment (EDM)
Principal Investigator: David Kilcoyne
Co-Investigators: Harvey Gould, Charles Munger, Benedict Feinberg, Juris Kalnins

Project Description:

The purpose of this project is to develop the technology needed to increase signal intensity, improve systematics suppression, and reduce magnetic field noise as the start of a new experiment to discover or rule out a permanent electric dipole moment (EDM) of the electron as small as 2×10^{-50} C-m (a factor of 100 below the present limit).

Since 1990, almost all improvements to the electron EDM upper limit have come from a series of thermal atomic beam experiments at LBNL, begun in 1987 by Harvey Gould and Eugene Commins and disbanded in 2002. To make further progress, a proof-of-principle laser-cooled fountain EDM experiment was performed. The analysis of that experiment and an internal LBNL review identified signal intensity, systematics suppression, and magnetic noise as needing further improvement to reach an electron EDM limit of 2×10^{-50} C-m. Electron EDM experiments search for a difference in energy between an unpaired electron aligned and anti-aligned with an external electric field. High atomic number paramagnetic atoms such as Cs, Tl, and Fr provide test systems of zero net charge and enhanced sensitivity to an electron EDM.

The aim is to complete a linear optics solution for focusing Cs atoms that will result in most of the atoms passing through the electric field and being detected, to have performed calculations that show how to reach systematics limits well below 2×10^{-50} C-m, and to have constructed a 4-layer prototype magnetic shield designed to reach a transverse shielding factor of 5×10^{7}.

Accomplishments:

"Electrostatic end-field defocusing of neutral atoms and its compensation," by Juris Kalnins has been published in Physical Review Special Topics - Accelerators and Beams (14,104201 [2011]) which is an open access electronic journal.

The four-layer, half-scale prototype magnetic shield assembly test stand was fully assembled and used for radial and axial shielding factor measurements, end cap effect (including port hole-size effect) and effective permeability measurements, and demagnetizing and remnant field studies. Shielding factors came in near the upper (most optimistic) end of our calculations and field uniformity is satisfactory. The end caps work properly, and the port design is effective at preventing stray fields from penetrating the shields. The basic design used here, and extended to a fifth layer of shielding will shield external magnetic field noise to below the levels needed for a sensitive electron EDM experiment. After checking the measurements and completing a short follow-on study, a manuscript will be prepared for publication.

Calculations of electron EDM mimicking effects in cesium have been completed and a manuscript (of over 20 journal pages) is being readied for submission to Physical Review. In late 2010 we learned of the availability of francium beams at TRIUMF and estimated that relative to its EDM sensitivity, it could be two orders of magnitude less sensitive to systematic effects than cesium. However the francium isotopes available have total spin $F = I + J = 5$, compared to $F = 4$ for cesium. The difference in spin (higher is better) and especially the change from even spin to odd spin required extending the computer code and reworking some parts of the calculation.

In addition, francium being heavier than cesium and having lower scaler polarizability than cesium, it defocuses less than cesium upon entering electric field plates but also focuses less in the focusing lenses. The computer simulations for end field defocusing and focusing in cesium have been modified for francium and can be used for future studies on francium.

LB10011

Structure solution of inorganic materials using energy resolved Laue microdiffraction
Principal Investigators: Martin Kunz, Nobumichi Tamura (ALS)

Project description

Laue X-ray microdiffraction is a powerful tool for mapping grain orientation and strains in polycrystalline materials and single crystals with submicron spatial resolution. The use of white radiation allows simultaneously satisfying Bragg condition for a number of reflections. However, Laue diffraction is intrinsically "blind" to the energy attached to the individual reflection so that the use of their intensity is usually neglected. The purpose of this LDRD project was to develop software and experimental tools to enable routine structure solution and structure refinement from micron- and sub-micron grains as typically investigated in x-ray microdiffraction experiments. This opens ALS beamline 12.3.2 to an entire new set of scientific problems and thus increases its scientific impact.

Accomplishments

The successful completion of this project was divided into 3 steps.

1) Experimental procedure: The precise alignment of very small crystals on a very small beam is a non-trivial problem. We developed sample mounts, optical setup and appropriate software to correlate high-resolution optical images with XRF maps of defined markers to enable a fail proof sample alignment without long diffraction searches which could be potentially harmful to radiation sensitive samples. In addition the minimal requirements in terms of number of reflections necessary for structure solution or refinement as a function of structural complexity and structure solution method applied were mapped out.

2) Proper intensity correction: The main obstacle here is the proper application of energy dependent correction factors to each individual reflection. We succeeded in the development of a method to extract an effective flux curve for a given combination of X-ray source and area detector. Our approach is based on comparing the calculated structure factors of a well characterized standard sample with its Laue intensities after applying a suite of analytical corrections (absorption, polarization, harmonic deconvolution). This method is to the best of our knowledge the most direct way to measure the spectrum of a white X-ray source. The effective flux determined by this way is transferable and allows to extract structure factors for any indexable phase. As a first demonstration, we managed to assign the correct indexation of a material with primitive trigonal lattice, a task hitherto impossible due to the lack of intensity information.

3) The newly developed method was successfully applied to a series of inorganic test structures with increasing complexity ($KAlSi_3O_8$, $KTiOPO_4$, zeolite). In all three cases, the crystal structure was successfully solved and refined based on Laue data only. The method is now applied for the structure solution of an unknown materials embedded in a complex matrix within the Allende meteorite. This constitutes the first application to a regular user experiment

The project seeded within this LDRD is continued by a group at ETH Zurich where it is further developed in collaboration with ALS/BL 12.3.2 and Chevron Corp.

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) 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 1500^{o}C and 2) a novel 3D imaging detector with elemental specificity.

The High Temperature Load cell will be applied to the problem of investigating 3D crack propagation within silicon carbide composite ceramics whilst operating at high temperature. Silicon carbide (SiC) composites are the currently proposed materials that show the ability to survive at high temperature while maintaining a high strength to weight ratio. Typical applications include critical high strength components operating at high temperature in hyper sonic aircraft, space re-entry vehicles and high temperature turbines for jet propulsion and power generation. In the latter case, the higher the turbine temperature the greater the efficiency – this being of relevance for 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. Temperatures of up to 1500^{o}C have been obtained. Images of SiC composite materials made by Teledyne Inc. have been imaged in 3D showing crack propagation at high temperature. More samples are required to develop a statistical sample. The data is to be used in the modeling codes being developed at various US universities as part of the long term vision of how to develop new materials via computer modeling and virtual testing.

3D Elemental imaging camera. The performance of a proposed coded aperture with reconstruction algorithms have been modeled successfully. A virtual object is successfully imaged and reconstructed in the model. The fabrication of a coded aperture is in process. The fast CCD cameras being assembled at LBNL are scheduled for delivery in Spring 2012. In the meantime we propose to use a regular CCD to establish the performance of the coded apertures currently being fabricated.

The Nanoscale Surveyor

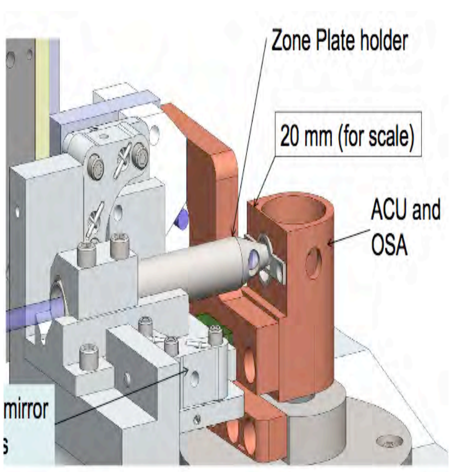
Principle Investigators: Stefano Marchesini (Advanced Light Source)

The purpose of the Nanoscale surveyor project is to develop the next generation x-ray nano-tomographic instrument. By exploiting diffraction and computational reconstruction techniques it is now possible to eliminate the tradeoff between resolution and depth of focus, enabling x-ray imaging of nanomaterials relevant to the energy mission, including nanoscale chemical imaging of nanoporous materials, polymer photovoltaics, and inorganic catalysts.

Accomplishments

In fiscal year 2011, we completed the nanosurveyor conceptual design, reconfigured beamline 9.0.1 at ALS to host the instrument, installed the instrument and received first light on Dec 11 2011. The instrument is set up for cryo- ptycho-tomography and the goal is to push the spatial resolution beyond 10nm. A new fast CCD camera collets high data rate diffraction measurements as the sample is moved across the beam with interferometrically encoded positions. The deep focus allows tomography, and the instrument is designed around this, with a cryogenic sample environment. Ultimately, this instrument will move to COSMIC at the new beamline 7.0.1.

We continued work on reconstruction methods to handle high rate vibrations, chromatic blurring and intensity fluctuations in the reconstruction process. We developed scalable high throughput code that can exploit GPU architecture to provide real time feedback. Data pipeline to be installed in the future exploits 10 Gbps connection to NERSC for processing.



Instrument
The instrument uses modest focusing to 300 nm using fresnel optical elements, sample motion of 5 mm in x-y-z, inteferometrically encoded position. rotation of 180 degrees.

LB09036

High quantum yield multi-alkali cathodes for psec pulsed electron sources

PI: Howard Padmore

Project Description

Many experiments require sources of psec dense electron beams, from those to be used for electron diffraction to free electron lasers. The generation of these beams is typically done using laser excitation on a metallic substrate. While robust, these cathodes are inefficient, typically having a quantum yield in the UV of 1e-4. The goal of this work therefore is to design and test new types of cathode based on high yield semiconductors. The system we have chosen to work with is K2CsSb, which in the green part of the spectrum can have a QE of > 5%. Our goal is to understand the growth and surface chemistry of this system so that it can be reliably used in high current pulsed electron applications.

Accomplishments

We followed on our FY10 work in which we demonstrated 6% 532 nm quantum efficiency with measurements of the growth and nano-roughness of the cathodes, and the transverse emittance.

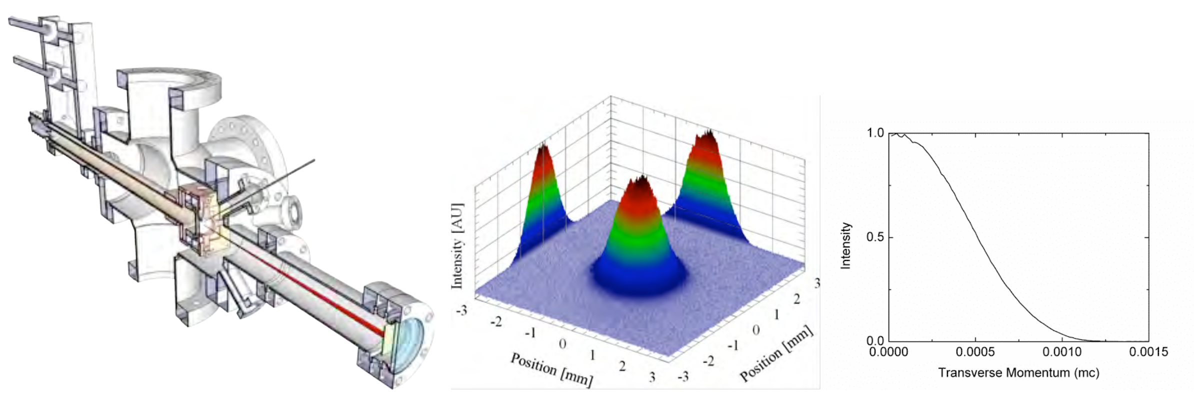


Fig. 1 Momentum analyzer (left), momentum 'image' (center) and transverse momentum distribution (right)

The growth chamber developed in previous years was modified to allow cathode transport into a new measurement chamber equipped with a new type of electron analyzer that in a simple way measures the transverse momentum distribution. This is shown in Fig 1 (left). It works by extracting electrons in a plane parallel field, through a grid, into a drift region and finally to a phosphor screen. A typical distribution is shown in Fig 1 (center). From this the normalized transverse momentum can be extracted (right). For 532 nm illumination, we achieved an emittance fo 0.36 microns / mm (rms). This is lower than that used at LCLS presently in the FEL. We also measured the effect of nano-roughness on the cathode by making 'thick' cathodes with 100 nm thickness at higher than optimum temperature, and could see a direct effect on transverse momentum. The cathodes were also tested over > 1 week, with no measureable change on the quantum yield. Finally we started experiments aimed at elucidating the structure of the cathode materials and the kinetics of growth, using in-situ x-ray diffraction.

Ambient pressure photoemission spectromicroscopy

Principal Investigators: Hendrik Bluhm, Zahid Hussain, and Tolek Tyliszczak

Project Description

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

In the new instrument under construction we are combining the principle approaches of zone plate based scanning transmission X-ray microscopy (STXM) and APPES. We are implementing the AP-SPEM in the new APPES endstation at beamline 11.0.2. This endstation features a 3rd generation differentially pumped electrostatic lens system with an acceptance half angle of better than 20 deg. Custom-designed sample cells can easily be attached and exchanged. The main challenges in the design and operation of a zone plate based APPES instrument are the due to the close proximity of zone plate and order sorting aperture (OSA) to the conical entrance aperture of the differential pumping system and the sample; the requirement for very precise alignment and motion of zone plate.

Accomplishments

We have designed and built the scanning zone plate microscope module for the ambient pressure spectrometer. At present, we are in a commissioning stage, characterizing the instrument. Initial measurements were very positive, all components of the project worked well. We were able to obtain the spectroscopic information of surface of test samples on the sub micrometer scale. The spatial resolution was lower than should be possible to achieve with the used zone plate. Investigation reviled that there are excessive vibration present. The instrument support was redesigned and the new setup made the instrument much more stable. The vibrations were lowered to the level of about 7 nm (RMS), which is very low for an instrument on the ALS floor. The beamtime is scheduled to continue commissioning in the first half of 2012.

The development of this stable platform is beneficial already in other measurements at the ALS-MES beamline 11.0.2. It should also influence design of many other endstations were stability is essential.

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

Further significant improvements have need achieved in the techniques of etching and coating faceted gratings. Etrching can now relaibly achieve facets sufficeintly smooth for multilaer coating. Several multilayer materials combinations have been studied wit h special ragard to the preservation of the initial blazeed grating structure after coating with the required number of layers. Al Zr is a candidate for soft x-ray gratings but exhibited large surface mobility and degradation of the profile. Models have been parametrized to quantify this effect in terms of power law smoothing as a fumction of spatial frequency. The degradation of diffrection efficiency has been measured and modeled and parameters determined that bring modeling into agreement with measurement. Mo/Si have exhibited less smoothing and will be adopted for spectrometer tests next year.

A UV lithography tool has been built and brought into operation and enables 20nm period gratings to be drawn in-house. This emplys a robust Lloyds mirror arrangement and the selection of process parameters has been confirmed.

This work will make possible the development of test spectrometers next year.

LB11039

Soft X-ray Spectroscopy of Lithium and Conductive Polymers for Li-Ion Batteries

Wanli Yang, Yi-de Chuang, Zhi Liu, Michael E Grass, Gao Liu, Lin-wang Wang

Project Description

The goal of this program is to establish a powerful spectroscopic probe for studying the electronic structure of Lithium ions and conductive polymers for high efficiency Li-ion batteries. Practically, the electronic structure will explain the performance and guide the optimization of the materials in a rational way. Scientifically, the accumulated efforts on soft x-ray spectroscopy will clarify many conceptual controversies to improve our understanding on the fundamental physics behind polymer conductivity, Li-ion diffusion process and the overall battery performance.

A combination of soft X-ray spectroscopy tools at three beamlines of the ALS, including X-ray absorption (XAS), X-ray emission (XES), resonant inelastic X-ray scattering (RIXS), ambient pressure X-ray photoelectron spectroscopy with spatial resolution in microns (ap-μ-XPS), will be utilized for this program. We will upgrade the *in-situ* sample preparation cells, develop new *in-situ* electrochemical cells for studying the Li-ions and polymers under real-world conditions. The spectroscopy will directly probe the density of both occupied and unoccupied electronic states of the polymers, electronic band gap and impurity states, the chemical environment of the Li-ions at different working stages, and the diffusion maps of the Li-ions in the charge and discharge process.

Accomplishments

The main accomplishments and developments of this project in this fiscal year could be summarized in three parts. (1) Established the new methodology based on soft x-ray emission spectroscopy for studying the critical energy levels in battery materials; (2) Rationalized the results on developing the new polymer binder for ultra-high efficiency battery anode through x-ray absorption spectroscopy; (3) Preliminary tests and setup of the dedicated soft x-ray instrumentation for in-situ battery material study.

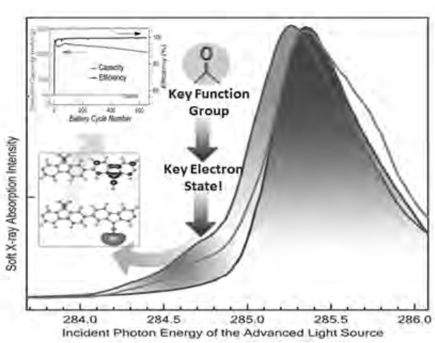


Figure: Soft x-ray absorption spectra collected on a series of polymer materials reveal key electronic states that triggered ultra-high battery performance.

Specifically, we have established EATH (Energy Alignment Through Hybridization) method for soft x-ray emission spectroscopy by studying transition-metal fluorides. EATH has empowered us to clearly define the transition-metal *3d* and oxygen *2p* states in one of the most interesting cathode materials, $LiFePO_4$.

Further, the soft x-ray absorption spectroscopy has delivered clear message on distinguishing a key electronic state in particular polymer materials, leading to a rational approach towards much higher capacity silicon based anode with hundreds of charge/discharge cycles (Figure).

LB09030

X-Ray Optical Metrology for Coherence-Preserving Adaptive Optics

Principal Investigators: Kenneth A. Goldberg, Valeriy V. Yashchuk

Project Description

This three-year LDRD project funded the successful development and demonstration of methodologies for x-ray nanofocusing. Integrating ex-situ optical testing and in-situ x-ray wavefront sensing, the project built on alignment techniques developed for state of the art visible-light profilometry and a successful program of EUV interferometry of diffraction-limited optics for photolithography. Extending these techniques to the unique problems of glancing-incidence soft x-ray beamline optics led to the creation of practical, quantitative, deterministic methods for x-ray nanofocusing of beamline optics with high accuracy and sensitivity required for sub-100-nanometer resolution, sub-100-nrad slope-error tolerances. These methods, which include slit-scanning versions of the Hartmann test for coarse adjustment, and shearing interferometry for fine alignment, are now being expanded and transferred to beamlines at the ALS and elsewhere.

While progress in nanoscience is driven by the development of high-resolution light probes on ultra-bright, third- and fourth-generation x-ray light source beamlines, advances have been frustrated by the unavailability of in situ metrology and mirror-alignment techniques with the required levels of sensitivity and accuracy. Our work is motivated by the desire to measure and overcome optical misalignment, mis-adjustment (from bending), thermal and mechanical drifts, and mirror fabrication errors that combine to blur focused beams, lower experiment resolutions, and reduce signal-to-noise ratios.

Accomplishments

In FY2011 based on research on the primary misalignment sensitivity modes, we created two thermally stabilized KB mirror benders (holders) robust in the presence of environmental changes, and each capable of 5 alignment degrees of freedom. To enable high-accuracy two-dimensional testing, we nanofabricated arrays of (object-side) spatial-filter slits and pinholes that produce coherent, cylindrical and spherical reference wavefronts. We also produced compact arrays of (image-side) nanostructures for interferometric and non-interferometric testing: these include gratings, slits, and knife-edges. Using surplus KB mirror substrates as the test optics, we demonstrated the measurement and elimination of wavefront aberrations up to 4^{th} order using a combination of mirror bending, tilting, and refocusing. This work proved the effectiveness of the *method of characteristic functions*—a linearization of the multi-parameter mirror optimization problem—for at-wavelength mirror alignment.

During the course of this project we developed and tested the mechanical components and optical elements necessary for a variety of complementary mirror-testing methods. This work demonstrated effective soft x-ray diffraction-limited nanofocusing with rapid, in-situ, at-wavelength interferometric and non-interferometric wavefront feedback; ultimately finding solid agreement with single-mirror, state of the art visible-light optical profilometry. The project created a vibration-isolated experimental test chamber at ALS Beamline 5.3.1 hosting multiple testing techniques for both single KB mirrors and KB mirror pairs.

This work continues with the transfer of knowledge and hardware to other beamlines where nanofocusing and wavefront preservation are important.

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 science case. The initial goal of the high intensity high harmonic system is to study the feasibility of localized excitation of valence states using non-linear stimulated Raman scattering in the extreme ultraviolet to lay the foundation for four-wave mixing in the soft x-ray regime. The coherent high repetition rate system will establish element specific coherent diffractive imaging that ultimately will provide the foundation for imaging of spatially resolved dynamics as it unravels in time.

Accomplishments:

Our most significant accomplishment has been to design and construct the experimental setup and the detection scheme both for the multi-dimensional spectroscopy experiment and the coherent diffractive imaging experiment. Two postdoctoral fellows lead these two parallel efforts. With help from the Center for X-Ray Optics (CXRO) we succeeded to deposit two separate coatings on the same face of a single focusing mirror with different multilayer structures that reflect the 17^{th} and 29^{th} harmonic, respectively. This approach facilitates the critical spatial and temporal overlap between the two different XUV pulses in the non-linear x-ray optics experiment. We designed and constructed the central components of a novel femtosecond EUV near-edge coherent diffractive imaging setup. The experimental setup consists of four major components: 1) A femtosecond laser driven high-order harmonic generation (HHG) light source. 2) An IR/EUV dichroic mirror. 3) A high transmission monochromator consisting of a toroidal mirror and a plane grating. 4) A home-built imaging EUV detector. We are in the process of testing the experimental set-ups at both Labs prior to the start of data taking in the next few months.

LB10002

Direct Comb Spectroscopy of Lithium in the Vacuum Ultraviolet and Beyond

Principal Investigator(s): Dmitry Budker and Holger Müller

Project Description

The purpose of this project is to develop technologies for coherent generation of femtosecond ultraviolet light, as a basis for later extension to soft x-rays. We will study the applications of such light in atomic and molecular physics by performing direct-comb spectroscopy of cold lithium atoms and using laser combs for atom optics. To achieve these goals we will initially work in the ultraviolet spectral region, but apply the technologies and methods envisioned for the soft x-ray region. Studying the advantages and limitations of these methods at low photon energies, where experiments are much simpler, will give us the necessary experience for finding an optimal experimental strategy for future x-ray experiments.

Our strategy is to trap lithium from background vapor in a two-dimensional magneto-optical trap (2D-MOT), transfer it into a 3D-MOT, further cool it in a 3D optical lattice, and finally perform atom interferometry measurements in a 1D optical lattice. A femtosecond oscillator will be stabilized to a high-finesse cavity and harmonics will be generated within a dispersion-compensated enhancement cavity. Methods for intracavity phase matching will be studied. Direct comb spectroscopy of laser-cooled lithium will be performed using single-photon and two-photon sum frequency excitation. This work will serve as a test bed and proof of principle for frequency comb metrology in the x-ray spectrum. Another important goal is to investigate the pressure broadening of the CO2 absorption bands, which is necessary to improve monitoring of atmospheric CO2.

Accomplishments

The frequency comb, a Menlo Systems FC8004 based on a mode-locked femtosecond Ti:Sapph laser, has been installed and stabilized. Fiber optic and electrical links were strung between the laboratories housing the frequency comb and spectroscopy experiments, and have been used to phase lock an infrared spectroscopy laser to the frequency comb.

A high finesse (nominally F = 100,000) Fabry-Perot cavity, based on a 5x5 cm cylinder of ultralow-absorption quartz glass (Suprasil 3001) coated with high reflectivity dielectric stacks, has been constructed and tested, and can be used as a frequency reference.

For the lithium spectroscopy, we have achieved trapping in both the 2D and 3D-MOT (see figure 1) using a combination of commercial diode lasers, tapered amplifiers, and home-built injection locked slave lasers. Two additional lasers needed for the optical lattice and interferometry have been built and stabilized; the former with feedback from lithium spectroscopy in a heat pipe, the latter with a phase lock to the master laser. Computer control and diagnostics, principally using absorption imaging, allow us to quickly evaluate and optimize experimental parameters. Post-project, we are currently implementing degenerate Raman sideband cooling in the optical lattice and plan on using the same laser system for a first demonstration of atom interferometry.

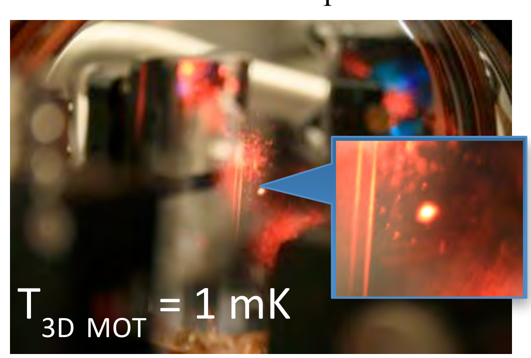


Figure 1. Fluorescence from lithium atoms captured in the 3D MOT.

LB09009

Development of *in situ* cells for Reactive Spectroscopic and Microscopic Studies
Principal Investigator(s): Mary Gilles

Project Description

This proposal is to develop *in situ* cells for scanning transmission x-ray microscopy (STXM) studies of nanoscale systems relevant to energy production. *In situ* cells are critical components for advancing studies in a wide range of fields; atmospheric chemistry, solar cells; electrochemistry (i.e. batteries), soil chemistry, magnetic systems, polymer processing, and catalysis. Commonalities between all of these include the need to understand detailed changes in chemical composition on the scale of 10's of nm to microns in reactive environments.

The goal is development of several *in situ* cells that are robust and can be adapted to other experimental platforms at the Advanced Light Source, including Fourier transform infrared spectroscopy, X-ray fluorescence microprobe techniques, or bulk near edge x-ray absorption fine structure (NEXAFS) measurements and micro-Raman. Since laboratory based ultrafast (femto or attosecond) transient absorption experiments share similar sample requirements with STXM, these cells could be readily adapted to laboratory-based experiments.

Essentially three types of cells are under development: a micro-fluidic cell; a temperature-controlled reactor (reactive gas flow and varying relative humidity); and a micro-fluidic cell.

Accomplishments

We have made significant progress developing both the micro-fluidic and the temperature controlled *in situ* reactor cells. Testing the cell revealed several shortcomings unique to the water vapor system. Accordingly, we designed a new reactor for use specifically with water vapor. The new reactor is shorter (compared to the previous design) along the optical path, mounts directly to the existing STXM sample holder, and contains a sensor to actively measure relative humidity and temperature at the sample position. The drawings for this improved version were finalized and additional post-project proof of concept experiments are scheduled.

The temperature distribution across the coils of the heater chips of the temperature controlled reactor cell was characterized using *in situ* measurements of micron-sized stearic acid particles during heating in the STXM. The temperature variation between the coils was estimated to be < 10 ºC. Micro-Raman spectroscopy on TiO_2 particles were also used to map temperature distributions and will be applied to the next version of the micro reactor.

Initial measurements of the micro-fluidic cell under flow (examining water across the oxygen K absorption edge) indicated that the liquid layer was ~4 µm thick; too thick for STXM applications. The micro-fluidic cell was redesigned to reduce the spacer layer thickness from ~2 µm to ~0.5 µm. Support pillars were added to the flow channel to prevent blocking of the liquid flow caused by the channel pinching shut. The redesigned cells were received and post-project preparations are underway for testing in the upcoming experimental cycles at the Advanced Light Source.

LB09011

Dynamics of homogeneous catalysis reactions investigated with transient two-dimensional infrared spectroscopy

Principle Investigator: Charles B. Harris

Project Description

Organometallic compounds have broad applications in synthetic chemistry, particularly as homogeneous catalysts. A full understanding of the mechanisms and associated dynamics of organometallic reactions allows new synthetic routes to be designed and current syntheses to be improved. Direct experimental observation of these dynamics is often the best way to determine the details of these transformations. We have previously studied organometallic catalytic systems using transient one-dimensional infrared spectroscopy, in which a reaction is photoinitiated by a UV pulse and then probed by an IR pulse. We are currently expanding our study of photochemical reactions using transient 2D-IR (T2D-IR). Thorough analysis of the T2D-IR spectra can give information on the structure of not only the transient intermediates but also the transition states connecting them—details that conventional spectroscopic techniques cannot provide. In order to show the efficacy of this technique, we are performing a proof of principle experiment in which we are studying the photolysis of iron pentacarbonyl to iron tetracarbonyl. We intend to use our expanded multidimensional capabilities to study important homogeneous catalytic reactions such as the activation of CO_2, a process that is of significant interest in the mitigation of the effects of fossil fuels.

Accomplishments

In the past year, we have made significant progress in our studies of the photolysis of $Fe(CO)_5$. Prior to performing these experiments, it was necessary to understand the rotational diffusion of the molecule in alkane solutions to remove these effects for the kinetics we wanted to monitor. This work resulted in a confirmation that $Fe(CO)_5$ rotates in the "slip limit;" these results, along with studies of a variety of other metal-carbonyl compounds in solution, are in preparation for publication *JCP*.

In the case of $Fe(CO)_5$, T2D-IR studies indicated that the vibrational label necessary to gain mechanistic information is annihilated by the effects of the UV light pulse. These experiments required an increase in the sensitivity of the apparatus. This increase in sensitivity allowed us to observe a stable, uncoordinated 14-electron species ($Fe(CO)_3$) in solution that had not been previously identified in earlier studies and only results from photolysis with higher-energy photons (Fig. 1). These results have recently been submitted for publication in *JACS*.

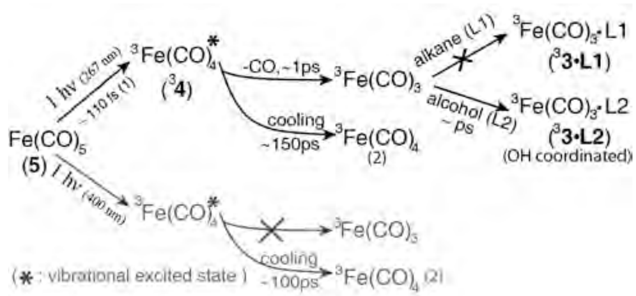


Fig. 1: Map of photolysis pathways for $Fe(CO)_5$ in liquid alkane phase. The 110 fs time is a gas-phase measurement. The chemistry of $Fe(CO)_4$ is absent to clarify $Fe(CO)_3$ processes.

Studies of CO_2-activating compounds are ongoing. Further investigation of *fac*-$Re(CO)_3(bpy)CN$ has shown that the dependence of this compound on an external, chemical electron source makes it infeasible to study, but we have shifted our focus to a series of heterobimetallic compounds of the form $Co(^iPr_2PNMes)_3Zr$ that show promise in CO_2 activation and should be fascinating targets for future study.

LB10037

Investigating f-Electron Exchange Coupling in Actinide and Lanthanide Complexes

Principal Investigator: Wayne Lukens

Project Description

The purpose of this project is to better understand exchange coupling in actinide and lanthanide (f-metal) complexes. Specifically, the goal is to develop techniques to quantify exchange coupling in these systems; currently, no general approach exists that allows quantification of exchange coupling involving f-electrons. This information will allow a better understanding of the roles that f-electrons play in bonding and determining magnetic behavior, especially as it relates to lanthanide-based single molecule magnets and to "Kondo-like" complexes of certain lanthanides, particularly ytterbium and cerium.

We will develop new techniques for quantifying exchange coupling in these systems, which use the crystal field information contained in the magnetic susceptibility of structurally similar complexes that do not display exchange coupling. In this approach, it is not necessary to determine the crystal field parameters, which is extremely difficult for low-symmetry systems. Instead, the magnetic susceptibility itself will be used to quantify the exchange coupling in other systems. We will prepare a series of lanthanide and actinide complexes to test and expand these techniques. If possible, the data obtained will be also be analyzed by traditional method, which does involve determining the crystal field parameters, which are then used to diagonalize the full Hamiltonian for the coupled system. In this way, the new, general approach can be compared to a more rigorous approach.

Accomplishments

The exchange coupling in $Cp^*_2Yb(bipy)$ has been quantified using the temperature independent magnetism of this complex at low temperature. The exchange coupling is very strong, 900 cm^{-1}, which extremely surprising for a lanthanide complex. The interactions between the electrons that leads to this strong exchange coupling was modeled using the Hubbard Model, which has been widely used in solid state physics but rarely used for understanding chemical bonding. The advantage of the Hubbard Model is that it allows electron correlation to be treated explicitly, which is impossible with any model of chemical bonding below the complexity of Hartree-Fock with configuration interaction.

Using the Hubbard model, the strong exchange coupling in this complex can be seen to arise from the mixing of a low-lying charge transfer state into the ground state. This result clearly establishes that very strong exchange coupling is possible in lanthanide systems. In addition, the model allows the rational design of lanthanide systems with very strong exchange coupling.

The results are relevant to the field of single molecule magnetism. The single molecule magnets with the highest working temperatures consist of two lanthanides linked by a ligand possessing an unpaired electron. The interaction between each lanthanide center and the unpaired electron on the bridging ligand determines the maximum possible working temperature for the single molecule magnet. The Hubbard Model shows that the strength of this interaction is related to the energy needed to transfer an electron from the bridging ligand to one of the lanthanide centers.

LB10027

Double-Auger Emission of small Molecules following Core-Excitation & Ionization

Principal Investigator(s): Thorsten Weber

Project Description

The goal of this project is to develop a 5-particle detection and analysis scheme and to prove its functionality in an ambitious research program, which focuses on the double Auger decay of small CO molecules after photo excitation and photo ionization of inner shell electrons. Here the aim is to understand the dissociation pathways during the Auger decay and the photo-electron valence-electron correlation; a fundamental correlation yet unexplored, which plays an important role in the understanding of the shape resonance energy-bond-length correlation in chemical compounds. Moreover, we want to investigate post collision interaction effects in the emission patterns of the outgoing electrons, and thus hunt for a breakdown of the widely accepted 2-step mechanism in small molecules.

As mentioned above, these complicated investigations will require coincident 3d-momentum measurements of up to 5 particles, a yet unprecedented experimental undertaking. These challenging experiments will lay the ground work for future many particle measurements with intense (x-ray) free electron laser sources and high harmonic generation laser systems and act as a proof of principle. Especially at free electron lasers the intensity of the incoming light will be that high that 2 photons can simultaneously couple to 2 core electrons, resulting in two vacancies, which initiate rich correlated multi-electron quantum dynamics and the emission of photo and Auger electrons to be measured time and position resolved. Currently we are setting up a so called Momentum Imaging Spectroscopy for TimE Resolved Studies (MISTERS) apparatus, which will function as a reaction microscope dedicated to experiments with ultrashort laser pulses. The project proposed here is directly linked to the completion of MISTERS.

Accomplishments

The accomplishments of the second and last year of the funding period strongly built on the technical advances and adaptations as well as the test measurements of the first half. We improved the experimental setup according to our first results on the Ne photo double ionization, i.e. we enhanced the available electronic readout and data acquisition to record up to 2 ions and 3 electrons in coincidence. We are now able to single out and process 36 correlated signals on 15 detector channels per photoionization event with a repetition rate of up to 30kHz. This enabled us to successfully perform the investigation of double-Auger emission of CO molecules after core excitation and ionization. The first fragmentation process leads to two correlated Auger electrons in coincidence with two recoiling nuclear fragments which serve as a benchmark for the second less likely process of an Auger cascade process after photo ionization resulting in 3 emitted electrons in the body fixed frame, which we successfully recorded as well for the very first time.

We finished the very complicated analysis of the 12d-phase space for the first breakup channel. This was time consuming but delivered rich results, which are currently discussed with theoreticians. We were able to investigate the angular correlations between the electrons and deduce the electron nuclei interaction in the emission patterns. They tell us about the ionization mechanisms at play. Building on this benchmark experiment we will finish the ongoing analysis of the 15d-dataset with two Auger electrons and one photoelectron. Together with the two ions this five-particle coincidence will allow us to look for possible symmetry breakings in terms of momentum, angular momentum and for the first time chirality. We immediately implemented our technologic advances in the spectrometer design of the MISTERS setup.

LB10001

Enabling HPC Workflows on Clouds
Principal Investigator(s): Deborah Agarwal and Keith R. 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.

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 are working 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. Through this work, we hope to identify common abstractions and techniques that enable effective use of the cloud infrastructure.

Accomplishments

Our most significant accomplishment this year has been the MODIS satellite imagery processing pipeline running in the standard Linux environment supported on the DOE Magellan cloud testbed at NERSC. In addition, we have gained an initial understanding of what cloud abstractions are useful for data-intensive computing.

The MODIS processing pipeline consists of spatial and temporal sub-setting or aggregation, resolution transformation, and re-projection from one map projection to another. An original pipeline implementation was written for the Windows Azure cloud platform in C#. For Linux we had to rewrite it in Python and C. Our target application, calculating global evapotranspiration, requires input datasets that are approximately 1.4 TB per year of data, and the output is on the order of 630GB per year.

Understanding how to effectively utilize the different abstractions provided in commercial Cloud infrastructures for scientific applications, and how these abstractions might be supported in an HPC environment is an important part of this research. Windows Azure supports a series of abstractions for developing highly-scalable, resilient distributed applications, e.g., reliable message queues, simple tabular data storage, etc. We have developed and deployed a simple queuing system, similar to that used in Azure, based on the RabbitMQ reliable messaging system. The MODIS pipeline components, use this messaging system to coordinate their activities.

We have also conducted research into the performance of storage systems for data-intensive applications at NERSC. Initial testing showed that the standard parallel file system, GPFS, did not perform well with the large number of small files used by the MODIS pipeline. Several alternatives are currently being explored, including the use of local flash based storage. The result of this work is a paper: *Assessing the Value of Cloudbursting: A Case Study of Satellite Image Processing on Windows Azure* – to appear in the proceedings of the IEEE eScience 2011 Conference, December 5-8, 2011 in Stockholm, Sweden.

LB11043

DEFINING AN ECOSYSTEM TO SUPPORT DATA-INTENSIVE SCIENCE

Shane Canon

Purpose

Across many domains, scientists are struggling with a tsunami of data. 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

As part of the LDRD, we have met with seven application groups from various disciplines and divisions including the Advanced Light Source, genomics, climate, financial analysis, and materials science. From these discussions we have extracted details about the structure of their data, the types of analysis there are performing on the data, and how they expect their needs to evolve. For example, we worked with a project that performs gene-centric analysis of microbial isolates. Analysis output was stored in a relational database and queries were used to translate the analysis into predicted gene function. Working closely with the scientists, we evaluated other models of storing and querying these results. These new approaches led to almost a 1000x improvement in end-to-end performance for a key step of the analysis and opened the door to new types of analysis that had previously been unfeasible. This experience highlighted the need and value to have experts working with scientists to implement new approaches and that new technology alone may not sufficiently address the challenges.

Another insight from discussions with scientist is the importance of running complex workflows that are often computational intensive in addition to being data intensive. HPC class systems could potentially help address these needs, but this can be difficult due to the complex workflows required. To address this issue, we developed a tool that allows users to instantiate a “virtual private cluster” within the HPC system. This cluster instance allows for more flexible scheduling options within the private cluster. This opens the door to a wider user community to exploit HPC class system for addressing data intensive problems.

Finally, we have also explored some of the performance characteristics of flash storage. For example, we studied how flash storage performs as a storage device in a parallel file system which is one model of how solid-state storage may be deployed for a purpose-built data-intensive, as well as exa-scale computing systems. Early results highlight the strong interplay between the storage device and the file system. The results also demonstrate that file systems and middle-ware may require significant improvements to fully exploit the full potential of these devices.

Next Generation Computing for X-ray Science

Principal Investigator(s) : Xiaoye S. Li

Project Description

We seek to develop new high performance computing (HPC) algorithms, codes, and software tools for the analysis of X-ray scattering data collected at the ALS. In conjunction with the implementation of a suitable theoretical framework for the analysis of novel scattering data, this task will produce fast and state-of-the-art capabilities for exploring the morphological and dynamical properties tied to photovoltaic materials, carbon capture and sequestration technologies, energy storage, and fuel cell devices. The latter applications directly advance the goals of Carbon Cycle 2.0.

We will develop new parallel algorithms and codes to use the ALS' in-house GPU clusters, the NERSC's medium-size Dirac GPU cluster, as well as the NERSC's most powerful massively parallel multicore system, the Cray XE6. We anticipate to achieve several orders of magnitude speedup for some commonly used analysis codes at ALS. 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 the ALS and NGLS.

Accomplishments

Reverse Monte Carlo (RMC) simulation is one popular analysis method used to extract information on material structure from small angle X-ray scattering (SAXS) data. In this fitting procedure, one attempts to simulate various configurations of the underlying atoms, molecules, or building blocks (e.g., nanoparticles) in a material until the scattering pattern from the simulated structure matches the real scattering data. The 3D RMC simulation codes for this application typically involve $\sim 10^4$ fast Fourier transform (FFT) kernels to be computed per iteration step of the algorithm, and the total number of iterations can approach $\sim 10^6$. Our initial in-house code was written in MATLAB and ran on one processor. We have ported this code to AccelerEyes Jacket to perform the simulations on graphical processor units (GPUs), which led to over 100x speedup in computing time on one GPU. Recently we have ported the MATLAB code to C++ code enhanced with NVIDIA's CUDA, which led to additional 9x speedup.

We have implemented a flexible Grazing Incidence Small-Angle Scattering (GISAXS) simulation code based on the Distorted Wave Born Approximation (DWBA) theory with C++/CUDA on GPUs. The software computes the diffraction image for any given superposition of custom shapes or morphologies (e.g. obtained graphically via a discretization scheme) in a user-defined region of k-space (or region of the area detector) for all possible grazing incidence angles and in-plane sample rotations. This flexibility then allows to easily tackle a wide range of possible sample geometries such as nanostructures on top of or embedded in a substrate or a multilayered structure. Preliminary tests on a single GPU show a speedup of over 200x compared to the sequential code. The new parallel GPU code is capable of computing GISAXS images from much larger samples and with higher resolutions than the sequential one.

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 iComputational 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 atracted a strong suite of collaborators from UC Berkeley and Gottingen University. 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. To this end, we have implemented 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.

Code-wise several advancements have been made in the past year. Dark matter particles have been put in as well as the equations for the expanding universe and an improved AMR solver has been implemented. The framework for Monte Carlo radiation transport via the *Sedona* code has been added as well. Heating and colling were placed into *Nyx* and cover hydrogen and helium and their ionic species. Weak scaling tests were carried out at ORNL on the jaguar computer and were excellent to 150,000 cores. Hopper has been used at NERSC to test and improve the hybrid MPI/OpenMP version of *Nyx* on 50,000 cores. The first paper from the collaboration, on the code framework, will appear this month and our first science paper will follow this one in the spring. The first *Nyx* simulations at a resolution of 1024^3 were presented at SuperComputing 2011 conference and demonstrated visualization over a 100Gb network.

LB10029

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

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 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 2011, we continued to focus on developing and experimenting with algorithms for determining relative orientations of diffraction images to be collected in single molecule diffraction imaging (SMDI) experiments. The main approaches we examined include the following:

1) Diffusion map based algorithm. In this approach, we construct a large diffusion map matrix whose entries are related to the pair-wise distances among 2D images. The eigenvectors associated with the 10 largest eigenvalues of this matrix are then computed. These eigenvectors are used to construct rotation matrices that describe the orientations of the sample used in the SMDI experiment through a nonlinear optimization procedure. We developed a parallel implementation of this algorithm because the construction of the diffusion map is computationally costly. Typically, more than 10,000 images are required in this approach.

2) Angular synchronization. We examined and implemented an angular synchronization algorithm used to identify 2D images that are associated with roughly the same projection direction but different in-plane rotations. These images can be used to create a class average that has a higher signal-to-noise ratio (but lower resolution). The algorithm first constructs an angular synchronization matrix whose eigenvector corresponding to the largest eigenvalue provides a global rotation that can be applied to align images associated with the same projection direction. These images can subsequently be identified through a spectral clustering or K-means algorithm.

3) Iterative refinement. We examined and implemented several iterative refinement algorithms for improving the initial reconstruction of the 3D diffraction pattern by using an ab initio orientation determination algorithm (e.g., a common curve based algorithm). In particular, we compared the projection matching algorithm and a statistical estimation approach which uses variations of the expectation maximization (EM) algorithm to improve the quality of the initial reconstruction obtained from a convex relaxation of the orientation determination problem.

In addition, we also investigated techniques for improving the robustness of phase retrieval algorithms. In particular, we developed strategies for automatically choosing a relaxation parameter in the hybrid input-output and a saddle point optimization algorithm. We also developed strategies for coping with the problem of noise in the data.

LB09035

Uncovering the mechanistic basis for soil microbial community response to altered precipitation patterns.

PI: Eoin L. Brodie

Project Description

The goal of this LDRD is to further understanding of potential changes in soil microbial community structure and function in response to altered precipitation patterns. This project will significantly increase our understanding of how anticipated changes in rainfall might affect the terrestrial carbon cycle. This issue is addressed across contrasting terrestrial environments with different annual precipitation regimes (desert, Mediterranean grassland and tropical rainforest). These three soil microbial populations have evolved under different rainfall regimes allowing for a comparison of the evolutionary constraints upon community adaptation to climate change. The workflow takes a bottom-up, three-pronged approach to this question by focusing on the properties of individual organisms, microbial communities and the biogeochemical processes they mediate.

Accomplishments

On of our most significant achievements is the development of a molecular biology and bioinformatics pipeline to generate and analyze next-generation DNA sequencing data from microbial communities. This pipeline has been adopted and implemented by other studies. Our approach has successfully demonstrated that rainfall exclusion reduces the diversity of naïve communities and changes the composition of communities to favor drought tolerant organisms. Such biodiversity loss may have important implications for ecosystem function. Indeed, in a laboratory microcosm experiment, rainfall excluded plots from the tropical rainforest environment became significant sources of nitrous oxide (a greenhouse gas with 230 times the radiative forcing of CO_2) upon resumption of rainfall. We are currently using a transcriptomic approach to understand the mechanism behind this.

We have successfully developed protocols for the extraction and analysis of the soil community metabolome to profile the metabolic pathways that are upregulated in response to drought stress. This is the first application of this technique in soils and shows great promise for understanding how energy is partitioned in communities under stress. We have shown that metabolic diversity is significantly different within drought plots, and indicate that a greater number of metabolic pathways related to stress are upregulated under rainfall exclusion. An example of this is the significantly higher concentrations of compatible solutes, used to reduce the deleterious effects of drought in rainfall-excluded plots. We have also identified potentially key influences of drought in tropical soils on the availability of phosphorus, a limiting nutrient to plant productivity and microbial growth and activity in these regions.

Finally, a comparison of the response of soil microbial communities from desert, grassland and tropical soils to simulated drought indicates common patterns of diversity change and alterations of soil microbial composition. These common alterations may be particularly valuable in predicting how microbial communities respond to decreasing precipitation.

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:

The nature of this project has been a focus on the development of the computational engines within the first part. With this stage now being completed, we are now able to carry out hydrological inversions with complex and thus computing-intense simulation domains within reasonable computing times. A parallel version of iTOUGH2 (inverse TOUGH2) has been applied to field tracer experiments at DOE's Integrated Field Research Challenge Site at Rifle, Colorado. We are now in the process of applying the different hydrogeophysical joint imaging approaches developed within this project using a combined inversion framework, called iTOUGH2-EMGeo. This framework is the aforementioned parallel iTOUGH2 combined with ESD’s parallel geophysical modeling/imaging package EMGeo into one computing engine. It allows investigating hydrogeophysical coupling processes with high-fidelity on large-scale models, typically occurring in the contexts of geologic CO2 storage, geothermal system characterization, and environmental remediation and monitoring applications.

Entering the “production phase” of this project, we are now applying two coupling approaches to environmental studies. In a first example, a direct coupling through a petrophysical model is used in order to merge hydrological tracer borehole measurements with field-scale geophysical data. The suite of geophysical methods – these are various electrical/electromagnetic, induced polarization and gravity methods – provided by EMGeo can now be exploited to incorporate multiple geophysical data types in the hydrogeophysical inverse problem. A second approach involves coupling hydrological and geophysical attributes through common-structure constraints, also referred to as cross-gradient constraints. Feasibility studies have been done and demonstration results are produced by carrying out simulations on complex models designed after DOE's Rifle site. The publications which have been drafted will be split by their focus on the computational aspects and the hydrogeophysics aspect.

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. We expect this research to improve our understanding of the impact of mineral-water interfacial processes on field scale behaviors of consequence to DOE.

Accomplishments

Progress to date includes the characterization of secondary mineral coatings on subsurface sediments from three different contaminated aquifers. Mineral phase characterization has been characterized at the Advanced Light Source (Berkeley, CA) using the micro-focused X-ray to collect diffraction data on hundreds of one micron square regions of coatings present on quartz grains. Analysis of the data is still in progress, but a preliminary analysis of the samples from two of the sites suggests that the coatings are a complex mixture of various clay mineral and iron oxide phases.

In separate experiments, the sediment samples were reacted with aqueous tracers for varying amounts of time (hours to one month), in synthetic groundwater solutions containing bromide, strontium, uranium, and arsenic. Analysis of the penetration of the tracers into the coatings and their reactions with the mineral phases was conducted at the Advanced Photon Source (Argonne, IL) using micro-focused X-ray fluorescence. These results indicate that bromide did not penetrate the coatings to a significant extent, presumably due to lack of chemical reaction and anion exclusion from the nanopore water phase. Strontium entered the coating and reacted with clays containing appreciate cation exchange capacity. Uranium and arsenic were observed throughout the coating regime in association primarily with the iron oxide nanoparticles. Concentration gradients in uranium and arsenic were not observed in these experiments, suggesting that the pore network did not constrain diffusion into the coatings, at least not in a manner that was observable in plan-view X-ray fluorescence observations at the micron scale.

We are in the process of scaling the experimental and analytical approach down further to examine grain coatings at the nanometer scale.

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 CO_2 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 point-source CO_2 to advanced biofuels using freshwater and marine cyanobacteria.

Accomplishments: We have produced more than ten engineered strains of a cyanobacterium with enhanced accumulation of a precursor for alkane biosynthesis. By constructing an artificial operon with two enzymatic genes, constituting the alkane biosynthetic pathway downstream of the synthesis the precursor, we demonstrated a five-fold increase in the endogenous accumulation of alkanes. We also showed that the artificial operon could direct biosynthesis of alkanes in a non-cyanobacterial microorganism. This work is part of a collaboration with one company and forms the basis for a submitted FY12 SBIR proposal. We have also engineered a means to control the chain lengths of the produced alkanes, for gasoline, jet fuel and diesel alternatives, in the cyanobacterial cells. We have also engineered two strains for isoprenoid (pinene and farnesene) biosynthesis, as jet fuel and diesel alternatives, respectively.

To optimize the activity of the two enzymes, and to allow for different substrate specificities, we have engineered an artificial enzyme harboring both activaties. We have named this novel enzyme alkane synthase (AS). We consider this first version of AS as a reference parent for further optimization by directed evolution. This optimization strategy is a collaboration with a second company, employing proprietary technology, and is the focus of a FY12 SBIR proposal. Meanwhile, by expressing referent parent AS in *E. coli*, we have demonstrated that it possesses the combined activity of the two enzymes, that it results in an accumulation of alkanes, and that it exhibits additional activities. Construction and the wider application of the novel AS enzyme is subject to IP protection.

Together with Hoi-Ying Holman, I have established synchrotron radiation Fourier transform IR (SR-FTIR) spectromicroscopy as a high-throughput diagnostic tool for real-time, single-cell metabolic analysis of genetically engineered cyanobacteria.

As a direct consequence of the CyanoAlkanes LDRD project, I initiated and headed an ARPA-E proposal, where a main objective is to install the biosynthetic pathway for alkane biosynthesis from cyanobacteria in tobacco for expression in the leaves. This proposal, FOLIUM, which is a collaboration between LBNL (lead), UC Berkeley and JGI, has been selected for funding by ARPA-E and will start in January 2012.

CO_2 as Cushion Gas for Compressed Air Energy Storage in Subsurface Reservoirs

Principal Investigator: Curtis M. Oldenburg

Project Description

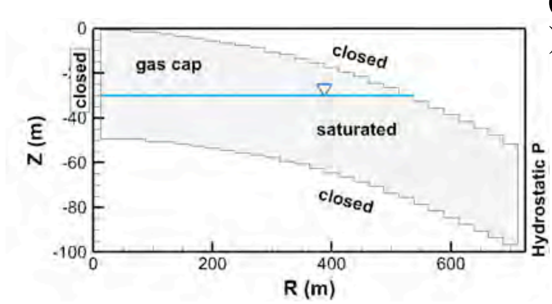
We are investigating the use of CO_2 as a cushion gas for Compressed Air Energy Storage in aquifers and in depleted gas reservoirs (referred to here as Aq-CAES, and DR-CAES, respectively). The advantage of using CO_2 as a cushion gas is that CO_2 compresses in a non-linear and advantageous fashion such 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 is to assess the feasibility of using CO_2 as a cushion gas for enhancing energy storage, while also developing expertise in the geoscience (hydrology, geochemistry, geomechanics) of CAES.

The approach we are using involves simulation of the coupled processes involved in Aq- and DR-CAES. Many of the processes associated with CO_2-enhanced Aq- and DR-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 are investigating 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 FY11, we continued refining our simulation capabilities and applying them to a prototype 2D radial DR-CAES scenario to investigate the performance of CO_2 as a cushion gas. The DR-CAES reservoir we model is 50 m thick, 500 m radius dome structure with infinite-acting boundary condition on the right-hand (outer radius) boundary as shown in Figure 1a. We have modeled the details of energy and mass flow in a 21-inch well and in the reservoir undergoing daily cycles of energy storage (air injection (recharge) and production). A comparison of results for DR-CAES with air cushion (i.e., no CO_2 cushion) and with CO_2 cushion are shown in Figure 1b. A very slight advantage of the CO_2 cushion is observed by the decreased pressurization that occurs during recharge. During FY12, we will delineate operating conditions that enhance the benefit of using CO_2 as the cushion gas.

(a
)



(b
)

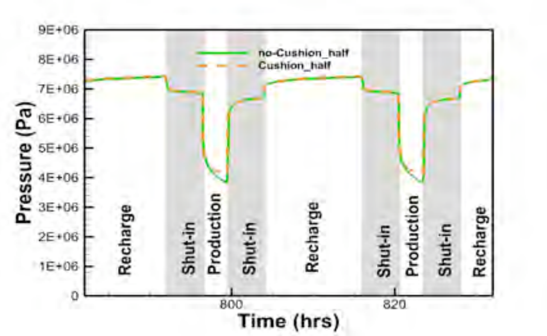


Figure 1. (a) Simple DR-CAES 2D radial model domain showing gridblocks, gas-water contact, and boundary conditions. (b) Results of recharge-production cycles of injection of air into the gas cap with air as cushion (green curve) and CO_2 as cushion (red dashed curve).

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

This year has seen the development of a novel technique for diagnosing convective entrainment and detrainment by clouds. As traditionally posed, entrainment is the rate at which air is entrained into a cloud as a function of height, and similarly for detrainment. As useful as these quantities are, they do not tell the whole story. The entrainment rate tells us how much mass is entrained into a cloud at a particular height, but it does not tell us where that particular mass is eventually detrained. Similarly, the detrainment rate tells us how much mass is detrained at a height, but not where that mass entrained. In a paper published in the Journal of the Atmospheric Sciences, a method is described for diagnosing the "transilient matrix," which gives the full history of air parcels entrained into and detrained out of clouds. As a first application of the technique, it is found that the sub-cloud-layer air in cumuli originates predominantly from within the first 100 meters of the surface. This result overturns the standard operational method for calculating instability in the atmosphere (CAPE), which assumes that cumuli pull their air uniformly from the first 500 meters.

Another line of investigation is the use of high-resolution large-eddy simulations to study entrainment rates in detail with novel methods. These simulations are beginning to yield new information on the dynamical processes of convective entrainment and their effect on the lifecycle of clouds. This characterization of the entrainment process will be used as one of the building blocks for the development of new convective parameterizations.

LB09023

Identifying and Predicting Climate Change Impacts on the Land-Based Components of the Water Cycle

Principal Investigators: Rohit Salve, William E. Dietrich, and Stefan Finsterle

Project Description

Our goal through this effort is to (1) document the importance of the fractured rock continuum that underlies most landscapes in regulating the hydrologic cycle and (2) determine how the hydrology of this zone can be impacted by climate change. We are using an unprecedented array of deep and shallow water-level and moisture-detection devices to document how pulses of rainwater pass through hillslopes, and how residual water is removed either through deep subsurface flow, plants, or transpiration during critical drying periods. We are also exploring the use of repeat geophysical surveys to detect moisture change in the deep subsurface. Key here is to identify and develop techniques to predict the influences related to meteorological and hydrological events, which may vary as climate may vary in the future.

The hypothesis of this proposal is that the underlying fractured rock in sloping landscapes regulates both the quantity and quality of water that becomes available to downslope ecosystems. An understanding of the physical makeup of this fractured continuum, and how water is stored and transmitted through it during and between precipitation events, will lead to improved predictive capabilities of trends in water quality and quantity, as dictated by changes in climate.

Accomplishments

We have concluded three years of high-resolution (temporal and spatial) monitoring of subsurface moisture. Data collected from this effort has been analyzed to explore potential mechanisms for moving water through the unsaturated fractured rock environment.

We have used an array of deep and shallow water-level and moisture-detection devices to document how pulses of rainwater pass through a hillslope in Northern California. We have observed rapid flow through the soil, into underlying weathered fractured rock, where it is either stored or transmitted to the underlying water table. We found no evidence of surface flow or of a conductivity barrier forming between soil and the underlying bedrock, to force lateral flow through the soil–a key assumption in most models of hillslope hydrology. These observations suggest that models treating soil as containing the water available for evaporation and transpiration need to consider moisture dynamics in the underlying bedrock to better explain land-atmosphere interactions.

Insights from this investigation are being used by ongoing research at the sight that is looking at the link between subsurface hydrology, vegetation and the atmosphere. This work has also informed research in two critical zone observatories that are set up in California and Arizona.

Testing a New Carbon Sequestration Strategy by Accelerating Calcite Precipitation in Soils

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 capturing CO_2 of soil respiration within surface soils. Soils comprise the third largest global carbon pool, are readily accessible, and hence are potentially more economical managed for C storage than deep subsurface reservoirs developed for geologic CO_2 sequestration. This study is investigating a new strategy for increasing C retention in slightly alkaline soils through supplying calcium ions to accelerate calcite ($CaCO_3$) precipitation and promote soil organic carbon (SOC) complexation on mineral surfaces.

With the addition of calcium ion to soils with pH > 8 often found in arid and semi-arid regions, the slow process of calcite precipitation may be accelerated. 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 to mix into natural slightly alkaline soils; which may promote the fixation of CO_2 as calcite and decrease leaching losses of organic carbon. To test this hypothesis, we have prepared laboratory soil columns (7.5 cm in diameter and 85 cm tall) with and without calcium sulfate-amended layers. The distributions of carbon in columns have been monitored in gaseous, aqueous and solid phases over a period of several months to test the effect of adding calcium ions on carbon distribution on soil columns. A relatively high fraction of ^{13}C-labeled bicarbonate has been injected to a column to differentiate the newly precipitated calcite from the initial calcite present in the soil.

Accomplishments

Our most significant accomplishment has been to identify conditions in which inorganic and organic carbon sequestration is practical in semi-arid and arid soils and to develop a method of measuring carbon balance in an unsaturated laboratory soil column to understand the distribution of carbon. Calcite mineralization is relatively slow process, making its quantification over a short period of time difficult. Therefore, it is necessary to measure the comprehensive carbon flow in gas, liquid and solid phases in well controlled laboratory simulations of natural surface soil environments in order to quantify the effects of gypsum treatment on C sequestration within relatively short times. At the current stage in the column studies, $CaSO_4$-treated soil is exhibiting lower losses of SOC and inorganic carbon, indicating SOC fixation, less calcite dissolution, and possible calcite precipitation. The isotopic ^{13}C analysis planned for the near future will also help to distinguish the amount of newly precipitated calcite from preexisting soil calcite which is often found at levels of several mass percent in arid soils.

The LDRD-supported second year's effort will focus on the impact of vegetation on the soil carbon balance under variable Ca^{2+} availability. The possibility of enhancing carbon sequestration within and immediately below the rhizosphere (root zone) of a biomass energy fuel crop will be tested in a greenhouse using switchgrass.

LB10022

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

Principal Investigator: Margaret Torn
Other Investigators: Janet Jansson, Christer Jansson & Eoin Brodie (ESD), Peter Nico (ESD/ALS), Susannah Tringe (JGI), Carolyn Ajo-Franklin (MSD/Molecular Foundry), Trent Northen (LSD/JBEI), Marc Fischer (EETD)

Project Description

Carbon (C) sequestration climate change mitigation is ripe for development based on advanced research. We are investigating biological C capture, compound production, and soil stabilization using a systems biology approach that engages the breadth of Berkeley Lab expertise. Our scientific aims are to understand: (1) mechanisms of soil C stabilization and how to influence them; (2) how to enhance or influence different means of biologically capturing CO_2; and (3) strategies to minimize loss of already sequestered terrestrial C. We also strive to integrate Berkeley Lab expertise for carbon cycling and biosequestration into the Lab's Carbon Cycle 2.0 Initiative. We are employing multidisciplinary research, including genomics, and biochemistry, molecular microbial ecology, imaging, molecular engineering, and biogeochemistry. This project showcases Berkeley Lab's strengths in carbon cycle research, addressing BER's interest in this area, and is producing novel results in only 3 years.

Accomplishments

Biochar incubations. We now have a good understanding of the impact of unlabeled biochar (BC) on soil microbial communities as well as the fate of ^{13}C-labeled biochar in soil. We set up incubation experiments to compare BC decomposition in soils from contrasting ecosystems (Puerto Rico Forest vs. Californian grassland), temperatures (ambient and elevated), and depths (surface and deep). Soil incubations containing pyrolyzed and unpyrolyzed ^{13}C-labeled wood were monitored for respiration, microbial community composition, and activity of extracellular enzymes. The samples were harvested after one week and three months, and a final harvest will be done after one year. Total respiration was 50-70% lower in incubations with BC vs. wood additions. In tropical soils, respiration of native soil C was slightly higher with BC; whereas in grassland soils it was slightly less. In both soils, respiration rates and temperature sensitivity of decomposition decreased with BC addition.

Microbial calcification. We used a multi-pronged approach to monitor cell properties and biomineralization in cells grown under different CO_2 concentrations, including (1) metagenomics and transcriptomics to characterize cyanobacterial consortia responsible for whiting events; and (2) cell surface assays with time-of-flight secondary ion mass spectrometry, synchrotron radiation Fourier transform infrared spectromicroscopy, Energy-Dispersive X-ray spectroscopy, Raman spectroscopy, Zeta Potential measurements, and electron and fluorescence microscopy. In our continuing study of the cyanobacterium *Synechococcus* sp. 8806, we demonstrated that it could grow at 15% CO_2 (typical of flue gas). Contrary to expectation, carbonate precipitation on the cell surface increased with higher CO_2 levels; the effect of photosynthesis on ambient pH and cell-surface charge allowed for calcification at high CO_2 levels, and the increase in carbonate precipitation coincided with a higher build-up of EPS. We also obtained evidence for the presence of an S-Layer in *S*. 8806. We submitted isolate S. 8806 to JGI for genome sequencing.

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 2011

In Task 1, we developed a set of scenarios of heterogeneity, from completely stratified systems to random fields of porosity, permeability, and pore compressibility. These random fields are generated using transition-probability-based geostatistics for a hierarchy of geologic units and sample semivariograms of sedimentary rocks. We are conducting simulation of pumping, thermal, and tracer tests to understand the effect of heterogeneity on pressure propagation, heat transfer, and tracer transport and the relationship between behavior of observed primary variables at wells and changes in the heterogeneity scenarios. Additional simulations of two-phase CO_2-brine flow will be conducted for CO_2 storage tests, with also random fields of entry capillary pressure and pore-size distribution parameters.

In Task 2, all available data on the pumping, thermal, and tracer tests, and the later-conducted CO_2 injection tests with phase-partitioning tracers have been collected from the Frio Pilot I Test. These observation data have been analyzed, with the borehole log and core data, to understand the different roles of the various field tests in characterizing the multiscale heterogeneity of the Frio Sand in the storage formation. For example, the temperature profile at the pumping well obtained during the dipole injection-pumping test signals a fast flow path whose effect on CO_2 migration was revealed in the CO_2 injection test. Further numerical simulations and model calibration will be conducted to test the developed methodology.

In Task 3, we presented our capabilities of forward and inverse modeling with case studies, while IGGCAS presented the site characterization of the Tianjin site and the planned pilot tests. Key scientific research topics identified include long-term geochemical responses to injected CO_2 during its migration from the injection well to monitoring wells, and the characterization of the interwell connectivity using pumping, thermal and tracer tests. The site-specific data has been collected from IGGCAS, and numerical modeling for designing these field tests is on-going.

Engineering Division

LB10018

Investigation of image current and magnetic field tolerance effects on high-temperature superconductor undulators for soft x-ray FEL's
Principal Investigator: Diego Arbelaez

Project Description

The purpose of this project is to develop undulators with very short periods and high magnetic field using the high-temperature superconductor (HTS) $YBa_2Cu_3O_7$ (YBCO). These devices show great promise for future light sources due to their potential to enhance brightness and spectral range at a reduced cost. The high magnetic field is required to provide a large spectral range, while the short period allows access to short wavelength radiation. Successful application of these devices in an FEL facility would result in substantial cost savings due to the low cost and shorter length of the undulator, and the reduction in the required electron beam energy necessary to access high energy photons.

YBCO conductors can be commercially obtained from vendors in the form of a tape. A layered winding approach, usually used for wire-wound undulators, is not readily applied with tape conductors, as some degree of hard-way bend of the tape is usually required, or a large number of joints must be made. This issue has been circumvented by incorporating the current path directly onto the tape; eliminating the need for winding altogether. Tapes can then be stacked together and joints can be formed so that the current travels from one tape to the next in such a way that the line currents from the individual tapes are superimposed to generate a high on-axis magnetic field.

While these devices promise to provide high fields and short periods at a reduced cost, there are several possible technical limitations that must be addressed for practical application of this technology. These include: understanding the effects of fabrication tolerances on the quality of the magnetic field and field integrals, development of magnetic measurement techniques that are compatible with small gap devices operating at cryogenic temperatures, and understanding the heat loads due to image currents.

Accomplishments

With respect to the HTS tape undulator fabrication, we have developed and tested the lithographic process for creating the cuts in the YBCO tapes. We developed a sample holder to test the samples at 4.2 K and performed transport current measurements on single tape samples. For the single layer samples with a period of 5 mm, we obtained the expected transport current of 400 A. We are now working on creating stacks of tapes to further test the undulator concept.

For the characterization of short period and small gap undulators, we have constructed a pulsed wire magnet measurement bench. We performed various studies on the accuracy and repeatability of the measurement technique. Of particular importance is the mitigation or correction for dispersive wave motion in the pulsed wire measurements. We developed an algorithm to correct for dispersive and finite pulse width effects by post-processing the wire motion data. For application to the measurement of cryogenic devices, we have developed an in-vacuum pulsed wire measurement system, which will be compatible with a cryostat that is currently being designed for testing superconducting undulators. We have also performed an initial analysis of the effect of fabrication tolerances on magnetic field errors.

LB10007

Parallel Microfluidic Synthesizer: A Fully Automated Chemical Evolution Platform for Novel Materials Discovery

Principal Investigator(s): Rafael Gómez-Sjöberg

Project Description

We aim to develop a parallel microfluidic organic synthesizer (PMOS) chip capable of both chemical synthesis and biological assays. By integrating these functions on the same platform, we can perform iterative cycles of parallel chemical synthesis and compound evaluation, where information from the assay can feedback into the design of the next set of compounds. Cycles can be repeated to converge on compounds with desired properties, resulting in fully automated chemical evolution of new compounds. Thanks to the low reagent consumption afforded by microfluidics, the PMOS chips can run continuously at low cost – sifting through sequence space around the clock until a hit is found. To be able to build such a synthesis system, we first need to develop chemically-resistant microfluidic devices with microscopic, integrated valves, which would allow for on-chip automated fluid handling operations.

The successful realization of this proposal would lead to a device that is capable of rapidly evolving novel materials with far ranging potential applications in nano-technology, energy, biology, and medicine. Initial tests of the device will attempt to synthesize peptoid ligands to protein targets. Peptoids are a class of non-natural biomimetic oligomers based on an achiral N-substituted glycine backbone and have a similar polarity and side chain spacing to that of proteins.

Accomplishments

We have successfully developed protocols for fabricating chemically-resistant microfluidic devices with integrated valves, made of Teflon membrane sandwiched between two glass plates, for the automated synthesis of peptoids. We have also built a semi-portable chip control system that allows the synthesis device to be used in different locations for testing. The prototype device has inputs for 7 synthesis reagents, and a synthesis chamber featuring a switchable sieve for the reversible capture of microbeads (Fig. 1). When the sieve is closed, beads can be collected in the chamber to act as substrates for solid-phase synthesis of peptoids. At the end of a synthesis run, the sieve can be opened to retrieve the beads for further processing or analysis. The biggest challenges in the development of a fabrication process have been the achievement of a strong and durable bond between the glass plates and the Teflon membrane, finding an optimal valve geometry, developing loading/unloading procedures for the micro-beads that minimize clogging and bead loss, and finding a fluidic network design that minimizes dead volumes and cross-contamination while maximizing manufacturability. Extensive reliability testing of the microfluidic valves shows that properly fabricated valves have leak rates of less than 70pL/s at 5psi when closed (vs. 3.5µL/s at 5psi when open), even after half a million actuations in the presence of aggressive chemicals. However, the current yield of functional synthesis devices is still relatively low (~50%), due to valve leakages caused by defects in the Teflon membrane.

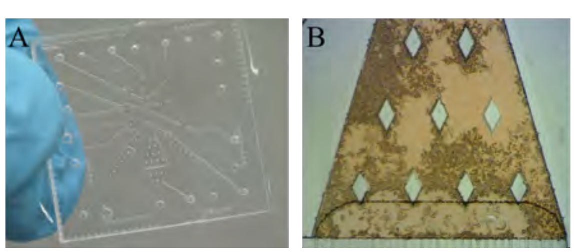


Fig. 1: (A) Microfluidic device for chemical synthesis. (B) Micro-beads packed inside the microfluidic synthesis chamber after a peptoid synthesis run.

LB11012

REAL-TIME DATA COMPRESSION FOR HIGH SPEED IMAGING X-RAY DETECTORS FOR THE NEXT GENERATION LIGHT SOURCE

Principal Investigator: John Joseph

Project Description

The Next Generation Light Source (NGLS) will provide ultrafast, high-brightness soft x-ray beams at a repetition rate far higher than any current or proposed x-ray Free Electron Laser (FEL), and experiments at NGLS would require sustained imaging detector readout at 100 kHz which is 1000 times faster than any detector system available today. An imaging detector used at NGLS will be required to produce images at a rate of at least 100,000 frames per second in order to capture shot-by-shot x-ray events. The current mode of operation in the user community (ALS, APS, LCLS, etc.) is to preserve all of the information recorded in each image by storing raw data. If we assume that the minimum acceptable detector size is a 1 Megapixel camera, imaging x-rays at 100k fps will produce a raw data volume at roughly 200 Gigabytes per second. A single minute of exposure time will produce approximately 12 Terabytes of raw data that must be stored and analyzed if signal processing algorithms are not developed and implemented into the readout system hardware. The magnitude of the data volume that will be produced by the next generations of x-ray detectors places a high demand on the development of hardware based image processing solutions.

This LDRD aims to understand what potential technical solutions could realistically be deployed in 10 years, when the NGLS turns on, and what a development roadmap would consist of. The project goals are to create a technology development roadmap, create a complete complex system model, identify and catalog candidate applications, develop loss-less software compression algorithms, and implement the compression algorithms in hardware using Field Programmable Gate Array (FPGA) devices.

Accomplishments

Because the topic of this LDRD is multidisciplinary, the road map to successful completion of our research goals requires a close collaboration between Engineering, Advanced Light Source (ALS), National Energy Research Super Computing Center (NERSC) and Physical Biosciences Division (PBD). To address this requirement we created an informal collaboration that includes individuals from each of the above mentioned divisions to discuss scientific applications that can be targeted for algorithm development, to share information and image data, and to review the completed R&D tasks. The collaboration produced a detailed work plan that included complex modeling of the complete system in order to understand the non-intuitive aspects of large data volume generation and transmission system bottlenecks. The base complex system model was completed and validated successfully using the Matlab and Ptolemy software tools. We also performed extensive research on lossless compression algorithms that can be implemented using fixed point arithmetic, required for future FPGA implementation, and to understand if different applications can accept a minimum level of information loss. Using the research results, were able to identify candidate applications and implement software and hardware compression algorithms that reduced the data volume by 800 times from the raw format. The creation of an Image Library that includes actual experimental data captured by the detector user community has also been started at the request of the working group. The collection includes image data from diffraction, single photon images for energy resolved Laue diffraction, tomography, ptychography and coherent images from experiments performed at LCLS and APS using the LBNL Fast CCD Camera system.

Development of variable-polarization superconducting undulators for soft X-ray FEL radiators

Principal Investigator: Soren Prestemon

Project description:

Soft X-ray science depends strongly on variable-polarization sources. Currently the only options are permanent-magnet variants, typically the APPLE-II type undulator used in most 3rd generation sources. These devices have massive moving structures subjected to large and varying forces, making precise trajectory control difficult. New approaches to generate variable polarization with static superconducting coils promise improved performance with superior trajectory control.

Two different approaches will be investigated for the generation of variable polarization light using superconducting coils. The first, proposed by the authors in 2007, provides access to all polarization modes as well as the possibility for period-doubling, yielding significantly enhanced spectral range over the permanent-magnet devices currently in service. The second is a new concept in which left and right circular polarization, each produced by the well-known and proven technique of bifilar helical windings, are superimposed to yield variable elliptic polarization.

Detailed analysis of performance characteristics will be developed for both concepts, including field-error tolerance analysis. The concept with most promise to significantly enhance FEL performance will be pursued in the form of a detailed design for fabrication.

Accomplishments:

The detailed design of a variable-polarizing, superconducting undulator concept (SC-EPU) has been developed. Spectral performance under various polarization modes has been analyzed. Working with a small business specializing in state-of-the-art superconductors, a conductor design has been established that is particularly well-suited for this application, having a small (~0.25mm) diameter compatible with the small coil corss-sections envisioned in the design. Furthermore, the conductor has small (<25 micron) superconductor filaments, which are expected to perform well in the low-field, high current-density regime of the SC-EPU.

Due to the long delivery time for the conductor, no coil fabrication was performed during this LDRD, but additional design effort was invested in developing a detailed design of a cryostat for future testing of an SC-EPU when built. The cryostat is compatible with the use of a pulsed-wire magnetic field measurement system developed under a parallel LDRD project. Furthermore, analysis tools have been developed to allow for parametric optimization of the SC-EPU design, and detailed analysis of the performance of an alternative variable polarizing design using left and right circular bifilar helical devices has been developed.

The superconducting wire has now been delivered and will be insulated with a thin ceramic insulation developed under follow-on support from the DOE SBIR program. Coil prototyping will commence in the next few months.

LB11029

Development of a colorimeter for the measurement of image-current heating on wakefield-surfaces for high-performance undulator applications
Principle Investigator: Soren Prestemon

Project description:

High performance undulators, in particular superconducting and cryogenic permanent magnet concepts, yield best performance at narrow magnetic gaps. Image current heating scales with 1/r, and for storage rings and for high-repetition rate, high-current FEL's the resulting heat flux can be a limiting factor in device implementation. Measured data under various beam, gap, and material configurations is critical for optimal undulator design. The proposed calorimeter will be implemented at diverse rings and linacs to measure heat loads under different operational parameters.

A calorimeter concept recently proposed by the authors will be finalized. The design will provide diagnostics to redundantly measure heat loads and to isolate known sources, including synchrotron radiation, conduction from end-transitions, and possible electron-cloud effects. Construction will be performed in partnership with collaborators from the Shanghai Light Source (SSRF). The device will be thoroughly calibrated and sensitivity to various heat sources will be determined in advance of implementation on storage rings and/or linear accelerators.

Accomplishments:

The detailed design has been finalized and device components are under construction by our collaborators at the Shanghai Light Source. All diagnostic equipment supported by this LDRD have been procured, and all schematics for the diagnostics and controls developed by LBNL have been completed and are being supplied to SSRF.

A detailed analysis of the thermal performance and behavior of the system has been made, yielding error bounds on the measurement accuracy. A model has been developed that will provide a means of discerning various thermal sources, including image currents and synchrotron radiation generated upstream. In-situ calibration has been incorporated so that drift in cryocooler performance can be measured and compensated for over time.

Initial commissioning will be done in Shanghai in spring 2012, with first installation and experimental results planned for summer 2012 in SSRF. After the first experimental campaign, the calorimeter will be shipped to LBNL for additional measurements on the ALS using follow-on support.

LB10004

Physical Accounting for Alternative Energy Pathways

Principal Investigators: Katie Coughlin and David Fridley

Project Description

In this project is we develop a new conceptual model for evaluating different resource allocation scenarios, and apply it to the study of industrial-scale production of biofuels from a variety of biomass feedstocks. Our approach is an analogue of ecological food web modeling, applied to the energy “production web”, which takes in raw materials and produces a wide variety of products in addition to energy. Most studies of the feasibility of industrial-scale biofuel production focus on the economics, and the conditions under which a particular biofuel will become cost-competitive with fossil fuels. The results are strongly dependent on assumptions about the rate at which agricultural yields (feedstock output per unit area) and process yields (fuel output per unit feedstock input) will increase over time. The physical-accounting approach provides a framework that allows these assumptions to be tested for consistency with what we know about the relevant physical constraints, and so produce more reliable quantitative estimates of the potential total output of biomass-based energy systems.

Accomplishments

The physical accounting methodology is implemented as a system of dynamic equations that define the input-output relationships of energy production. The principal results are: 1) We show that, under steady state conditions, the equations can be used to derive rigorous metrics for resource use efficiency. These metrics can be used to resolve some inconsistencies in published estimates of the net energy output for different biofuel production chains. 2) This methodology clearly distinguishes between an energy *source* and a conversion process that changes the form of a material but doesn’t increase the total energy output of the system. As with item 1, a number of published studies fail to make this distinction and so provide inaccurate estimates of the energy potential of biomass. We show that, for any input feedstock and output fuel, there is a maximum yield beyond which the process cannot be energetically self-sufficient. This means that, if yields are assumed to be above this maximum value, then the additional input energy required to reach these yields must come from an external source. Hence, the additional output is the result of a conversion process, and does not constitute a net increase in total energy output. 3) The carbon-neutrality constraint, under steady-state conditions, means that GHG emissions from biofuels are balanced by the net primary productivity (NPP) of the feedstock. Potential NPP in the United States is constrained by water availability. Using these relations we derive an estimate of the potential gains in NPP from re-allocating water use. These gains are not large, and suggest that increasing agricultural water use efficiency is a key component of an effective biofuel development strategy. 4) The physical accounting approach makes it clear that biofuel feedstock production must be modeled as a fraction of total agricultural output. This output is vulnerable to climate change. We calculate that the increase in crop evapo-transpiration (ΔET) with increased average temperature (ΔT), *i.e.* the ratio $\Delta ET/\Delta T$, is about two in the large agricultural states, with corresponding reductions in potential output under different climate scenarios. 5) Our approach requires information on the energy use of the biorefinery process, which is rarely available. Using the JBEI model, we show that this energy use can be estimated from thermodynamic data (temperatures, pressures, *etc*.) that could easily be measured for processes still in the laboratory stage. This information would be very useful in evaluating the potential output, as a net energy source, of different processes while they are still in an early stage of development.

LB10044

Toward a US Greenhouse Gas Information System
Principal Investigator(s): 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. First, we completed an analysis of seasonality in regional CH_4 and N_2O emissions from Central California. We found that both CH_4 and N_2O are emitted in at levels of 1.5 to 3 times those reported in the existing State inventory (Jeong et al., 2011). Second, we completed analysis of a one-year record of atmospheric fossil fuel CO_2 for Central California, which we combined with collaborative measurements from the Los Angeles area to evaluate statewide fossil fuel CO_2 emissions a full year in Central California and the entire State for June, 2010. Here we found that the atmospheric measurements suggest that actual fossil fuel emissions are consistent existing state inventory to within 10% (Fischer et al., 2011). In FY12 we plan to submit manuscripts describing these results and expand upon the work to design a network of measurement sites to capture emissions from California's South Coast air basin.

LB10041

Haiti Cookstove Project
Principal Investigator: Ashok Gadgil

Project Description

In January 2010, a 7.0 magnitude earthquake struck near Port-au-Prince, Haiti, displacing hundreds of thousands of people. As Haitians primarily cook with inefficient charcoal cookstoves, cookstoves were an important avenue to pursue in the rebuilding effort.

A fact-finding mission was conducted in the summer of 2010 to discover the cookstove needs in post-earthquake Haiti. As many cookstoves were already being considered for dissemination in Haiti, an assessment of these cookstoves was deemed necessary to suggest the most efficient candidate for the field so informed dissemination could occur.

The Haiti Cookstove Project sought to provide an unbiased, independent assessment of the performance of different charcoal cookstoves proposed for dissemination in Haiti. Testing included Water Boiling Tests (WBTs) and Controlled Cooking Tests (CCTs) to determine the efficiency and emissions associated with each cookstove. The WBT is an international standard that allows for cross comparison of cookstoves, while the CCT is a lab-reproducible test that incorporates culture-specific cooking practices. For this reason, CCTs typically provide a better prediction of actual performance in the field when compared to WBTs.

Accomplishments

We performed WBTs for five commercial cookstoves as well as the traditional cookstove. With one substitution, these cookstoves were included in the CCTs. For both the WBTs and CCTs, cookstoves were tested for specific fuel consumption, total carbon monoxide emissions, total carbon dioxide emissions, and the ratio of carbon monoxide to carbon dioxide. The WBT also tested cookstoves for time to boil and thermal efficiency. Additionally, both sets of tests included comments of usability of the cookstoves compared to the traditional stove.

For the WBTs, we found that all improved cookstoves were more efficient than the traditional cookstove. However, the traditional cookstove boiled water faster than the improved cookstoves. Two of the commercial products had the highest efficiency, while another had the lowest emissions. No one cookstove emerged as a clear winner in all performance categories.

For the CCTs, we developed a Controlled Cooking protocol, mimicking the preparation of *diri kole*, a bean and rice dish that is very popular in Haiti. The protocol consisted of three phases: cooking beans, vegetables, and rice. Precise amounts of ingredients were used for each test.

We found in these tests that two of commercial stoves had the lowest specific fuel consumption, while the one of the two had the lowest emissions. The traditional cookstove consumed more fuel than any other cookstove in the tests. Similar to the WBTs, no one cookstove emerged as a clear winner in all performance categories. Additionally, since more replicate tests were performed for the CCTs than for the WBTs, differences between cookstoves were more often statistically significant, when compared to the results of the WBTs.

This team played a valuable role in providing an unbiased assessment of cookstoves to enable non-governmental organizations (NGOs) to make more informed decisions. Results will be distributed to organizations involved in cookstove programs in Haiti, allowing them to better assess which cookstoves operate with high efficiency and are suitable to the cooking styles prevalent in Haiti. Both the WBT and CCT reports will be available online at http://cookstoves.lbl.gov/haiti.php.

LB11021

Developing Analytical and Communications Frameworks to Enable Breakthrough Low-Carbon Technologies

Principal investigators: Eric Masanet, Surabi Menon

Project Description

This project will develop new analytical methods and tools to bridge information gaps between basic, applied, and analysis research at LBNL. The goal is to accelerate LBNL's development and delivery of advanced science and technologies for sustainable, low-carbon energy systems by providing robust estimates of future technology performance under different economic, environmental, and technological conditions to guide today's R&D decisions. The research is comprised of five tasks: (1) market and technology characterization, which will develop credible estimates of the future application market and deployment-stage energy, environmental, and cost data for each technology; (2) deployment assessment scenarios, which will explore and quantify potential market barriers and net changes in energy use, global warming potential (GWP), and select environmental impacts under various scenarios for policy, development, and energy demand trajectories; (3) impact assessment science, which will provide the necessary scientific frameworks and tools for developing market, technology, and scenario data such that net systems-level benefits and impacts can be quantified credibly and using meaningful metrics; (4) identification of technology deployment barriers and research opportunities for select technologies to provide quantitative feedback into the innovation pipeline; and (5) identification and implementation of important feedback loops for institutionalizing critical information flows and collaborations between LBNL basic, applied, and analysis research moving forward..

Accomplishments

To date we've focused on four high-impact energy technologies under development at LBNL—advanced biofuels, solar photovoltaics, building technologies, and carbon capture and sequestration – to build a portfolio of tools for consistent and scientifically-sound analysis of technology performance in each domain. This portfolio includes a range of life-cycle inventory (LCI) data for energy and resource systems; geospatial data on land use, infrastructure systems, and resource systems, and data modules on power plant emissions, locations, and fuel use relevant to the four targeted research domains. We're also building an integrated energy and resource systems supply and demand forecast model for parametric analysis of technology scenarios within each domain, and have begun to couple data from U.S. county-level health impacts models with atmospheric chemistry models and point source emissions data to assess human health cost implications of various technology scenarios. These new analytical capabilities have been applied to R&D relevant case studies for advanced window technologies, engineered switch grass, aquifer brine disposition, artificial photosynthesis for hydrogen production, and large-scale deployment of solar PV.

LB11022

Life-Cycle Analysis of Geologic Carbon Sequestration

Principal Investigator(s): 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

In FY2011, we built the capacity to map and evaluate brine production in all regions of the United States and have compiled a range of brine management options, which require LCA. We have now 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. For each candidate GCS site, we evaluate the depth and properties of saline aquifers that offer potential disposal sites. For these sites we are characterizing the CO_2 storage capacity, the porosity continuity, brine composition, and brine temperature. We have selected three sites to characterize in detail.

We find that impacts and the potential commercial value of brine vary substantially between regions due to differences in brine composition and in market data. Water residing in the three saline aquifers spanned a range of temperatures and compositions. Economic value was sensitive to regionally-specific electricity providers, salt and mineral markets, and water scarcity. Net values for management scenarios ranged from a cost of \$50/tCO_2 to a return of \$50/tCO_2. The unexpected finding that pressure management could mitigate the cost of CCS in certain regions of the United States would not have been recognized if national averages were used in calculations.

LB11023

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

Principle Investigators: James McMahon, Larry Dale and Gary Fitts, EETD; Pamela Ronald and Dan Putnam, U.C. Davis; Sarah Lewis, U.C. Berkeley

Project Description

This LDRD address three broad questions: (1) Can we identify grass genes that confer enhanced tolerance to drought or salt? (2) How much biofuel could be produced from salt and drought tolerant switchgrass? (3) How could production of stress tolerant switchgrass proceed, with minimal impact on food and other crop production and prices? We address these questions in turn, working with a geneticist to identify grass genes for stress tolerance and with GIS analysts to assess the scale of potential switchgrass production on dry and salty lands. The U.C. Davis genetics lab is identifying genes for stress tolerance and testing their function in engineered rice, a model for switchgrass; analysts at LBNL and UC Berkeley are using GIS information to assess where the newly developed varieties can successfully produced on marginal or low value farmlands, or if further enhancements are needed.

Accomplishments

The focus of our work this fiscal year has been on a spatial analysis using land selection criteria and GIS to estimate suitable locations for growing engineered switchgrass feedstock. The benefit of the genetically modified plant is that it can maintain the same yield by getting the same amount of precipitation overall, but has the advantage that it can withstand intermittent periods of drought where other varieties cannot. The land selection criteria used in our analysis target low-value, marginal lands in California and selected Midwestern States. One question we explored is whether the variability of rainfall actually causes drops in land values. It is clear that agricultural land values drop off in water-limited areas; however we also identified areas with a constant average rainfall that instead experience intermittent periods of drought.

We have developed a multi-criteria dryness index to explore this question at a course level across California and Midwestern States and determined that land value in non-irrigated areas is related to average rainfall and rainfall variability. The dryness index is an indicator of rainfall variability used to refine the suitability analysis. This indicator identified northwestern Kansas to be potentially suitable for drought tolerant switchgrass. This analysis using this indicator is being expanded to other states to assist our search for areas with ideal temperature and yet limited water, i.e., periodic drought situations on low-value land.

We have been working with Dr. Pam Ronald at UC Davis to identify grass genes that confer salt or drought tolerance that can be used to engineer switchgrass and with econometricians and agronomists at U.C. Berkeley and Davis to estimate the likely yield and production response of engineered switchgrass to variations in soil type, climate, salinity, and precipitation. Pamela Ronald and her UC Davis genetics team have identified rice genes that enhance the tolerance of rice to drought, and are now testing their function in the model grass, rice. Her long term goal is to transfer genes that are proven to function in the model to switchgrass.

Going forward, we will expand the list of target areas for growing stress tolerant switchgrass, work with crop extension specialists to characterize switchgrass yields across different soil and climatic conditions and feed our results back to the genetics team, allowing them to fine-tune their efforts to target the desired drought/salt tolerance genes.

LB11024

From Fossil Fuel to Photovoltaics: Economic, Environmental and Health Impacts for Policy Considerations

PI: Surabi Menon
Co-Is: Dev Millstein, Pei Zhai, Jeff Urban and Joel Ager

Project Description

Substitution of traditional energy generation sources with photovoltaics (PVs) will change surface albedo and emissions of CO_2 as well regional pollutants such SO_2, NOx and carbonaceous particles. To guide policy decisions on strategic deployment of PVs, associated changes in regional climate, air quality, and public health are to be quantified. Life cycle costs for new materials used for manufacturing PVs are to be evaluated as well.

The regional climate and air quality effects of large-scale PV adoption are simulated with a regional climate and air quality model (Weather Research and Forecasting model -WRF-Chem). Economy-wide inventories for NOx, SOx, organics and primary particulate emissions were created for a 2030 base scenario. Future emission inventories were created by including over 80 economic sectors and combining published economic and fuel-use growth estimates with in-depth analysis of technology and regulatory changes likely to affect emissions over the time frame of interest. To incorporate new emission inventories into WRF-chem, a software framework was developed that projects county level emission estimates onto the sub-county modeling grid. The overall emissions framework created is an important tool that can be used for many future investigations, bringing increased capability for scenario modeling compared to currently available emission tools available for WRF-Chem.

Accomplishments

A recent journal article, "Regional climate consequences of large-scale cool roof and photovoltaic array deployment," described the regional climate effects of land-use changes (specifically albedo changes) associated with massive (terawatt) deployment of PV arrays in the Mojave Desert of California. The article included a quantitative analysis of surface temperature changes due to PV installation, and compared the magnitude of PV induced surface temperatures changes to those that may occur with albedo changes associated with installation of cool reflective roofs and pavements in cities. Associate emission changes with PV deployment were not accounted for and is the subject of ongoing work described below.

To estimate avoided emissions of CO_2, SO_2 and NO_X, due to 10% PV penetration level, an hourly dispatch energy system simulation model (EnergyPLAN) was used given generation and insolation data for 10 U.S. states. This research shows how the existing mix of generation resources and the amount and timing of solar irradiation affects the amount of emissions that are offset with PV integration. Technical constraints, such as power plant ramping rates and minimum operational capacity were taken into account in the analysis. This research is currently being submitted to a relevant peer-reviewed journal.

In ongoing work, WRF-chem will be used to determine the effects of PV integration in a future year 2030. The inputs for this modeling investigation have been developed as described above. Specifically, for a 10% PV integration into the power sector, avoided emissions for the 10 U.S. states obtained with EnergyPlan will be extrapolated for the continental U.S. This would allow for an evaluation of regional climate, air quality effects of PV integration for 2030.

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.

Dynamic Light Redirection by Optical Metamaterial Coatings

Principal Investigator(s): Stephen Selkowitz, Delia Milliron, Brett Helms, Stefano Cabrini, Andrew McNeil, Eleanor Lee, Jacob Jonsson, Andre Anders

Project Description

Lighting is the largest end-use of electricity, accounting for about 25% of all electric generation. The luminous flux in 1 m^2 of sunlight could offset electric lighting in over 200 m^2 of floor space, if it could be redirected efficiently. Prior efforts using static optical solutions have failed. The purpose of this research is to develop microscale, electro-actuated optical metamaterials that could be used in windows and skylights to provide this unique dynamic optical control, saving potentially 25% of all lighting use or $15B/yr in building operating costs.

Metamaterial properties can be dynamically tuned in response to angle and wavelength through electro-actuated inverse polymer opals. The optical characteristics of inverse opals made from soft materials have recently been shown to be tunable over a broad range through mechanical deformation. The development of dynamic holographic and prismatic optical elements (POE) will be explored. Numerical models of the optical metamaterials will be developed to understand the interaction between the electromechanical response and changes in refractive index. Full optical characterization of laboratory scale prototypes will be carried out using a scanning gonioradiometer and other optical assessment methods. Daylighting simulations will be used to inform and guide the design of the coatings by defining the required performance attributes. Lab-based coating R&D will provide proof of concept demonstration that one or more optical metamaterial systems shows promise to meet redirection requirements.

Accomplishments

Dynamic POEs consisting of an elastic electro-active polymer film with a periodic grading were developed. Materials were prepared by scalable synthesis protocols and used for fabrication of prismatic glazings by nano- or micro-imprinting lithography and hot embossing of polymer coatings. Issues associated with photo-curing and surface chemistry (polymer-substrate or polymer-mold interface) were resolved. Samples of ~1 in^2 were prepared and the resulting electro-active gratings were characterized by imaging and spectro-electrochemical analyses. We demonstrated that POE's with electro-active coatings can be created in various geometries by reproducible fabrication processes. Electromechanical induced structural changes as a function of applied potential are currently under investigation.

To guide development of early prototypes, finite-difference time-domain (FDTD) simulations were carried out to test the response of several proposed grating geometries. Initial designs were ineffective, but significant improvements were made by making the features larger. More improvement was found as a result of strategically adding thin metal layers to the design. Response of several hypothetical dynamic gratings was also explored with the FDTD-simulations by applying a simple model for the grating movement. The next step is to verify the simulated data by measuring the response of the recently fabricated polymer gratings. Daylighting simulations were conducted to quantify annual lighting energy use savings from alternative dynamic refractive POEs. Design optimization was constrained by a requirement to maximize energy savings while minimizing glare. Simulated annual lighting energy savings were estimated at 16% compared to the same window with a conventional shade in a 12 m deep open plan office. Samples large enough for measurement by the scanning gonioradiometer are anticipated to be fabricated at the next stage of development.

LB10028

Building Systems for Net Zero Energy Buildings

Principal Investigators: Michael Wetter (LBNL), Wangda Zuo (LBNL), Alberto Sangiovanni-Vincentelli (UC Berkeley)

Project Description

This project is to prototype how integrated building systems with very low energy use can be designed using *model-based rapid prototyping* within a *formal design process* based on a platform-based design (PBD) methodology. For the rapid prototyping, the equation-based, object-oriented Modelica language has been used. Research challenges included how to scale equation-based models from component level to whole building level for annual energy optimization. To formalize the design methodology, we prototyped the PBD flow for building automation systems. PBD is based on the usage of formal modeling techniques, clearly defined abstraction levels and the separation of concerns to enable an effective design process. Research challenges included how to define abstractions for the variety of building control algorithms and product lines to ensure a robust design flow that reuses system models for energy analysis, design of the building automation system and deployment of control sequences.

Accomplishments

Our first accomplishment is the inclusion of building envelope heat transfer simulation natively in Modelica as opposed to using co-simulation with EnergyPlus and Modelica. This allowed significantly faster development of feedback control loops compared to the previous configuration in which control loops had to be closed across different simulators. Furthermore, it allowed the automatic extraction of models of the building and the air-conditioning system, linearized around prescribed operating conditions, for the subsequent use in Model Predictive Control algorithms.

Our second accomplishment is related to addressing numerical problems that were caused by the coupling of the building envelope heat transfer with the air-conditioning system. Compared to the previous co-simulation implementation, the system of strongly coupled differential equations became large. Furthermore, the pressure dynamics of supply and return air path become coupled through the room air. This caused new numerical problems at near-zero air flow rate. We solved this problem through the development of new model formulations for fans, heat exchangers and sensors, and through embedding of state-selection rules in the underlying base models that allowed graph-decomposition algorithms to create smaller coupled subsystems.

Our third accomplishment is the full demonstration of the PBD flow for energy efficient buildings. We are now able to go *seamlessly* from a control algorithm described in Simulink and Modelica via an intermediate format to an implementation platform, including sensors, actuators, processors, and communication network for a floor of a real building. To demonstrate the full power of the methodology, we have chosen a popular vendor specific platform as a particular implementation platform. In this general framework, we developed a new control algorithm for energy efficiency and a novel tool with a graphical user interface to perform possibly the most complex step in the flow: the choice of the topology of the communication network that connects the components of the implementation platform. In particular, the synthesis algorithm targets wireless sensor networks with guaranteed performance.

Genomics Division

LB11030

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

Principal Investigator(s): Sam Deutsch, Eddy Rubin

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 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 aim 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 the Pacific Biosciences 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. These genes have been over-expressed, with over 65 % showing soluble expression. Biochemical characterization of the first 30 proteins has confirmed the predicted enzymatic activities, and has revealed significant variability in terms of enzyme thermostability and tolerance to pH changes. We aim to complete the biochemical characterization of all synthesized proteins, and use this information to derive structure-function relationships that might help to rationally engineer these proteins. In addition, we have started the synthesis of PKS modules for the biological production of 1-hexene as a potential biofuel precursor.

LB11036

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

Principal Investigators: Axel Visel (Lead Investigator), Zhong Wang, Stephen Gross

Project Description

The future success of lignocellulosic biofuels—those derived from the entirety of plant biomass rather than solely easily fermentable sugars and starches—is dependent upon development of additional plant feedstocks with high productivity yet minimal resource needs and low impacts on staple crop production. Agaves, exceptional desert plants capable of withstanding sustained droughts, high temperatures, and nutrient-poor soils, have recently been proposed as an additional lignocellulosic feedstock for arid (desert) and semi-arid (seasonally dry) environments inhospitable to other bioenergy plant species and unsuitable for food production. Though some *Agave* species are cultivated for fiber and distilled spirit production and the physiology and biochemistry of some species has been well-studied, the molecular genetics of agaves remains unexplored. The current lack of gene sequence information prohibits deeper investigations of the genes underlying the tolerance to the stresses of arid climates and the development of bioenergy-optimized agaves through modern plant breeding techniques.

To address the need for a sequence resource aiding development of bioenergy-optimized agave varieties, we are using massively-parallel sequencing technologies to assemble a reference transcriptome, a set of expressed genes, for *A. tequilana*, the *Agave* species with the most promise as an initial bioenergy feedstock. Such an approach avoids costly and time-consuming genome sequencing and is a faster route to protein-coding sequences. Short-read sequence data will be assembled using a novel computational pipeline for *de novo* transcriptome assembly (Rnnotator) developed at the Department of Energy Joint Genome Institute. Following sequence analyses, the *A. tequilana* transcriptome will be released as a community resource. Further planned experiments will profile gene expression of agaves under stress in order to understand molecular mechanisms of stress tolerance that distinguish agaves from other plant species.

Accomplishments

The assembly of plant transcriptomes without aid of a reference genome is challenging, especially in the case of plant genomes where repetitive sequence and gene duplication are common. To optimize methodologies in anticipation of the *A. tequilana* transcriptome, a parallel transcriptome project for *Zea mays* (maize) has allowed optimization of the Rnnotator pipeline and downstream annotation and analyses. Comparison of the *de novo* assembled maize transcriptome against the current annotation finds that ~80% of all known maize transcripts can be assembled by sequencing RNA isolated from tissues of juvenile stage maize seedlings.

Sequencing libraries originating from RNA of four distinct *A. tequilana* tissues from two developmental stages were constructed. Sequencing libraries with the Illumina HiSeq platform with the latest version of sequencing reagents yielded approximately 368 billion base pairs of sequence data. Computational analysis of these data sets is in progress.

Life Sciences Division

LB10040

Synchrotron-Based Microtomography for Functional Analysis of Normal Tissue and Tumor Molecular Markers, and their Perturbation by Low-Dose Radiation Exposure

Principal Investigator: Eleanor Blakely

Project Description

The first goal of this project is to explore novel nanoscale methods to optimize micro-tomography to generate a molecularly-defined, cell-type-specific 3D-image of a mouse. A second goal is to use these enhanced contrast techniques to identify functional physiological changes in multiple organ systems after exposure to low doses of radiation in intact animals. The third goal is to detect microscopic cancer cells potentially distributed in multiple organs of a tumor-laden mouse *in situ*.

We will image rodents with and without an intravenous injection of high Z-loaded caspids coated with antibodies to cell-specific structural proteins. High Z elements in the range from Ru to I will be tested. The microtomographic imaging will be done with both dual-energy- and fluorescent-tomography at the Advanced Light Source. The contrast sensitivity of this technique will be much higher than conventional single energy imaging. The protein specific antibodies will allow specific targeting to particular cells and will allow us potentially to generate an atlas of normal tissue markers for several strains of mice. Using the contrast enhancement techniques developed in our first goal we will identify functional physiological changes in multiple organ systems after exposure to low doses of radiation in intact animals, or in tumor-laden animals, in order to detect microscopic disease. In a time course extending up to 10 months after a low-dose radiation exposure, animals will be injected with antibody-coated caspids, and the distribution of organ-specific changes or nascent tumor cells will be tomographically imaged *in situ*.

Accomplishments

We have completed a total of six experimental runs at the ALS Microtomography beamline 8.3.2 over the past two years of LDRD funding, in which we have imaged 15 intact mice using beam energies from 22 to 35 keV. High quality 3D images of the intact mouse, mammary glands, lungs, tumors and kidneys were obtained with a pixel size of 18 x 18 x 18 microns. Some of the mice were imaged following a tail-vein injection of Iohexol, an iodine containing contrast agent. The addition of contrast agent enhanced the image contrast of the lung and kidneys dramatically. Additionally we have successfully imaged *in situ* lungs. Using standard solutions of Pd containing compounds, a beam energy of 25 keV and a single element Si(Li) detector we measured the elemental sensitivity of both dual energy absorption and fluorescent K X-ray techniques for 3D imaging of trace elements. We found that the concentration of Pd needed to have good quality images was not currently possible with the high Z-loaded caspids that we can make. However, based on these measurements, we have developed a fluorescent imaging system based on a coded aperture plate and a high-speed, many-pixeled CCD camera that should allow us to take fluorescent tomographic images of high Z-loaded capsids that are present in achievable concentration in various organs of an intact mouse following injection in a tail vein. With follow-on funding, this proof-of-principle study should result in a system that provides a unique capability at the ALS to obtain high-resolution tomographic images of dilute concentrations of many elements in complex samples with no sample preparation.

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. Information obtained from the *Drosophila* studies will be used to determine if similar proteins and mechanisms are utilized by human cells to regulate the response of heterochromatin to DSBs.

Accomplishments

We have successfully screened over 7,000 genes (out of 15,000 total) and have already identified candidate novel regulators of the heterochromatic DNA damage response (hDDR). These candidate genes implicate several of the pathways already known to be involved in hDDR, while also identifying completely novel pathways which will increase our understanding of this response. Additionally, we have identified new candidate genes which may regulate the proper localization, recruitment and/or maintenance of heterochromatin and repair foci.

Another important accomplishment has been the continued development and refinement of the computational tools necessary to extract as much data from this image-based screen as possible. Our software is now able to characterize 39 unique imaging features on a per nucleus basis. This allows us to utilize the screen to identify regulators of additional molecular pathways (such as maintenance of heterochromatin or recruitment of repair proteins to DSBs) in addition to regulators of hDDR. Identification of regulators of these additional pathways provides a valuable resource for researchers studying a broad range of topics. Additionally, new molecular pathways critical for regulating hDDR are identified by determining the common pathways linking genes whose silencing led to a loss of hDDR. This allows us to test a larger, yet more focused array of potential targets as follow-up experiments in order to better understand the hDDR pathway.

LB11016

Determination of Impact of the Microenvironment and Tissue-level Self-organization on Cell Fate Decisions and Homeostasis in the Mammary Gland, to Ultimately Inform Drug Discovery.

Principle Investigator(s): Mark LaBarge

Project Description

The purpose of this project is to dramatically improve our ability to understand the effects of therapeutics on human tissues at higher orders of organization than just cells in a dish. We will do so by systematically determining the functional response of tissue specific stem cells, groups of cells, and malignant derivatives to pathway-targeted therapeutics in the contexts of hundreds of unique and defined combinatorial microenviroments. These data will aid in better design and deployment of therapeutics and therapeutic regimens. The technologies and methods developed will also aid in the determination of tissue-level effects of chemical and radiological carcinogens (they are just wayward therapeutics after all).

We will further develop the microenvironment microarray (MEArray) platform for high throughput functional screening of combinatorial microenvironments as modulators of drug effects, and we will develop a microwell self-organization assay for quantifying rudimentary tissue-level organization in the presence of therapeutics and carcinogens. After establishing these methods for this purpose, we will perform proof of principle experiments to demonstrate and dissect specific drug and carcinogen response patterns that are correlated with specific properties and molecular constituents of microenvironments. These data combined with our recently developed unique cell human mammary epithelial cell culture collection will allow a first ever dissection of human tissue-level responses to drugs and carcinogens.

Accomplishments

We have improved upon the MEArray technology in two important ways: (1) We have altered the printing substrata, allowing us to control both the molecular content and elastic modulus of the microenvironment. We can now print arrays on surfaces, which allows us to better mimic in vivo conditions. (2) We now use higher resolution light-based imaging techniques to analyze MEArrays, which enables single cell analysis when desired. Using the improved MEArray platform we showed that the molecular constituency of and the modulus of microenvironments determine the responses of breast cancer cell lines to cancer therapeutics. These data help make sense of the many observations that cancer therapeutics often succeed in killing a primary tumor in breast, but fail to treat metastases.

Using the microwell self-organization assay together with a new algorithm for quantifying the dynamics of movement of communities of cells we proved that human mammary epithelium organizes into bilayers according to differential adherens junction activity. Recent innovations in the microwell's polymer chemistry have begun to identify physical characteristics of the microenvironment that are crucial to tissue organization.

We are in the process of applying these data and technologies to understand the effects of low dose ionizing radiation in communities of mammary epithelial cells.

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 generated 407 F1Bx mice that have been subjected to a single dose of 4Gy whole body x-radiation and are being monitored for tumor development. Some of them have developed thymic lymphomas. So far we have collected about 100 thymic lymphomas and other tissues including tail, lung, liver, kidney and spleen, and have stored them in tissue bank. The tail DNAs from all F1Bx mice have been made. A portion of them have been proceeded for SNP genotyping, the rest are in the process of SNP genotyping by Illumina Mouse LD Linkage panel that contain an optimized array of 377 loci in the mouse genome. In addition, the total RNAs have been made from thymuses for gene expression analysis using Affymetrix platform. We anticipate we will generate gene expression networks for the normal unperturbed thymus and to characterize the changes in gene expression networks that take place during perturbation by radiation. Now we will continue to monitor the F1Bx mice until all mice have developed tumor and to collect tumors. Thymic lymphomas will be analyzed by LOH, CGH, gene expression micorarray. Based on some of these preliminary results, I have submitted one R01 grant to NCI in October, 2011.

TITLE: SPARKLE

Principle Investigator: Cynthia T. McMurray

Purpose/Goals. The goal of the proposal was to create quantum dot(s) (QD) system in which transient interactions could be monitored inside cells. The interactions between components would be monitored using Fluorescence Energy Transfer (FRET). The purpose of the proposal would allow a glimpse into the inner workings of protein complexes in cells as they undertake biological transactions, and increase our understanding of their regulatory processes. The goal was to be carried out in three parts: (1) To generate non-toxic quantum dot reagents suitable for FRET analysis, (2) to test the uptake of the QDs and monitor their distribution in cells, and (3) to measure FRET inside cells as proteins interact.

Approach/Methods. Our most first goal was to prepare QDs that were aqueous soluble, non-toxic, stable in solution without aggregation, non-immunogenic, cell-permeable. We have developed new methods to optimize production quality of QD, which improve homogeneity and usefulness for tissue penetration and cellular uptake *in vivo.* In a typical preparation, we synthesized oleates from inexpensive hydrates of the corresponding chloride or nitrate salts. We then decomposed them at high temperature in a controlled manner using varying amounts of oleylamine in a mixture of coordinating and non-coordinating solvents. QDs were prepared in sizes ranging from 2 – 100 nm, suitable for use in the SPARKLE assays. As synthesized, our QDs are passivated with oleic acid and oleylamine and are only soluble in organic media. For aqueous transfer of QD, we employed a ligand exchange process whereby the nonpolar residual passivating ligands were exchanged for higher affinity, multivalent polysaccharides ligands. For example, we were able to obtain QD passivated with a well-known non-toxic FDA-approved polymer for *in vivo* work. Cells were cultured on plastic plates and the QD were visualized by microscopy.

Accomplishments: Our most significant accomplishment was to generate CM-dextran QD which were non-immunogenic, and stabilized folded (active) conformation of bound proteins. We developed several novel techniques for the chemoselective ligation of biomolecules to be used for successful conjugation of polymer to the donor protein. The advantage of chemoselective bioconjugation was orientation control. Since the interaction of the proteins to be tested was unknown, we standardized the conjugation procedure by measuring the antibody-binding capacity of protein G chemoselectively ligated to the polymer. After conjugation to the polymer, protein G was able to bind an antibody 4 times better relative to a comparable substrate where protein G was immobilized non-specifically. We also developed catalysts to accelerate these reactions in aqueous media. The coated quantum dots have been tested for their ability to enter cells. We find that the dots successfully enter cells by endocytosis. We are currently testing QD sizes to exclude vesicle encapsulation. We have obtained recently a Zeiss 710, which has enabled us to visualize FRET. We are currently optimizing FRET intensity and background subtraction.

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 environmental 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, 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 BSCs.

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

The research team has collected the requisite field samples and performed the planned wet-up experiment. Using 16S rRNA profiling we have confirmed that the dominant bacterium in the soil sample is *Microcoleus vaginatus.* We have obtained an isolate that has now had its genome sequenced. To help interpret the metabolic, respiration, and photosynthetic data we have annotated the major metabolic pathways in *Microcoleus vaginatus* genome and used these annotations to constructed a flux balance model. Custom microarrays were designed and used to study the expression dynamics of the pulsed activity (wet up) event. Results suggest the existence of a series of transcription modules. We have also completed sequencing and assembly of the crust (meta)genome and have compared the annotation enzymes in *M. vaginatus* with those in the community and found a large fraction of the total enzymatic capabilities are found within *M. vaginatus*, however, our results suggest that many critical functions such as nitrogen fixation require additional community members. This work was presented at the 11th Biennial conference of research on the Colorado Plateau in October, at the 1st Conference on Soil OMICS in Nanjing, China, in November, and at the LBNL open house and was met with great enthusiasm by both the scientific and lay community in all these venues.

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) being proposed 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 or any comparable future machine.

We have built on our experience at the ALS beamlines SIBYLS in structural investigations of macromolecules.. Key features of NGLS, which we intend to design our analysis tools around, include high average power, high repetition rate and short pulses in the soft X-ray spectrum. We will shrink the scale of biomass required for fractionation and purification of macromolecules. The strategies will build on our previous work on native biomass purification for small angle X-ray scattering at the ALS.

Accomplishments

A primary system of interest is gold end-labeled DNA molecules. We are investigating 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.

Utilizing X-ray scattering from our gold label system to measure the end-to-end distance of one sequence of DNA we have found that MutS specifically bends mismatched DNA and not fully complimentary DNA. However a second sequence bends regardless of whether a mismatch has been designed into the DNA. The purification of such particles remains non-trivial and we continue to improve our yield and the purification process. A conclusion of our studies will result in a publication with high impact on DNA mismatch repair, DNA repair in general and a natural application for the NGLS. The methods we are developing should fill a particularly important niche in the study of DNA repair processes as the signal from the gold labels acts as an accurate rulers over “long” (50nm) distances.

At the NGLS the technique may be applied 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 imbed in a phospholipid membrane.

Over the last year we have significantly enhanced our high throughput SAXS data collection pipeline. SAXS provides a fingerprint (low information content) by which the entire entity (high information content) may be reconstructed. This can be done by constraining modeling of the data by known information which is readily available. SIBYLS is the place where high throughput structural biology is being conducted and a paradigm for a beamline at NGLS.

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 electrospray mass spectrometry for single cell metabolomics. 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 Omics presents 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 of in single cell metabolomics. Specifically, we will fabricate prototype multinozzle arrays, measure their physical characteristics, perform surface derivatization, and demonstrate their proof-of-principle applications in metabolomics for human mesenchymal stem cells.

Accomplishments

We have made important progress for the project. Our most significant accomplishment has been to have published a major paper: Mao P., Wang H.T., Yang P., Wang D.*, "Multinozzle Emitter Arrays for Nanoelectrospray Mass Spectrometry," (2011) *Analytical Chemistry,* 83(15), 6282-6289. PMCID: PMC3146565.

In this paper, we report the silicon-based monolithic multinozzle emitter array (MEA), and demonstrate its proof-of-principle applications in high-sensitivity and high-throughput nanoelectrospray mass spectrometry. Our MEA consists of 96 identical 10-nozzle emitters in a circular array on a 3-inch silicon chip. The geometry and configuration of the emitters, the dimension and number of the nozzles, and the micropillar arrays embedded in the main channel, can be systematically and precisely controlled during the microfabrication process. Combining electrostatic simulation and experimental testing, we demonstrated that sharpened-end geometry at the stem of the individual multinozzle emitter significantly enhanced the electric fields at its protruding nozzle tips, enabling sequential nanoelectrospray for the high-density emitter array. We showed that electrospray current of the multinozzle emitter at a given total flow rate was approximately proportional to the square root of the number of its spraying-nozzles, suggesting the capability of high MS sensitivity for multinozzle emitters. Using a conventional Z-spray mass spectrometer, we demonstrated reproducible MS detection of peptides and proteins for serial MEA emitters, achieving sensitivity and stability comparable to the commercial capillary emitters. Our robust silicon-based MEA chip opens up the possibility of a fully-integrated microfluidic system for ultrahigh-sensitivity and ultrahigh-throughput proteomics and metabolomics.

LB10039

Functional Characterization of *NUCKS* - a Potential Cancer Susceptibility Locus Required for Recombination
Principal Investigator: Claudia Wiese

Project Description

NUCKS (Nuclear Ubiquitous Casein and Cyclin-dependent Kinases Substrate): NUCKS is a nuclear, DNA-binding and highly phosphorylated protein of unknown function. The amino acid composition of NUCKS and its DNA-binding domain each show some resemblance to high-mobility group A (HMGA) proteins, chromosomal proteins known as modulators of chromatin conformation and regulators of transcription. NUCKS is subject to extensive posttranslational modifications and has been investigated in several proteomic studies. As yet, these studies have not helped in describing a biological role for NUCKS.

In an attempt to identify proteins with sequence homology to RAD51AP1, a protein that we have characterized in the past, we have discovered that RAD51AP1 and NUCKS share extensive sequence homology throughout, suggesting that these two proteins can be considered paralogs of each other. In our sequence analysis, which is based on the comparative alignments of NUCKS and RAD51AP1 from several vertebrate species, human NUCKS and human RAD51AP1 are 28% identical and 11% similar. Apart from RAD51AP1, NUCKS shares no further major regions of homology with any other protein in protein or translated cDNA databases.

Paralogs are related proteins that have arisen from gene duplication. While evolving new functions, paralogs also can retain very similar functions (*i.e.* can be part of the same pathway). Here, we tested whether NUCKS and RAD51AP1 would have similar functions.

Accomplishments

Based on sequence homology with RAD51AP1, a RAD51-binding protein intimately involved in homologous recombination DNA repair (HRR) and characterized by us, we have tested and validated a role for NUCKS in DNA double-strand break repair (DSBR). To the best of our knowledge, our data are the first to demonstrate a biological function for NUCKS. Taken together, our results show that NUCKS is required for HRR, and that NUCKS is epistatic with both XRCC3 and RAD51AP1, two well-established HRR factors. In addition, our results also show that NUCKS is required for the repair of ionizing radiation-induced DSBs in G1-phase cells, suggesting that NUCKS could be a multifunctional protein.

Given the well-established tumor-suppressor role of the HRR pathway, we speculated that mice with targeted inactivation of one or both *Nucks* alleles, if viable, would show increased susceptibility to tumor formation. We find that *Nucks* KO mice are viable in either a *Trp53* wild type or *Trp53* mutant context and that, compared to *Trp53* single heterozygous mice, *Nucks Trp53* double heterozygous mice show increased sensitivity to radiation-induced tumor formation. These results show that partial deficiency of *Nucks* reduces tumor latency in a *Trp53* heterozygous genetic background and strongly suggest tumor suppressor role for the Nucks protein in mice. As with our results from human cell lines depleted for NUCKS (decribed above), both *Nucks* mice and *Nucks* MEFs show phenotypes consistent with a role for NUCKS in DSBR, and this will be assessed in future investigations.

LB11002

Induced "Bucket Brigade" Photovoltaic Effect
Principal Investigator: Joel W. Ager

Project Description

Ferroelectric materials have a built-in, spontaneous electrical polarization whose direction can be switched by an applied electric field. The electric fields caused by the polarization influence charge flow and, as a result, ferroelectrics have found numerous applications as sensors and in solid-state memory. It is an attractive idea to use the built-in electric fields to drive a photo-voltaic (PV) current. Indeed, it has been known since the 1950's that some ferroelectric materials can develop very large photovoltages under illumination. Although the effect can be quite spectacular, with photovoltages far exceeding the band gap of the ferroelectric, its detailed understanding had been elusive.

A major limitation in the understanding of these ferroelectric PV effects is incomplete knowledge of the exact nature of the electric fields proposed to produce the effect, e.g. whether they are supposed to be around impurity atoms or between different grains in polycrystalline materials. This uncertainty is eliminated in thin films of ferroelectric bismuth iron oxide ($BiFeO_3$ or BFO). Thin films of epitaxial, single-crystal BFO can be made with exquisite control over the areal patterning of domains of differing electrical polarization; this material was the key to understanding the origin of the high-voltage PV effect in ferroelectrics.

Accomplishments

Thin films of BFO were synthesized with a simple periodic pattern of ferroelectric domains: 150 nm of one polarization direction adjacent to 150 nm of the opposite polarization with a 2 nm thick "domain wall" between them. The electric potential produced by this structure has a simple sawtooth shape with sharp steps at the interface. Careful electrical measurements established that the large photovoltages produced by illumination of BFO thin films are associated with absorption across the band gap and thus involve the motion of both negatively charged electrons and positively charged "holes." Also, it is observed that the photovoltage is linear in the distance between the contacts on the surface of the film, suggesting a crucial role for the nanometer-scale domain walls.

These measurements enabled the fundamental mechanism for the ferroelectric PV effect is be discerned for the first time, solving a 50 year old mystery. The nanoscale source of the photocurrent is field driven charge separation caused by the potential steps at the domain walls. On one side of the wall, electrons accumulate and holes are repelled. On the other side, holes accumulate and electrons are driven away. As a result, the carrier recombination rate (the key PV loss mechanism) is reduced next to the walls as both an electron and hole are required for this process to occur. The domain walls act in this way as current sources, pumping electrons from one domain to another in a "bucket brigade" fashion. Analysis of the internal quantum efficiency (IQE) for individual domain walls shows it can be surprisingly high and approaches 10% for photons of energy above the bandgap.

Although the effect was experimentally in $BiFeO_3$ thin films, this LBNL work shows that it should occur in any system with a similar periodic potential. Work is underway to amplify the effect by coupling BFO to materials with greater light absorption, such as lower bandgap semiconductors and/or molecular absorbers such as dye molecules.

Heating rates of planar ion traps for quantum information

Principle Investigators: John Clarke and Hartmut Häffner
December 10, 2011

Project description

The main goals of this project are (a) to study the source of fluctuating patch charges and (b) to device methods to build small traps which feature heating rates on the order of 0.1 quanta/ms or less at room temperature. So far systematic studies of ion heating have concentrated on traps at cryogenic temperatures demonstrating that heating can be suppressed by many orders of magnitude by cooling the electrodes. Here, we will concentrate solely on fabrication methods and materials to create traps which work satisfactory at room temperature. Successful operation at room temperature will facilitate ion trap experiments considerably and allow for many applications ranging from ion trap quantum computing with segmented planar ion traps, extremely sensitive quantum detectors, and interfacing trapped ions with solid state systems. Understanding how to reduce these fluctuating patch charges could also impact other fields like nanomechanics and single spin detection.

For our experiments we fabricate planar ion traps with different methods. Planar traps have the advantage that they can be produced fast and are cost-effective. Furthermore, planar traps have been proven to be easily taken into operation. Finally, the monolithic design of planar traps helps a lot to speed up turn-around times. Traditionally, gold has been employed as an electrode material.

Accomplishments

We set up a testing apparatus and all the laser sources necessary for loading ions. We trapped ions at Berkeley using a trap fabricated at Zürich. However, the performance was orders of magnitude worse than observed by us previously. This lead us to the conclusion that the trap performance is limited by surface deterioration even inside ultra-high vacuum (UHV), shifting our emphasis to establish surface analysis tools.

We fabricated ion traps using photo-lithography. In our approach, we pattern trenches with a depth on the order of 15 μm and a width 10 μ in a quartz substrate. Evaporating this substrate under an angle on the order of 60 degrees to the trap surface normal, yields the trap electrodes electrically disconnected from each other. As trap electrode materials we used gold, platinum and copper. We also successfully grew graphene onto the copper trap. We expect graphene will passivate the surface thus reducing heating from surface adsorbates considerably.

To clean the traps, we build an annealing oven. Along similar lines, we evaluated cleaning procedures inside the UHV chamber. This includes plasma cleaning, photo-desorption as well as heating the trap in situ.

LB11013

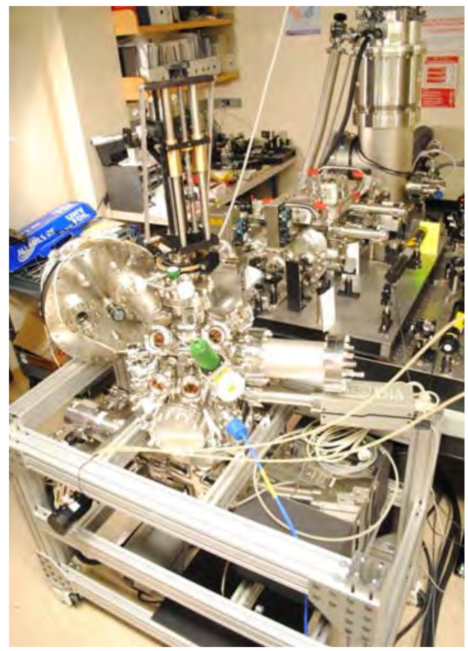
Attosecond XUV Condensed-Matter Science: Electronic Wavefunction Coherence and Correlated Dynamics

Principal Investigator(s): Robert A. Kaindl, Joseph Robinson, and Zahid Hussain

Project Description

The purpose of our project is to directly probe coherent electron dynamics in solids on the attosecond time scale for the first time. On these timescales, the effect of light waves on the material can be observed with sub-cycle resolution, yielding a measure of the time-dependent perturbation and evolving coherence. 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, our project helps establish a novel experimental technique to investigate condensed-matter processes on the shortest timescales.

In solids, the eV-scale electronic excitations are fundamentally linked to attosecond dynamics of the wave functions. Our approach to study this physics employs a customized scheme that combines few-cycle light fields, attosecond XUV pulses, and 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 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.



Attosecond condensed-matter setup developed during this first LDRD year.

Accomplishments

Our main accomplishment during this first LDRD project year has been to build a unique condensed-matter attosecond instrument. This effort involved the detailed CAD design, procurement, and assembly of the complex setup which includes the vacuum chambers and pumps, optics, interferometer, electronics, etc. Our setup, shown in the adjacent figure, avoids the split-mirror time delay conventionally used for gas-phase attosecond studies which is incompatible with UHV vacuum conditions. True solid-state properties are only observed on clean surfaces, critically necessitating $\approx 10^{-10}$ Torr vacuum conditions. Therefore, we separated the attosecond timing and UHV sample environment into different chambers.

Precise time delay in our setup is achieved by a piezo-stabilized Mach-Zehnder interferometer, connected to a reconfigurable XUV optics chamber. This also provides space for attenuation, polarization modulation, and nonlinear frequency conversion of the few-cycle pulses to enable tunable THz streaking experiments. The bakeable UHV experimental chamber incorporates the sample load-lock and transfer, electron spectrometer, and manipulator. With the assembly of this complex instrument completed, optical alignment is now underway to enable the 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

The goal of our LDRD is to study the femtosecond dynamics of complex semiconductor nanostructures relevant for photovoltaic applications using broadband 2D Fourier-transform spectroscopy (2D-FTS). Nanoscale heterostructures offer important new possibilities for controlling exciton creation and coupling, and for achieving ultrafast and directed charge separation – essential components for efficient solar energy conversion in photovoltaics or photocatalysts. At present, their dynamics is only poorly understood. Conventional ultrafast pump-probe experiments are hampered by the typically broad optical features of photovoltaic nanomaterials, making it difficult to isolate specific energy eigenstates and mutual couplings. The broadband 2D-FTS studies pursued here, in contrast, can reveal coherent and incoherent dynamics underlying the congested multi-component optical spectra, providing insight to exciton creation, energy transfer, charge separation, or coupling to surface states.

Our experimental approach is based on an ultrafast laser system 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 efforts and with 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 nanomaterials and physics, to investigate e.g. high-energy carrier relaxation in nanorods, coherent exciton coupling in superlattices, or electron transfer in photocatalytic structures.

Accomplishments

During the first project year we have developed the 2D-FTS interferometer instrument suitable for broadband coherent multi-dimensional spectroscopy of photovoltaic nanomaterials. The experiments are based on a 250-kHz high-repetition rate femtosecond amplifier system, combined with broadband parametric frequency conversion into the near-infrared and visible and a custom-designed 2D-FTS interferometer. Here, the high repetition rate ensures high-fidelity in the data collection while providing large pulse energies to efficiently convert the output into laser wavelengths over a broad spectral range. The 2D-FTS interferometer encompasses four arms arranged in a compact way to ensure high phase stability. Motorized nanopositioning is employed to achieve precise timing in a large range, from sub-cycle phase shifts up to nanosecond delays. Moreover, the setup is constructed such that digital software loops replace the analog feedback electronics of conventional interferometers.

We are in the process of finalizing the optical setup and its alignment, and applying it towards first experimental 2D-FTS studies. To this end, CdTe/CdS core/shell nanocrystals have been synthesized at the Molecular Foundry and spectrally characterized in the visible and near-IR. These samples are suitable for investigations of exciton coupling dynamics. While initial work has focused on developing the instrumentation, we expect to expand the efforts in the second year to exploit its scientific potential for studying the ultrafast physics of photovoltaic nanomaterials.

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 have been synthesized and characterized by transport and magnetic measurements. The proper protocols for synthesis of crystals of Sr_2IrO_4 are being developed. In collaboration with a team at the Advanced Light Source, infrared transmission has been performed on Sr_2IrO_4 and the spectra thus obtained show clear evidence of the large spin-orbit interactions that are needed for TI materials.

LB09029

Tuning the self-assembly of membrane proteins
Principal Investigator(s): Berend Smit

Project Description

Our understanding of the role of the cell membrane has evolved from a passive bilayer limiting the boundaries of a cell to an integral part of the regulatory system of the cell. Linked to this regulatory system are the mechanisms the cell membrane is using to modulate its structure. In this model, the cell membrane contains different morphologically distinct regions or domains specialized in different functions ranging from nutrient adsorption, cell-to-cell communications, or endocytosis. In this proposal we address the question of how cells modulate the structure of membrane proteins and the self-assembly of membrane proteins. In this project we use coarse-grained molecular simulation to study the effect of changes in the structure of the bilayers on the interactions between objects embedded in the membrane.

Accomplishments

Our most significant accomplishment has been a detailed comparison with the experimental technique, calorimetry to determine phase boundaries. With this method we studies the phase behavior of saturated lipids as a function of temperature and tail length through changes in structural properties and we introduce a computational method to monitor changes in enthalpy, as is done experimentally with differential scanning calorimetry. The lipid system experimentally presents four different bilayer phases – subgel, gel, ripple, and fluid – and the DPD model describes all of these phases structurally while MARTINI describes a single order-disorder transition between the gel and the fluid phases. Given both models' varying degrees of success in displaying accurate structural and thermodynamic signatures, there is an overall satisfying extent of agreement for the coarse-grained models. We also study the lipid dynamics displayed by these models for the various phases, discussing this dynamics with relation to fidelity to experiment and computational efficiency.

In addition we developed the software to run our DPD code on GPUs (graphical processor units). Tests show that this new code speeds-up the calculation by a factor of 30.

LB10021

Project Title: Structured Charged Polymers

Principal Investigator: Matthew Tirrell

Project Description

Polyelectrolyte applications are continuing to emerge and expand in novel materials and interactions with physiological systems, driven in part by a growing demand for polymeric materials that respond to environmental changes. Current efforts in fields of multilayer formation and behavior, chemical gating, and drug delivery, all exploit polyelectrolytes that respond to external stimuli ranging from electrical and mechanical to environmental changes in pH and salt concentration. This increase in interest necessitates a deeper fundamental understanding of the structure and properties of these complex materials. End-tethered polyelectrolyte brushes, coated onto surfaces or onto colloidal particles in solution, constitute an interesting and substantial portion of the applications in these areas, as well as a well-defined experimental system for examining intermolecular interactions in polymers. Although polyelectrolyte brushes have been well-studied in environments consisting exclusively of mono-valent ions, much less attention has been given to their behavior in the presence of multi-valent species. This is despite importance of multi-valent ions in many situations of practical interest ranging from commercial products and processes, to environmental technologies, to biology. Oppositely charged macromolecules are an especially interesting type of multi-valent species.

Accomplishments

This work has explored the structure and properties of end-tethered anionic polyelectrolyte brushes containing tri-valent ruthenium hexamine ($Ru(NH_3)_6^{3+}$) and mono-valent sodium (Na^+). Detailed studies of these planar, strong polyelectrolyte brushes composed of poly(sodium styrene sulfonate) were performed *via* electrochemical experiments using cyclic voltametry (CV) and surface force experiments using the Surface Forces Apparatus (SFA). A comparison between CV and SFA measurements provided physical information regarding polyelectrolyte brush height and the population of tri-valent $Ru(NH_3)_6^{3+}$ ions inside a brush. Polyelectrolyte brushes were observed to transform from extended brushes dominated by the presence of mono-valent counterions, to collapsed brushes saturated with tri-valent ions. This transformation occurred as a result of $Ru(NH_3)_6^{3+}$ uptake into polyelectrolyte brushes. The collapsed state, seen only with brushes dominated by multi-valent counterions, also corresponded to strong adhesion between brushes. Adhesion was never seen with only mono-valent ions present in solution. Experiments were performed in solutions of three fixed ionic strengths, with brush collapse occurring more suddenly and producing higher adhesion at lower ionic strength.

In closely connected work, interfacial tension of polypeptide complex coacervates was measured using a Surface Forces Apparatus (SFA). Poly(*L*-Lysine hydrochloride) (PLys) and Poly(*L*-Glutamic Acid sodium salt) (PGA) were investigated as a model pair of oppositely charged weak polyelectrolytes. The interfacial energy of these polypeptide coacervates was separately found to increase with both decreasing salt concentration and increasing polypeptide chain length. In most of the above cases, interfacial tension measurements were found to be very low, below 1 mJ/m^2. Biocompatible complex coacervates with low interfacial energy have strong potential for applications in surface coatings, adhesives, and encapsulation of a wide range of materials.

Intermediate Band Solar Cell – Proof of Concept and Search for New Materials

Principal Investigator(s): W. Walukiewicz and Kin Man Yu

Project Description

Using the unique features of the electronic band structure of dilute GaN_xAs_{1-x} alloys, we have designed, fabricated and tested a multiband photovoltaic device. The device demonstrates an optical activity of three energy bands that absorb, and convert into electrical current, the crucial part of the solar spectrum. The results demonstrate the feasibility of using highly mismatched alloys to engineer the semiconductor energy band structure for specific device applications. However, in this work one of the key features in a multiple band solar cell, light absorption from the intermediate band to the conduction band was only indirectly demonstrated through the current-voltage and external quantum efficiency measurements. We propose to perform two photon experiments on this dilute nitride based multiple band gap solar cell to directly probe the absorption of light from the intermediate band to the conduction and thus unambiguously show the basic operation of this device.

Accomplishments

In the two photon experiments we have used an intermediate band solar cell with GaNAs active layer and AlGaAs layers blocking the charge conduction in the intermediate band. We have designed two different experimental set ups to measure the electrical current produced from the absorption of two low energy photons in an intermediate band solar cell.

In the first experiment the samples were mounted in a He cryostat with two transparent windows. The intermediate band solar cell structure was illuminated with two photon beams: a modulated beam from tungsten (W) lamp and a constant illumination from a xenon (Xe) light source. Proper filters were used to eliminate effects of second harmonics and to restrict the photon energies of the Xe source to a specific single photon transition. In the second experiment an unmodulated W source is used to produce monochromatic light whose energy can be varied from UV to near IR whereas the light of the second Xe source is filtered to eliminate higher energy optical transitions except the transitions from the intermediate to the conduction band.

Both experiments have demonstrated photocurrent extraction when the sample is illuminated with two light sources that can selectively excite electrons from the valence to the intermediate and from the intermediate to the conduction band. This provides the first proof of the generation of electron hole pairs by two photon absorption with the intermediate band serving as a “stepping stone” for the valence to the conduction band optical transitions. The results of these experiments provided important insights into operational principles of the intermediate band solar cells. They have highlighted the importance of matching the strengths of optical transitions to and from the intermediate band and have shown how these strengths can be controlled by the intentional doping. In addition the experiments reinforced the significance of the proper electrical isolation of the intermediate band from the charge collecting contacts.

LB10025

Integrated Optoelectronic Devices Based on Graphene

Investigator: Feng Wang

Project Description:

Graphene, a single layer of honeycomb carbon lattice, is emerging as an exceptional new material for future electronic technology. One reason for this is that graphene exhibits many novel behaviors. Electrons in graphene, for example, move as if they have zero mass and display strongly quantum mechanical behavior even at room temperature.

In contrast to the great activity in graphene electronics, studies on graphene optoelectronic properties have been few. However, our recent studies show that graphene optoelectronics can provide exciting opportunities for physics and technology. For instance, we demonstrated that graphene couples to light strongly and the infrared *optical* transitions in graphene monolayers can be switched on and off by *electrical* gating. Understanding of such optoelectronic reponses can lead to novel graphene based optoelectronic devices.

Accomplishments:

We have made exciting progresses in studies of tunable electro-optical behavior in graphene in the LDRD project.

We demonstrate for the first time the capability to control Raman scattering quantum pathways in graphene. Raman has been an indispensable tool in physical science to probe elementary excitations. In the quantum mechanical picture of Raman scattering, incident photons first excite a set of intermediate electronic states, which then generate crystal elementary excitations and radiate energy-shifted photons. The intermediate electronic excitations therefore play a crucial role as quantum pathways in Raman scattering, and this is exemplified by resonant Raman scattering and Raman interference. The ability to control these excitation pathways can open up new opportunities to probe, manipulate, and utilize inelastic light scattering. We achieved excitation pathway control in graphene with electrostatic doping. Our study reveals quantum interference between different Raman pathways in graphene: When some of the pathways are blocked, the one-phonon Raman intensity does not diminish as commonly expected, but increases dramatically. This discovery sheds new light on the understanding of resonance Raman scattering in graphene. This work has been published in Nature.

Design and Surface Properties of Semiconductor Nanowires

Principal Investigator(s): Peidong Yang, Ali Javey, Junqiao Wu

Project Description:

This collaborate effort seeks to explore the controlled fabrication/synthesis and chemical doping of nanostructured materials, including oxides and III-V compound semiconductors. Our goal is to discover, understand, control, and exploit the functionalities of individual phase boundaries in these nanowires. The experiments are designed to address the following outstanding questions: (1). Is there any fundamental difference between doping in nanowires and doping in bulk semiconductor (single crystal and thin films)? (2). How to quantitatively evaluate the dopant environment, uniformity and induced lattice modification, and consequently any electrical/optical property modification? (3). For surface functionalized nanowires, what are the effects on surface states, wire conductivity, carrier mobility and other optoelectronic properties?

Accomplishments:

The Yang group**:** P-type doing in ZnO has been highly elusive, and yet it is extremely important for the realization of ZnO based active optoelectronic devices. Li-doped ZnO nanowires were synthesized via an in situ CVT approach. While Li ions are incorporated within the crystal, the as-synthesized nanowires exhibit lower mobility and higher resistivity than pure ZnO. This is due to the Li ions residing predominantly as an interstitials and/or defect pairs, which do not act as electrical dopants yet still adversely affect the mobility. However, upon thermal annealing, Li ions are able to diffuse to Zn vacancies and act as shallow accepters, changing the majority carriers from electrons to holes. While p-type conductivity was measured via NW-FET, a positive Seebeck voltage also gave confirmation.

The Wu group: 1) We performed a comprehensive numerical modeling of the electrothermal dynamics of free charge carriers in nanowires. The simulation allows us to reveal and predict important, surprising effects that are previously not recognized, and assess the limitation as well as potential of scanning current techniques in nanowire characterization. 2) We elucidated the mechanism of a novel photovoltaic effect which occurs in ferroelectrics with periodic domain boundaries. Under sufficiently strong illumination, domain walls function as nanoscale generators of the photovoltaic current, and photovoltages are additive and voltages much larger than the band gap can be generated. And 3), we revealed that in the metal-insulator transition of single-crystal vanadium dioxide, a large kinetic asymmetry arises from the distinct spatial extension and distribution of two basic types of crystal defects: point defects and twin walls.

The Javey Group**:** We have explored the controlled ex-situ *p*-doping of InAs quantum membranes (QMs) with thicknesses down to just a few atomic layers. The electrically active [Zn] is estimated to be $\sim 1\times10^{19}$ cm^{-3} , which is among the highest reported acceptor concentration in InAs. In a second project, monolayer S-doping of InP nanopillars (NPLs) were explored for the fabrication of high efficiency solar cells. We implemented sulfur monolayer doping scheme to achieve conformal ultra-shallow junctions with sub-10nm depths and a high electrically active dopant concentration of $10^{19}\sim10^{20}$ cm^{-3} in arrays of InP NPLs. The enabled solar cells exhibit a respectable conversion efficiency of 8.1% and a short circuit current density of $25mA/cm^3$. The work demonstrates the utility of well-established surface chemistry for fabrication of non-planar junctions for complex devices.

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). The most straightforward method for the fabrication of graphene nanoribbons, which is based on e-beam lithography patterning and plasma etching, however, has the difficulty to reach widths bellow 10 nm and results in rough GNR edges that will reduce the carrier mobility and deteriorate the device performance significantly.

This project aims at developing new methods to grow GNRs on a selected surface of a nanowire (NW) template. The surface-selectivity of GNR growth can be based on different lattice mismatch and epitaxial rates on different crystallographic planes of a single crystalline NW template. It can also be based on the catalytic reactivity of a specific surface that promotes the graphene formation in a chemical vapor deposition process (CVD). By understanding the surface-selectivity and the nucleation/growth process of graphene synthesis on NW templates, we aim to achieve GNRs with a well-defined width down to nanometer scale, controllable crystallographic orientation, and smooth edges. We will characterize the GNRs and verify the bandgap-GNR width relations predicted by various theoretical models.

Accomplishments

In this phase of the project, the growth of graphene by using nickel as the catalysts material in CVD processes has been established. In parallel, the patterning of nickel catalyst layers has been optimized so to fabricate nickel nanowide paths. These paths result in the growth of GNRs because of the catalytic selectivity for graphene growth on the paths with respect to the substrate. At present, the conditions for the growth of single and few layer GNRs are being optimized.

In addition to graphene growth optimization, GNR based test structures and devices have been designed, and the first prototypes have been fabricated. The structural characterization and the electrical testing of these devices are on-going.

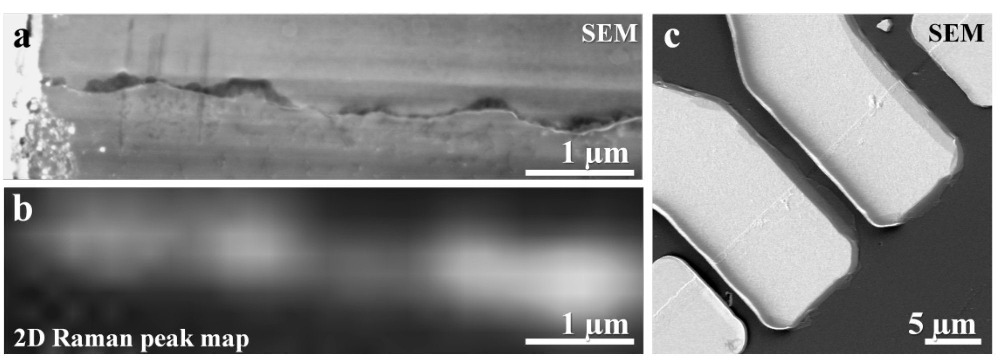


Fig. 1: (a) Scanning Electron Microscopy (SEM) image of a GNR and (b) a mapping of the characteristic Raman peak of graphene for this GNR. (c) SEM image of a GNR test structure.

Imaging Through Liquids Using A TEM

Principal Investigator: Haimei Zheng

Project Description

The goal of this project is to study of nanocrystal growth and structural dynamics in liquids and image biological materials in their native environment at high resolution using a transmission electron microscope (TEM).

We develop liquid environmental cell using silicon-based microfabrication process which allows imaging through liquids with subnanometer resolution using a TEM. Low stress silicon nitride membranes for the imaging window will be developed so that it is thin enough to achieve high resolution yet it is strong enough to achieve robust operation. We apply such development along with other advanced TEM to investigate colloidal nanocrystal growth mechanisms and structural dynamics at nanometer or atomic scale, which are mostly not accessible by any other approaches. In addition, we also use liquid cell TEM to image proteins in liquid water, which will establish technical advances on imaging biological materials in their native environment with nanometer resolution using a TEM.

Accomplishments

One of our most significant accomplishments has been on the study of nucleation and growth at pseudoequilibrium states. Firstly, we engineered a precursor scarce environment in a liquid cell to study growth of bismuth nanoparticles in a solution mixture of oleylamine and dichlorobenzene. By controlling the slow releasing of bismuth precursor, we observed the oscillating growth and dissolution of bismuth nanoparticles with subnanometer resolution. We quantified the growth kinetics and directly measured a mass transport zone presented around each nanoparticle. This study shed light on engineering growth processes to reverse nanoparticle coarsening by Ostwald ripening. These findings may be highly beneficial to improve the reactivity and life time of nanoparticle catalysts. Secondly, we used an aberration corrected TEM to study solid-solid phase transition of a single nanocrystal at atomic level. It demonstrated that advanced TEM is critically important complimentary approach to the liquid cell TEM. Phase nucleation, propagation and phase fluctuation dynamics at the transition point were observed with an unprecedented level of detail. This study may contribute to understanding ion transport in electrodes and many other material processes.

We have also succeeded in imaging proteins in liquid water with 2.7 nm resolution using liquid cell TEM. The solution of acrosomal bundle is loaded into a liquid chamber with a 300 nm gap between two identical 10 nm thick electron transparent Si_3N_4 windows. Low-dose imaging using a TEM operated at 120 keV was applied. We find the tolerable dose to be $D_{1/e}$ *(293K)*= 35 e/A^2, which is higher than the expectation that the effect of temperature on radiation damage is at least 10 times worse at room temperature compared to that at cryogenic conditions. This enhanced resistance to radiation damage of proteins in aqueous environment at room temperature suggests that it might possible to image dynamic processes of biological materials with high resolution using a TEM.

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 and dark matter. The project plan includes constructing a cryogen-free ^3He-^4He 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 second year of the LDRD a Triton-400 cryogen-free dilution refrigerator from Oxford Instruments was successfully commissioned and temperatures as low as 6.6 mK have been achieved - well within the target range. We mounted the refrigerator on a specially modified frame which we designed to meet our eventual goal of easily relocating to a low background facility; a test-move within our lab was successful. Our system is capable of cooling from room temperature to below 10 mK within ~24 hours and possesses a cooling power of 300 μW at 100 mK, we have grown the expertise within our group necessary to operate the refrigerator, successfully completed many warm-to-cold cycles, and characterized key diagnostic parameters to monitor the stability of the system. Remote monitoring and control capabilities, necessary for operations envisioned at a distant underground facility, have been demonstrated. A portable clean room has been installed to establish a clean perimeter around the refrigerator. We completed the design of a lead-shield which will encapsulate the refrigerator sample-volume, the shielding system includes a mechanism to safely move the shield when access to the sample volume is necessary. Construction of this system is now advancing.

We have set up a nuclear-orientation thermometry system consisting of a Co-crystal with implanted ^{60}Co, two NaI gamma counters, and a data acquisition (DAQ) system. We have achieved reliable and independent temperature measurements below ~100 mK with this system and used it to calibrate secondary thermometers. We have also designed and built an AC resistor bridge circuit capable of measuring resistances up to 1 GΩ, it is being used to characterize NTD-thermistor samples in our refrigerator. To streamline these characterization runs we have designed a versatile, dedicated sample holder; a prototype has been fabricated and deployed in the refrigerator, optimization of the design for thermal balance and wiring is progressing.

In addition, we have acquired two $5 \cdot 5 \cdot 5$ cm^3 and several $1 \cdot 1 \cdot 1$ cm^3 TeO_2 crystals for bolometric measurements; the necessary front-end electronics have been sourced and implementation of the associated DAQ system has begun.

LB10008

Heavy Element Mass Analysis and Detector Facility

Principal Investigator(s): Kenneth E. Gregorich

Project Description

The purpose of this project is to do the initial design work and planning for a single-atom mass analyzer and detector station to be run in conjunction with the Berkeley Gas-filled Separator (BGS).

Since prediction in the 1960s of superheavy elements (SHE) stabilized by spherical nuclear shells, the production and study of SHE has been considered the Holy Grail of Low-Energy Nuclear Science. During the last 10 years, we have seen several claims of SHE production in Dubna, using ^{48}Ca projectiles with actinide targets. There have now been several *independent confirmations* of some of the Dubna SHE claims. However, the atomic number (Z) and mass number (A) assignments of all SHE isotopes are, to a large extent, based on comparison of measured and alpha-decay energies with those predicted using nuclear mass models. Before using the measured alpha-decay energies to refine the nuclear mass models, we must be certain that the Z and A assignments are correct (otherwise, refinements to the mass models will reinforce the incorrect Z and A assignments).

An RF gas-stopping cell will be installed at the BGS focal plane. After initial separation with the BGS, heavy element recoil ions will pass through a thin HAVAR window, and stop in high-purity He gas inside the RF gas-stopping cell. Because of the high ionization potential of the He, these heavy element ions will retain a 2+ charge state. Application of focusing RF+DC fields will direct the heavy element ions toward an orifice. Once they near the orifice, they will be swept through with the gas flow. Subsequent gas skimming will result in a “beam” of 2+ ions which will be accumulated in a radio frequency quadrupole (RFQ) trap. Periodically, the ions accumulated in the RFQ trap will be sent through a mass analyzer to a low-background detection facility. Highly-efficient delivery of mass-separated heavy ions to a low-background detector facility on a 10-ms timescale will facilitate a broad, world-leading heavy element nuclear physics research program.

Accomplishments

For the mass separator section, we spent much effort comparing the time-of-flight “reflectron” technique with the crossed electric and magnetic field “trochoid separator”. The reflectron concept was interesting because of its ability to simultaneously use 1+ and 2+ ions coming out of the RFQ trap, resulting in an increased efficiency. However, it was found that the large longitudinal emittance of ions ejected from the RFQ trap resulted in insufficient mass resolution. Simulations of the trochoid separator were refined, with realistic magnetic and electric fieldmaps, and realistic values for longitudinal and transverse emittance of the incoming beams. The mass separation using the trochoid separator is sufficient to give unit mass resolution for single atoms of heavy and superheavy elements.

In FY 2011, we were successful in obtaining follow-on funding for the components of this project. Presently, we are obtaining quotes for the separator magnet, and designing the vacuum chamber and electric field shaping circuit boards. We have also chosen a commercially available ion source for testing the mass separator.

The detector system is being constructed. A DOE Subcontractor Agreement between LBNL and ANL was signed where ANL will construct the RF catcher, RFQ trap, and post-trap acceleration sections of the facility.

LB11010

Lattice QCD Codes by Discretizing Time and Space
Principle Investigator(s): Wick Haxton

Project Description

The project is focused on advancing lattice QCD (quantum chromodynamics) calculations of observables important to nuclear physics/astrophysics. QCD is the fundamental theory of the strong interaction, the force responsible for binding nuclei and for generating approximately 99% of the universe's visible mass. The theory is both nonlinear and non-perturbative, so that analytic techniques are of little use in evaluating the theory. Lattice QCD is a formulation of QCD in which both space and time are discretized, so that a four-dimensional lattice represents our world, up to corrections associate with the finite extent and nonzero grid spacing of the lattice. With this formulation the theory can be solved numerically by methods based on Monte Carlo sampling of the path integral. With the leadership-class machines now becoming available, realistic predictions of nuclear properties can be made.

In collaboration with our partners from Lawrence Livermore National Laboratory – together we form the CaliforniaLattice collaboration – we have made significant progress on several problems connected with the structure of the lightest nuclei, the interactions of strange matter important to the neutron star equation of state, and the strength of the parity-violating weak nucleon-nucleon interaction. We are particular excited about our efforts to use lattice QCD calculations to determine properties of the two-baryon system, as we see this as a possible road to connecting lattice QCD to standard nuclear structure techniques. Our work is now at an important point because Sequoia, the new 20 petaflop computer at LLNL, will be assembled over the next several months. This machine, which will be the fastest in the world, could take lattice QCD calculations to a new level. Our group is working with the CPS and Chroma codes in preparation for turn-on of Sequoia.

Accomplishments

While we were able to make good progress on several fronts, three accomplishments stand out from the past year's work:

1) Group member André Walker-Loud was able to make an estimate of the mass of the H-dibaryon, a conjectured bound state of two strange baryons. The calculations were able to constrain the binding energy to a relative narrow band that includes zero. Because the band is consistent with both an unbound state and one barely bound, the conjecture of the di-baryon is not yet resolved. However, the worked demonstrated the feasibility of a definitive calculation, as computing resources continue to grow.

2) Walker-Loud and group member Sergey Syritsyn used lattice QCD techniques to determine properties of the nucleon. Walker-Loud demonstrated that background fields could be introduced into a lattice QCD calculation to determine nucleon polarizabilities. Syritsyn, in a calculation using domain-wall fermions as a device to exactly impose chiral symmetry, determined the fractions of the nucleon's spin and momentum that are carried by the quarks.

3) CaliforniaLattice member Joe Wasem (LLBL) was able to make the first lattice QCD estimate of the parity-violating pion-nucleon coupling. This project required nearly dedicated use of LLNL's Edge GPU cluster for a period of 10 months. His result provides importance guidance for an upcoming cold neutron experiment, $\vec{n} + p \rightarrow D + \gamma$, planned for the SNS at ORNL. A paper has been submitted to Physical Review Letters (arXiv:1108.1151). This coupling depends on the only interaction in the Standard Model of particle physics not yet detected in the laboratory, the weak neutral hadronic current.

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.

We will develop a realistic simulation of the physics capabilities of ALICE' current setup together with the projected LHC performance for 2010 and 2011, and develop the trigger strategy to exploit the full statistical reach provided by the delivered LHC luminosity. First, we will develop the reconstruction methods for neutral mesons, mainly pions, to be able to gauge the electromagnetic calorimeter, and to study the background of decay photons. Then, we will develop the reconstruction method for photons the standard approach of shower shape analysis in the calorimeters, and of alternative reconstruction algorithms outside of or complementary to the applicable region of the shower shape method. In particular, we will also investigate an hybrid algorithm where one conversion electron is identified using the TPC, and the other using the calorimeter, and explore if direct photon measurement via measurement of low mass electron pairs far below the π_0 mass can be pushed to high transverse momentum. Further investigations include the application of new isolation strategies using modern jet finders.

Accomplishments

We have carried out realistic simulations of the physics performance of ALICE for the 2011 proton–proton and lead–lead runs, and convincingly argued for, and then implemented, the trigger strategy for photons for the 2011 runs.

Our most significant accomplishments are the measurements of neutral pions, the main background source for decay photons, both in proton–proton, as well as in lead–lead collisions at 2.76 GeV per nucleon pair. First, uncorrected results have been shown at the Quark Matter conference in May 2011. The fully corrected spectra are expected to be published within the next months.

Furthermore, we have obtained first spectra of raw, isolated photons in proton–proton collisions, using standard shower shape cuts, and isolation criteria derived from neutral meson production in jets. Currently we are working on a data driven procedure to improve the predictive power of the MC simulations for the calorimeter response. This will be a crucial step to arrive at an isolated photon measurement in proton–proton collisions.

Physical Biosciences Division

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

We have derived macromolecular aspherical atom densities for specific chemical environments oriented to conform to the local bonding environment, from which aspherical-atom scattering factors are calculated. These aspherical densities can be 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) contains atom-types occurring in light-atom proteins and nucleic acids.

We have identified the components of the XD program that are relevant to the calculation of aspherical scattering factors. We have also worked on automated translation of the XD code to C++ for use in Phenix. This work will lead to an implementation of the aspherical atom scattering calculation in the Phenix software. This relies on algorithms to identify the appropriate patterns of atoms (including their local environment) to retrieve the correct aspherical fragment from the database for calculation of scattering factors. We are currently testing whether these algorithms can be generated as an extension of the structural analysis performed in the assignment of rotatable torsion bonds for constrained molecular dynamics in our Tardy algorithm.

Once the appropriate scattering factors can be calculated it will be possible to generate improved electron density maps that account for the aspherical electron density distribution. However, for each structure these scattering terms need to be refined to optimize the fit of the model to the experimental data. Procedures for this optimization have been developed for small molecular systems (up to 100 atoms). However, they scale poorly with the size of the system (number of atoms) and become challenging for large macromolecular systems. This results in computing times of days for a single refinement run, of which many must be performed interspersed with manual analysis using interactive molecular graphics. To make the method practical for a broad range of systems and researchers we have developed code for GPU architectures to rapidly calculate atomic structure factors using a direct summation method. The initial implementation shows a speed up of a factor of 500 using NERSC GPU systems.

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 first year of this project, we have developed reagents and methods necessary to dissect the assembly and function of the carboxysome. We have constructed BglBrick compatible expression vectors for E. coli and tools to fuse proteins, purify them and regulate expression as well as fluorescent reporter proteins (GFP, YFP, CFP). We have also cloned and expressed fusions of carboxysome proteins to try to control the size of the carboxysome compartment. Initial results in E. coli have been characterized by TEM and show single compartment-like structures of ~200 nm. To track the dynamics of carboxysome assembly, we have developed an atomic force microscopy (AFM) method for imaging carboxysomes in vitro, and this method will be augmented and extended by the addition of fluorescent reporters to the shell proteins.

While many of the individual subunits of the carboxysome shell have been characterized there is still little information on how the protein shell assembles in vivo. To help elucidate the mechanism for this process, we are using Monte Carlo (MC) and molecular dynamics (MD) simulations. A coarse-grain model of the shell subunit hexamers and pentamers are used, and each subunit is represented as either hexagonal or pentagonal prisms with interactions between the subunits occurring on the vertical faces of the prisms. Preliminary MC results have successfully replicated the crystal packing of the carboxysome hexamers into molecular layers.

Further MD simulations and experimental studies of carboxysome assembly will hopefully not only replicate the assembled carboxysome shell but also provide answers to how the size of the carboxysome shell is uniquely determined, what number of pentamer subunits are needed for complete shell closure, and how the necessary substrates and enzymes are enclosed within the shell during assembly.

Metafluxomics of a phosphorus removing microbial community

Principal Investigators: Héctor García Martín and Aindrila Mukhopadhyay

Project description

We propose 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 will develop 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 will unfold in three different phases of ascending complexity: the first step will involve computationally testing that the same results are obtained with the proteomic method and the standard amino-acid based method. The second one will involve the experimental check that, for *E. coli*, the same results are obtained using both methods. The third phase involves checking that from the combined lysate of *S. cerevisiae* and *E. coli* grown separately, it is possible to obtain flux distribution and assign it to each of the species.

Accomplishments

Whereas in the first year 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, in this year we have 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 have 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 have also found that for longer peptides (10 amino acids) increasing the number of peptides counters the loss of information but it cannot help produce the same amount of information content as the amino-acid based. Our next steps involve confirming this fact with peptides of non-random composition and use the experimentally obtained data to test the method as explained above.

We have been forced to abandon Enhanced Biological Phosphorus Removal (EBPR) sludge as our initial target for applying this method to a full community due to its instability and are looking for more stable communities for a full test.

LB10042

Advances in Standardized, Scar-less, Sequence-Independent Cloning Methods
Principal Investigator(s): Nathan J. Hillson

Project Description

A diverse array of biological endeavors, spanning from the production of clean renewable sources of biofuels and chemicals, to environmental stewardship, to the development of cancer therapies, share in common labor-intensive molecular biology procedures. There is significant promise that standardization, coordination, and consolidation of multiple independent cloning projects could be achieved though the use of automated design and with methodological advances. Such advances would be driven by software improvements as well as by redesigning protocols with robotics and automation integrated into process workflows.

This project will accelerate progress towards these advances in standardized, scar-less, sequence-independent cloning methods. A graphical user interface will be developed that will facilitate and standardize DNA assembly design for molecular and synthetic biologists. The resulting experimental designs will be aggregated into 96-well plates, enabling a single researcher (utilizing multi-channel pipettes and/or liquid-handling robotics) to perform the synchronized cloning tasks of several people. As part of the workflow optimization process, cost/benefit analyses will be investigated. Following preliminary screening, DNA constructs will be submitted for sequencing and analysis; successful clones will be delivered to end-users.

Accomplishments

We have completed designs for three large combinatorial DNA libraries (48 plasmids with 29 parts each; 500 with 7 parts each; and 50000 with 8 parts each, respectively), which are critical to experiments that will improve our understanding of how we can best improve biofuel production and microbial biofuel tolerance. We have constructed and sequence validated the components required (55, 28, and 156 parts, respectively) to assemble all three of these libraries. One half of the first of these libraries has been successfully constructed and sequence validated and is now being experimentally assessed for improved biofuel production by our collaborators. The latter two have been handed off to their respective collaborators for completion, as this project has come to a close. This project has pushed the limits of our technical capabilities, and has demanded that we develop refined experimental DNA construction methodologies and strategies, such as hierarchical sub-cloning and DNA digest patterning screening protocols. Going forward, these new practices will be incorporated into our protocol design software.

Improvements have been made to the graphical user interface software that aids the design of the DNA to be assembled. A small subset of new features include: the design file XML schema has been updated and documented; refinedment of combinatorial bin forced assembly strategy determination; additional error-checking routines; hyperlinks from designed sequences to VectorEditor for immediate visual assessment; extensive user-interface modifications; built-in example designs; and the option to generate empty Master List files. A new web server has been dedicated to the developed software tools, which has been made publicly available (http://j5.jbei.org) at no cost to academic, non-profit and government institutions. There are now 161 institutions on 6 continents that are registered users of the developed software. A major bio-based chemicals company has site-licensed the software, and the software has spurned the creation a new start-up company that will further commercialize the software.The work supported by this project has recently resulted in two scientific manuscripts, one of which is under revision, and the other which is under review (see attached publications list).

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 phage-based electrical generator producing up to 6 nA and 400 mV, that was enough to operate liquid crystal displays.

We are in the process of enhancing the piezoelectric properties of the phage through the directed evolution and enhancing the piezoelectric power through serial connection of the self-assembled piezoelectric devices through microfabrication approaches.

LB10019

Engineering of Drought and Heat Tolerance in Bioenergy Crops

Principal Investigator(s): Henrik Vibe Scheller

Project Description

The aim of the project is to engineer stress tolerant plants that accumulate the thermo and osmoprotectant mannosylglycerate in response to abiotic stress. Bioenergy crops growing on marginal lands will often be exposed to such stress factors and will be particularly important targets for engineering of these traits. Mannosylglycerate may protect plants against several different kinds of stress, and in addition to drought and heat stress, salt stress and cold stress will be investigated in the most promising plant lines.

Plants (arabidopsis, *Brachypodium* and rice) will be transformed with constructs encoding mannosylglycerate synthase from the lycophyte *Selaginella moellendorfii* under control of constitutive and stress-induced promoters. Constructs using the bifunctional mannosyl-phospho-glycerate / mannosyl-phospho-glycerate phosphatase from *Dehalococcoides ethenogenes* will also be tested as an alternative route of synthesizing mannosylglycerate. The accumulation of mannosylglycerate and other metabolites during and after stress will be analyzed and related to stress tolerance of the obtained plants.

Accomplishments

In the first year of the project, the gene encoding mannosylglycerate synthase from *S. moellendorfii* was codon optimized for efficient expression in plants. The synthetic gene was engineered into vectors for transformation of plants, and the vectors were used to generate stable transformants of Arabidopsis and rice, and for transient expression in tobacco. In all three species, it was determined that mannosylglycerate was produced.

In the second year, the enzyme was expressed in *E. coli*, purified and used in enzymatic assays to determine the kinetic properties. These studies showed that the enzyme is able to catalyze the production of mannosylglycerate from GDP-mannose and glycerate in vitro.

Metabolites were extracted from plants expressing the mannosylglycerate synthase. In general the levels of mannosylglycerate were rather low, i.e. less than 5 mM. In an attempt to generate plants with higher content of mannosylglycerate, a codon-optimized version of the mannosyl-phospho-glycerate / mannosyl-phospho-glycerate phosphatase gene from *D. ethenogenes* was used to transform Arabidopsis. Since phospho-glycerate is present in plants at much higher levels than glycerate this approach could potentially lead to a higher concentration of mannosylglycerate. However, transformed plants did not show a significant accumulation of mannosylglycerate.

The mannosylglycerate gene was originally found in *S. moellendorfii*. However, mannosylglycerate was not detectable in the leaves of this plant. The highly drought tolerant *Selaginella lepidophylla* was also analyzed both in non-stressed and drought stressed conditions but no mannosylglycerate was detected. Hence. the mannosylglycerate synthase must be active in *Selaginella* only under special conditions, perhaps in spores. A moss, *Physcomitrella patiens* was found by genome sequencing to have a putative mannosylglycerate synthase. In this species, mannosylglycerate was detected at levels similar to those obtained in the transgenic plants.

The major breakthrough in the project was that stress experiments with young Arabidopsis plants expressing mannosylglycerate synthase showed a significantly improved tolerance to salt in spite of the rather low concentration of mannosylglycerate. Further experiments will be required to determine the tolerance to other types of stress.

LB11037

Engineering Thermophilic Bacteria For Converting Hydrocarbon To Valuable Chemicals, Methyl Halides

Principal Investigator: Christopher Voigt

Project Description

The purpose of this project is to dramatically increase the bioengineering capacity on thermophilic bacteria using synthetic biology tools and bioinformatic data resource. Direct syntheses of selected gene pools of interesting will dramatically increase the accessibility of rich gene resources. High-throughput screen and analysis methods will also be applied and developed to construct genetic parts, explore novel enzymes and assemble useful pathways in thermophilic bacterial hosts. This pipeline can be applied to engineer specific thermophilic bacteria for broad applications in converting hydrocarbon to high value chemicals, bio-energy production, microbial enhanced oil recovery and bioremediation.

We will first focus on oil-eating thermophilic microorganisms to develop more active, cost-effective process to convert petroleum to voluble molecules, methyl halides. We will screen a set of selected thermophilic bacteria for good growth properties on alkane and relatively convenient genetic manipulation. Expression plasmids, promoter libraries including constitutive and inducible promoters and fluorescent protein reporter will be developed for selected thermophilic bacterial species. After constructing all genetic tools, a set of methyl halide transferase (MHT) genes from a synthetic metagenomics pool will be expressed in selected bacterial hosts for screening a better enzyme to produce methyl halides. Various alkane substrates including the collected crude oil spill will be test for the conversion efficiency. This pipeline can be further used to engineer oil-eating thermophilic bacteria for a broad potential application.

Accomplishments

We have accomplished most of designed goals and are in the progress of the final steps. We have screened a set of thermophilic bacteria isolated from high temperature oil reservoirs and various terrestrial environments; several *Geobacillus* and *Pseudomonas* species have been selected as suitable host for parts development and for the final alkane conversion respectively.

A genetic tool box has been developed for Geobacillus and Psuedomonas including a self-replicated expression plasmid and an integrative expression plasmid, superfoldGFP reporter and constitutive and inducible promoter libraries covering a broad transcription activity range.

The successfully developed tools have been used to express and screen a set of methyl halide transferases which are directly synthesized according to the Genebank DNA sequences. The methyl iodide (MeI) synthesis has been achieved in Geobacillus by 9 MHTs. *In vitro* evolution method is also successful applied to MHT from Kordia algicida to make thermostable MHTs. The method to efficiently transform Pseudomonas with the integrative plasmid has been developed and the plasmids bearing all select MHTs has also been constructed.

We are in the process of transforming Pseudomonas with integrative plasmid bearing the selected MHT pool. Hopefully we can get all selected MHT expressed and screen better MHT enzymes to produce methyl halide.

Development of Reusable Software Modules for the Analyses of bioSAXS Data.
Principle Investigator: Petrus H. Zwart

Project Description

The purpose of this project is to develop a reusable software modules for the analyses of bioSAXS data. Over the duration of this project, we have invested our effort in developing a reusable computational infrastructure for the analyses of bioSAXS data. BioSAXS is the predominant technique for determining the structure of macromolecules in solution. The technique is experimentally straightforward but the interpretation of the data can be non-trivial. Current scientific software available for the analysis of SAXS data is not easily accessible for novice users and lacks the automation that the current high-throughput SAXS beamlines demand for efficient analyses of results. The sastbx addresses both of these issues.

Accomplishments

The main accomplishments of this project are is the development of a basic infrastructure for the analyses of SAXS data. The software is available upon request or via the web at http://sastbx.als.lbl.gov. The software we have developed is use friendly and covers the most important analyses tasks for the bioSAXS community, namely 1) Model data calculation 2) Determination of the distance distribution function 3) Determination of the low resolution shape of macromolecules 4) Multi resolution model superpositioning 5) Normal model refinement of existing crystal structures against SAXS data. The first four tasks are available online for structural biologists to use on our servers. The most used application is the structure determination from SAXS data only. Traditionally, this computational task is very time consuming, typically taking hours to days to converge. A novel approach developed in this project has however resulted in a significant speedup of this process, resulting in accurate structural models from SAXS data within 60 seconds. The results of this procedure have been validated against existing methods and have shown to produce highly comparable results in a highly automated fashion. The other most significant application is a novel method to compute SAXS data from known molecular models. The method we have developed is not only more computationally efficient it also has a more accurate method for handling surface bound solvent. This becomes more important for irregular shaped proteins, such as macromolecular machines. Our automated method for determining the distance distribution produces highly similar results as compared to existing software and is available on our online webserver as well. The tools developed for multi resolution structure super positioning is mainly used to compare low resolution models derived from SAXS data against existing structures. Given the open source nature of the development of these tools, this particular tool is now used in automated ligand fitting in macromolecular crystallography. The refinement module in the SASTBX works well for structural changes that are pure normal mode motions. Unfortunately, a significant number of structural changes in macromolecules, cannot easily be described by normal mode transitions. Further research is required to make this tool generally applicable.

In summary, the SASTBX has been developed up to a point where it can provide most routine tasks to bioSAXS users. Further external funding is actively pursued.

LB11042

Feasibility and development of Flutuation Xray Scattering for the NGLS
Principle Investigator: Petrus H. Zwart

Project Description

The purpose of this project is to develop a novel biophysical technique named Fluctuation Xray Scattering (fXS). fXS utilizes the ultrashort X-ray pulse lengths from free electron lasers such as the NGLS to enhance the information content in solution scattering data. The increase in experimental information obtained in these experiments as compared to standard SAXS/WAXS techniques, can be utilized to significantly reduce ambiguities in the determination of the structure of macromolecules in solution. The project aims to further develop this technique via model experiments, numerical simulation and algorithm development.

Accomplishments

Our most significant accomplishments in this project are: 1) Derivation of a computationally efficient procedure for computing model data. 2) Development of computational tools for time resolved fXS. 3) Developing computational tools for determining structural models from 2D and 3fXS data. Our first accomplishment, the efficient generation of model fXS data allows us to quickly compute model data from proposed structures. This step is a main bottleneck when determining structural changes in solution given measured fXS data and a known crystal structure. The structural changes one aims to determine are either due to different packing forces or drug-induced. The second accomplishment is the discovery that fXS data of mixtures can be expressed as a linear combination of fXS data from the individual components. This basic principle has been derived analytically and is backed up by extensive simulations. The implications of this finding will enable time resolved fXS experiments on macromolecules in solution aimed at elucidating structures of short lived intermediates in macromolecules. Current technology to determine these structures has a large associated uncertainty with the proposed models. Because fXS data has a higher information content, the derived models will provide more details. The theoretical and analytical models are put to the test using model systems at the ALS. Thirdly, we have developed a novel method for determining the structure of scattering bodies from fXS data using real space modeling. Existing methods have not been able to produce structures from fXS data for the 3D case. For this particular part of the project, we have first developed a real space method for determining the projected 2D structure of nano-particles from 2D fXS data. The success of this method has lead to a similar algorithm for the 3D case. As far as we are aware, this is the first demonstration of an ab initio structure solution from 3D fXS data. A similar algorithm has been developed that allows the determination of relatively minor real space changes to existing models. The later method is of importance when studying drug-induced structural changes in macromolecules.

In summary, our work has provided the experimental, theoretical and computational framework for the further development of fXS and will ultimately allow for a more accurate understanding of macromolecules in solution utilizing state of the art X-ray facilities.

Physics Division

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 (BAO) technique, the BigBOSS collaboration is proposing to construct a 5000 fiber-fed, multi-object spectrograph for the prime focus of the Mayall telescope. The concept requires the fibers to be robotically placed on target galaxies that transport photons to the spectrographs, approximately 40 m distance. High efficiency coupling and transport and minimal f-number degradation of the light is required, all impacting the required integration time to achieve a given signal to noise ratio, that in turn impacts the amount of sky covered during the 500 night program. 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, and the effects of multiple bendings on focal ratio degradation and fiber transmission efficiency at the positioner and telescope mount pivot points. Initial fiber installation and positioner maintenance may require an intermediate connector with near zero insertion loss.

Losses will occur at the fiber ends due to cutting, polishing quality and index mismatch even with the best of anti-reflective coatings. Propagation of ab initio microcracks as the fiber is flexed during actuator motion may lead to a time dependent degradation of transmission efficiency.

Accomplishments

We have terminated individual fiber ends in various ways, compatible with how they would be mounted in a robotic actuator. To measure termination and polishing performance we have developed a focal radio degradation (FRD) apparatus and have been able to identify classes of termination processes that work much better than others. FRD can be measured with a collimated or focused light beam at the fiber input. That former is easier to implement at a mass production site. Experimental and theoretical correlation of the two techniques is underway.

We have also fabricated and evaluated a variety of single and multiple fiber connectors. The FRD apparatus has proved useful here. We are able to eliminate many connector types as unsuitable. As part of this study, we have acquired and measured thermally fused fibers from several vendors. This technique is promising, showing the least FRD any connectorization scheme.

At the spectrograph input, 500 fibers need to be placed in a precise arc to match the input pupil. We have explored several assembly scenarios for this and consulted with manufacturers. A promising technique that we will prototype is a meniscus lens that can be shaped and glued directly to the tips of a subgroup of fibers. The lens can be antireflective coated prior to gluing and the optical polish of the fiber tips on a curved surface can be relaxed since the glue will compensate for imperfections.

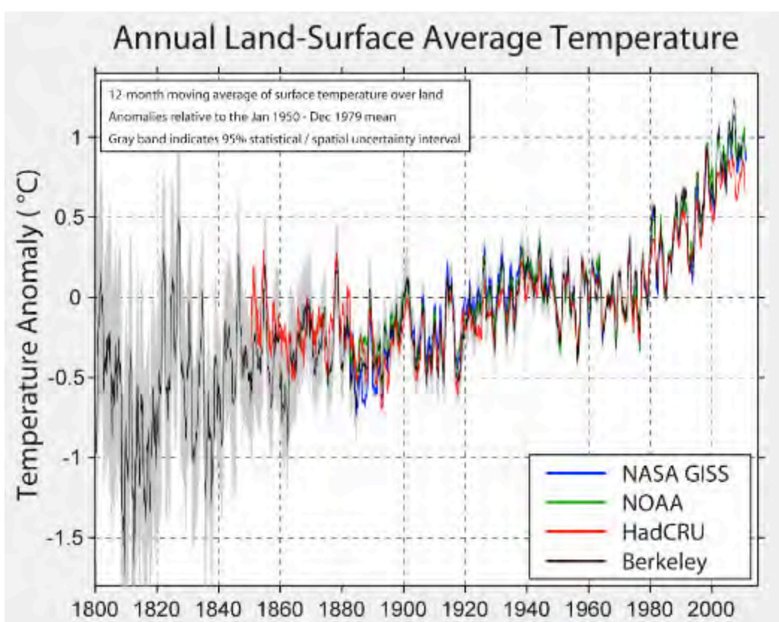
Study of History of Global Surface Temperatures
(Berkeley Earth Surface Temperature)
Principal Investigator(s): Richard A. Muller

Project Description
Analyzing temperature data from 15 sources, in some cases going as far back as 1800, the Berkeley Earth study directly addressed scientific concerns raised by skeptics, including the urban heat island effect, poor station quality, and the risk of data selection bias.

On the basis of its analysis, the group concluded that earlier studies based on more limited data by teams in the United States and Britain had accurately estimated the extent of land surface warming.

Accomplishments
We have reached all major milestones of the Berkeley Earth Surface Temperature project. Specifically:

- Berkeley Earth has developed analysis techniques that do not require long continuous records, therefore allowing us to use virtually all of the available data.
- We have released the analysis results, together with our programs, and including error bars, on our website (www.BerkeleyEarth.org/analysis). I have posted a chart below, more are available on the website.
- We have made all of our data available to the public on our website (www.BerkeleyEarth.org/dataset)
- Berkeley Earth has submitted 4 scientific papers to major peer review journals.



Theoretical Studies of Dark Matter Beyond the Standard Model

Principal Investigator: Yasonori Nomura

Project Description

There is incontrovertible evidence for an unknown form of "dark matter" comprising roughly 25% of the universe, while no possible dark matter candidate can be found within the Standard Model of elementary particle physics. On the other hand there is a tantalizing clue that weakly interacting particles with masses around the scale of electroweak symmetry breaking (i.e., WIMPS), have just the right ratio of mass to interaction strength required to populate the universe at precisely the density required for dark matter. Dark matter may then be tightly linked to the puzzles about the origin of mass (through electroweak symmetry breaking) that are not satisfactorily addressed in the Standard Model, and that will soon be addressed at the LHC.

Accomplishments

According to recent progress in string compactification, it is plausible that there are multiple separate sectors at the TeV (or lower) scales, which are hidden from current experiments simply because they interact very weakly with the standard model particles. Phenomenology of such scenarios depends on details of interactions between the sectors. In pub. [1] I proposed a new way that the standard model sector interacts with these sectors: through kinetic mixing between singlet fields, where one of these singlets is identified with the singlet field in the next-to-minimal supersymmetric standard model. In the context of supersymmetry, this scenario is the only alternative to the well-studied case in which the interaction occurs through U(1) gauge kinetic mixing, if the connection between sectors is provided by marginal interactions. We studied implications of this scenario to collider physics and cosmology in detail, and found that it elegantly accommodates dark matter while leading to distinct signatures at the LHC, which can be tested by future data.

In a last year's work, I showed that weakly interacting massive particle (WIMP) dark matter can arise naturally as a consequence of environmental selection in the multiverse. There is, however, a well-known problem in theories of the multiverse---probabilities are not well defined because of the eternally inflating nature of spacetime (called the measure problem). In pub. [2] I proposed a novel solution to this problem based on the principles of quantum mechanics. I showed that a consistent quantum mechanical treatment of the multiverse leads to well-defined probabilities, free from many of the problems and paradoxes associated with earlier measure proposals. Moreover, I found that the same probability formula can be used to predict probabilities for both global properties of the universe and outcomes of quantum measurements, providing complete unification of the eternally inflating multiverse and many worlds in quantum mechanics. As the first application of this framework, I calculated the probability distribution of the cosmological constant/dark energy, and found that the distribution agrees with the observed value at an order of magnitude level [3].

LB11038

High voltage up- and down-converters for low power, low density detector instrumentation

Principal Investigator(s): Henrik von der Lippe

Project Description

The physical size of experimental physics detectors has been increasing with time and will continue to increase. For detectors at accelerators this is to extend particle energy range and event density capabilities, while for non accelerator or long baseline detectors this is to increase acceptance and thus statistical sensitivity. At the same time the operating voltage of microelectronics has been decreasing with time as a consequence of Moore's Law and will continue to decrease. The confluence of these trends results in a widely recognized problem of power distribution efficiency within new detectors. A related problem is the distribution of high voltages within detectors, for example for phototubes, gaseous detectors, and silicon sensors. In this case the issue is not power efficiency but complexity of wiring and inherently high cost of high voltage channels. The trends of decreasing operating voltage of microelectronics have also led to a need for improved power distribution in consumer products. In this case efficiency losses are compounded not by increasing physical size, but by the desire to increase battery life. While research at LBNL has been exploring power distribution and voltage conversion within physics detectors for some time, independent work on the UCB campus has been focusing on power conversion for mobile applications. While many requirements are quite different for physics instrumentation and consumer electronics, the ultimate goal of these efforts is the same: to distribute a single moderate voltage (of order 10V) to microelectronic components and internally convert it to whatever values are needed with high efficiency. The goal was to develop a system-on-a-chip integrated circuit block that would combine techniques developed for long battery life with requirements of physics instrumentation, such as radiation hardness and increased reliability. The goal is to explore both down conversion and up converter.

Accomplishments:

The effort in the first year of this study has been on IC technology analysis of circuit analysis for up and down converts. Several integrated circuit technologies have been studied that can accommodate detector readout electronics and detector biasing electronics. For low mass detector systems 65nm CMOS was identified to satisfy the needs of low voltage readout electronics and due to the 11V deep Nwell breakdown voltage also enables the implementation of a 10V : 1V, 0.5A down converter. With these deep Nwells we can design cascades of 2V stages that do not exceed the 2.5V breakdown voltage for the transistors and thus implement high voltage circuits in the 2.5V process. For up converts the there have been identified two promising IC processes. A 0.8um 120V SOI process and a 0.35um 50V CMOS process. The 0.8um is best suitable for a pure bias circuit and the 0.35um process is well match for up converters that need to be integrated together with readout electronics. This process the up converts can be design as 3.3 V stages that pump the voltage up or the standard parallel-serial cap switching. To meet the extreme low mass requirement internal integrated capacitors are needed. These have large bottom plate parasitic capacitance with reduces the efficiency significantly. In the demonstrator that will be tested out we have chosen to implement the converters with external capacitors. The goal for year to is to build and test a 10V : 1V down converter in 65nm CMOS technology for readout electronics biasing in low mass instrumentation.

LB10010

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

Principal Investigators: Cheryl Kerfeld, Adam Arkin, 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 CO2 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 second year we have continued to obtain cyanobacterial carboxysome mutants, characterized their ultrastructure and physiology and refined methods for their genetic manipulation. One of the mutants is particularly of note in that we have shown that this previously uncharacterized carboxysome component is essential to the organelle. This protein can also target heterologous proteins to the carboxysome. Moreover, we were able to identify specific functional regions in the protein including a domain for organizing other CO2 fixation enzymes and a domain for adherence to the shell. These data are summarized in a submitted publication. We are expanding on these results by testing synthetic constructs to replace/augment these functions. 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. At the same time we are learning fundamental principles of structure and function of the carboxysome.

In anticipation of having to carefully control the stoichiometry of these carboxysome components we have successfully completed the adaptation of a novel system for transcript processing that makes prediction of multigenic operon expression possible. We use a protein from *Pseudomonas aeruginosa* UCBPP-PA14 to cleave transcripts at precise locations, and have shown these leads to far more reliable and predictable expression of proteins.

LB10015

Multifunctional Window Coatings for High-Performance Buildings

Principal Investigators: Delia Milliron, Jeffrey Urban, Andre Anders, Thomas Richardson

Project Description

The goal of this project is to develop materials necessary to support key technological advances in window coating technology for improved building efficiency. In particularly, we are motivated by a potential breakthrough technology of spectrally selective dynamic coatings for climate responsive NIR transparency. To enable these technologies, we aim to develop NIR- and visible-transparent conductors and to investigate electrochromism in nanostructured metal oxides. For both transparent conductor and active materials, we will focus on earth-abundant compositions and scalable deposition processes, smoothing the path toward eventual large-scale deployment of the resulting technologies.

NIR- and visible-transparent conducting oxide (TCO) are to be developed using a variety of sputtering techniques, including advanced plasma technology, applicable to deposition in large format, to control doping levels and minimize roughness. Spectral and electrical properties of the TCO films will be evaluated over systematically varied deposition conditions. For the active material in the NIR electrochromics, TCO nanocrystals will be prepared by colloidal synthesis, using the Molecular Foundry's automated synthesis station, which facilitates high throughput, systematic variation of composition. Their spectroscopic properties across the visible and NIR will be characterized first in dispersions, then integrated into thin film devices. Electrochemical characterization techniques will be employed to assess the operating principles of the devices.

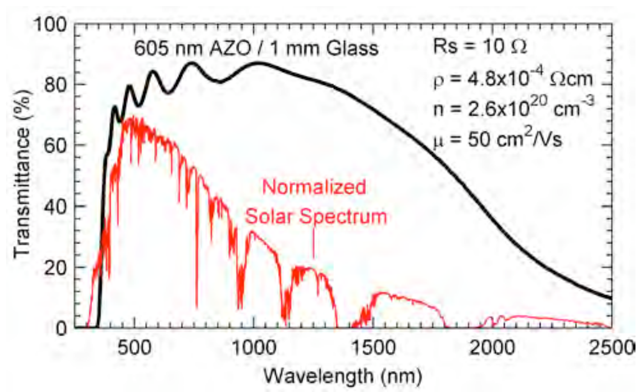


Fig. 1. Transmittance of an AZO film on glass.

Accomplishments

While indium tin oxide (ITO) is today's standard TC material, indium's relative scarcity has driven us to focus on aluminum-doped zinc oxide (AZO) for window coatings, which will ultimately be broadly deployed. Using our newly developed compact arc deposition arrangement, we can now deposit very high quality AZO films with exceptional transmittance across the solar spectrum and very low sheet resistance (**Fig. 1**). The key factor in their performance is a high carrier mobility, which has reached 60 cm^2/Vs in our samples; this is the current record for AZO as-deposited on glass.

Colloidal nanocrystals of ITO and AZO form the basis of a new dynamic electrochromic coating we have developed. Using solution-based low temperature processing, we use these to prepare nanostructured TC oxide thin films with excellent visible transmittance and whose NIR transmittance depends predictably on the chemically controlled doping level. Evaluating such films in an electrochromic half cell, we have demonstrated – for the first time – selective electrochromic switching of NIR transmittance while maintaining near unity transmittance of visible light. Thus far, our best performing films modulate solar NIR transmittance by 35%, while visible light transmittance remains above 92%, suggesting a unique window coating technology offering on-demand passive solar heating with continuous daylight illumination.

Publications List

AFRD-Anders LB10032 Plasma-assisted High Rate Deposition Concept for Energy Applications

Journal publications (refereed)

A. Anders, "Deposition rates of high power impulse magnetron sputtering: physics and economics," *J. Vac. Sci. Technol. A* **28**, 783-790 (2010), url: http://dx.doi.org/10.1116/1.3299267

A. Anders, J. Brown; "A plasma lens for magnetron sputtering," *IEEE Trans. Plasma Sci.* **39**, 2528-2529 (2011). url: http://dx.doi.org/10.1109/TPS.2011.2157172

R. J. Mendelsberg, S. H. N. Lim, D. J. Milliron, A. Anders; "High rate deposition of high quality ZnO:Al by filtered cathodic arc," *Proc. Mat. Res. Soc.* **1315**, mm03-25 (2011). doi: 10.1557/opl.2011.1285

R. J. Mendelsberg, S. H. N. Lim, Y. K. Zhu, J. Wallig, D. J. Milliron, A. Anders; "Achieving high mobility ZnO:Al at very high growth rates by dc filtered cathodic arc deposition," *J. Phys D: Appl. Phys.* **44**, 232003 (2011). url: http://dx.doi.org/10.1088/0022-3727/44/23/232003

A. Anders, J. Čapek, M. Hála, and L. Martinu, "The 'recycling trap': A generalized explanation of discharge runaway in high power impulse magnetron sputtering," *J. Phys D: Appl. Phys.,* accepted and in press (2011).

Conference presentations

A. Anders, J. Brown, S. Lim, R. Mendelsberg, L. Gontijo, K. M. Yu, M. Field; "Improving aluminum doped zinc oxide films by minimizing negative ion damage," *8th Int. Conf. Coatings on Glass and Plastics*, Braunschweig, Germany, June 2010, pp. 33-34.

A. Anders, R. Mendelsberg, S. Lim, Y. Zhu; "Hitting the energy sweet spot: How to make high quality aluminum doped zinc oxide films," *Proc. Ann. Tech. Conf. Soc. Vacuum Coaters,* Chicago, IL, April 2011, paper H4.

R. J. Mendelsberg, S. H. N. Lim, Y. Zhu, D. J. Milliron, A. Anders; "Effects of oxygen plasma treatment before, during, and after growth of ZnO:Al by dc cathodic arc deposition," *2011 MRS Spring Meeting*, San Francisco, CA, 2011, paper G9.8/S8.8.

A. Anders, "Progress in understanding HIPIMS discharges (Invited Talk)," *6th Symposium on Functional Coatings and Surface Engineering*, Montreal, Canada, June 2011.

Invention Disclosures

A. Anders, IB-2823: "Method and Apparatus for Sputtering with a Plasma Lens", U.S. Provisional patent; International Patent Application filed 2011.

A. Anders, IB-2871: "High rate arc plasma deposition", LBNL disclosure filed 2010.

A. Anders, IB-2922: "Hot, nested plasma filter", LBNL disclosure filed 2010.

R. Mendelsberg and A. Anders, "IB-3018: "Method and appartus for locally enhanced thin growth", LBNL disclosure filed 2011.

AFRD-Byrd LB11006 Development of Attosecond Synchronization for Future Light Sources

R. B. Wilcox, J. M. Byrd, L. R. Doolittle, R. Holzwarth, G. Huang; "Towards attosecond synchronization of remote mode-locked lasers using stabilized transmission of optical comb frequencies," *J. of Modern Optics* **58**, 16, (1460-1468, Oct 2011). url: http://www.tandfonline.com/doi/abs/10.1080/09500340.2011.597520

R. B. Wilcox, J. M. Byrd, R. Holzwarth; "Optical Comb and Interferometer Development for Laser Synchronization in Femtosecond FELs", *2011 Free Electron Laser Conference*, Shanghai, August 2011.

AFRD-Ferracin LB11008 Fourth Generation Electron Cyclotron Resonance (ECR) Ion Sources

C. Lyneis, P. Ferracin, S. Caspi, A. Hodgkinson, G.L. Sabbi; "Concept for a Fourth Generation ECR Ion Source," accepted for publication in *Review of Scientific Instruments*.

AFRD-Li LB09007 Experimental Accelerator R and D Toward a Future Light Source at LBNL

J. Corlett, et al; "Next Generation Light Source R&D and Design Studies at LBNL," submitted to *2012 International Accelerator Conference,* New Orleans, Louisiana (May 20-25, 2012).

M. V. Orocz, C. Pappas; "Update on Kicker Development for a Next Generation Light Source," submitted to *2012 International Accelerator Conference*, New Orleans, Louisiana (May 20-25, 2012).

M. Reinsch, B. Austin, et al; "Machine Parameter Studies for an FEL Facility Using STAFF," submitted to *2012 International Accelerator Conference*, New Orleans, Louisiana (May 20-25, 2012).

M. Placidi, P. J. Emma, C. Pappas, D. Robin, C. Sun, W. Wan; "Design Concepts of a Beam Spreader for a Next Generation Free Electron Laser," submitted to *2012 International Accelerator Conference,* New Orleans, Louisiana (May 20-25, 2012).

AFRD-Robin LB10031 Novel Accelerator and Engineering Strategies for Ion Beam Cancer Therapy

D. Robin, D. Arbelaez, S. Caspi, C. Sun, A. Sessler, W. Wan, M. Yoon; "Superconducting toroidal combined-function magnet for a compact ion beam cancer therapy gantry," *Nucl. Instr. and Methods in Phys. Res., Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **659**, 484-493 (Issue 1, 11 December 2011).

S. Caspi, D. Arbelaez, H. Felice, R. Hafalia, D. Robin, C. Sun, W. Wan, M. Yoon; "Conceptual Design of a 260 mm Bore 5 T Superconducting Curved Dipole Magnet for a Carbon Beam Therapy Gantry," *IEEE Transactions on Applied Superconductivity*, **PP**, Issue: 99 (2011). doi: 10.1109/TASC.2011.2174568

C. Sun, D. Arbelaez, S. Caspi, D. Robin, A. Sessler, W. Wan, M. Yoon; "Compact Beam Delivery Systems for Ioon Beam Therapy," *Proceedings of the 2011 International Particle Accelerator Conference*, 3633-3635 (Marselle, 2011).

AFRD-Seidl LB10012 Ion Beam Driven Fusion and Fusion-Fission Hybrids

P. Seidl, J.L. Vay; "Formation Of High Charge State Heavy Ion Beams With Intense Space Charge," *Proc. of the Particle Accel. Conf.*, New York (2011). url: http://accelconf.web.cern.ch/AccelConf/PAC2011/papers/wep098.pdf

P.A. Seidl, J.J. Barnard (editors); “Summary Report of the Workshop on Accelerators for Heavy Ion Fusion, Berkeley, USA May 23-26, 2011. url: http://ahif.lbl.gov/workshop-reports

AFRD-Wurtele LB10024 Linac Driver and Coherent Soft X-ray Sources

J. Qiang, J. Wu; “The effects of jitters on coherent X-ray radiation using a modulation compression scheme,” in *Proceedings of 2011 Workshop on Free Electron Lasers*, www.jacow.org

J. Qiang, J. Wu; “Generation of multi-color attosecond coherent X-ray radiation through modulation compression,” *Appl. Phys. Lett.* **99**, 081101 (2011).

J. Corlett, B. Austin, et al; “Next Generation Light Source R&D and Design Studies at LBNL,” to be presented at *IPAC 2012*.

M. Reinsch, B. Austin, et al; “Machine Parameter Studies for an FEL Facility Using STAFF,” to be presented at *IPAC 2012*.

P. R. Gandhi, G. Penn, M. Reinsch, J. Wurtele; “High Repetition High Gain Harmonic Generation in the ‘Radiator First’ Configuration,” to be presented at IPAC 2012.

M. Venturini, et al; “Studies of a Linac Driver for a high repetition rate X-Ray FEL,” *Proceedings of the 2011 Particle Accelerator Conference (PAC11)*, p. 2450 (2011), LBNL Report LBNL-5005, url: www.jacow.org

E.M. Yoon, D. Filippetto, C.F. Papadopoulos, C. Pellegrini, G. Penn,S. Prestemon, F. Sannibale; "The BTFEL, an infrared free-electron laser amplifier based on a new-design short-period superconducting tape undulator," *Nucl. Instrum. Methods A* **660** 138-146 (2011).

G. Penn, M. Reinsch; "Designs and numerical calculations for echo-enabled harmonic generation at very high harmonics," *J. Modern Optics* **58**, 1404-1418 (2011).

J.N. Corlett, B. Austin, et al; “A Next Generation Light Source Facility at LBNL,” *Proceedings of the 2011 Particle Accelerator Conference (PAC11)*. Online at www.jacow.org

C.F. Papadopoulos, J. Corlett, et al; “Photoinjector beam dynamics for a next generation x-ray,” *Proceedings of the 2011 Particle Accelerator Conference (PAC11)*. Online at www.jacow.org

M. Venturini, J.N. Corlett, et al; “Studies of a Linac Driver for a High Repetition Rate X-ray FEL,” *Proceedings of the 2011 Particle Accelerator Conference (PAC11)*. Online at www.jacow.org

C. Sun, H. Nishimura, G. Penn, M.W. Reinsch, D. Robin, F. Sannibale, C. Steier, W. Wan; ”Study of Highly Isochronous Beamlines for FEL Seeding,” *Proceedings of the 2011 International Conference on Free Electron Lasers (FEL2011)*. Online at www.jacow.org

ALS-Hexemer LB10009 Long-range Ordering of Block Copolymers on Patterned Silicon

P. Zavala-Rivera, K. Channon, V. Nguyen, et al;; “Collective osmotic shock in ordered materials,”*Nature Materials* **11**, 53-57 (2011). doi: 10.1038/nmat3179

M. A. Modestino, E. R. Chan, A. Hexemer, J. J. Urban, R. A. Segalman; “Controlling Nanorod Self-Assembly in Polymer Thin Films, ” *Macromolecules* **44** (18), 7364–7371 (2011).

S. W. Hong, J. Huh, X. Gu, D. H. Lee, W. H. Jo, S. Park, T. Xu, T. P. Russell; "Unidirectionally Aligned Line Patterns Driven by Entropic Effects on Faceted Surfaces," accepted for publication in *Proceedings of the National Academy of Sciences*.

J. Xu, S. W. Hong, W. Gu, K. Y. Lee, D. S. Kuo, S. Xiao, T. P. Russell; "Fabrication of Silicon Nano-dots with An Areal Density beyond 1 Teradots/Inch^2," published online in *Advanced Materials*, 24 NOV 2011.

S. W. Hong, X. D. Gu, J. Huh, S. G. Xiao, T. P. Russell; "Circular Nanopatterns over Large Areas from the Self-Assembly of Block Copolymers Guided by Shallow Trenches," *ACS Nano*, **5** (4), 2855-2860 (2011).

D. H. Lee, S. Park, W. Gu, T. P. Russell; "Highly Ordered Nanoporous Template from Triblock Copolymer," *ACS Nano*, **5** (2), 1207-1214 (2011).

B. Kim, S. W. Hong, S. Park, J. Xu, S. K. Hong, T. P. Russell; "Phase Transition Behavior in Thin Films of Block Copolymers by Use of Immiscible Solvent Vapors," *Soft Matter*, **7** (2), 443-447 (2011).

S. Park, D. H. Lee, T. P. Russell; "Self-Assembly of Block Copolymers on Flexible Substrates," *Advanced Materials* **22** (16), 1882-1884 (2010).

ALS-Kilcoyne LB10034 Search for a Permanent Electron Electric Dipole Moment (EDM)

J.G. Kalnins, "Electrostatic End-Field Defocusing of Neutral Atoms and its Compensation," *Phys. Rev. Special Topics – Accelerators and Beams* 14, 104201 (October 11, 2011). url: http://link.aps.org/doi/10.1103/PhysRevSTAB.14.104201

B.J. Wundt, C.T. Munger, U.D. Jentschura; "Quantum Dynamics in an Atomic Fountain: Electric-field Induced Hyperfine Mixing and Electron Dipole Moment Measurements," in preparation for submission to *Physical Review*.

H.A. Gould, B. Feinberg; Multi-layer Magnetic Shielding for > 10^7 Shielding Factor," in preparation for submission to *NIMS*.

ALS-Kunz LB10011 Structure Solution of Inorganic Materials Using Energy Resolved Laue Microdiffraction.

Journal articles

C. Dejoie, M, KunzN. Tamura,C.Bousige,K.Chen,S.Teat, C.Beavers,C.Baerlocher; "Determining the energy dependant X-ray flux variation of a synchrotron beamline using Laue diffraction patterns," *J. Appl. Cryst*. **44**, 177-183 (2011).

K. Chen, C. Dejoie, H. R. Wenk; "Unambiguous indexing trigonal crystals from white beam Laue diffraction patterns: Application to Dauphiné twinning and lattice stress mapping in deformed quartz," submitted to *J. Appl. Cryst*.

C.DejoieM.KunzN.TamuraC. Beavers, S. J. Teat, K. Chen, L. McCusker, C. Baerlocher; "Toward structure solution and refinement of inorganic crystals using Laue microdiffraction," in preparation for possible submission to *J. Appl. Cryst*.

C.DejoieM.KunzN.TamuraO. Tschauner, C. Ma; "Structure solution of a new titania crystal coming from the Allende meteorite using Laue microdiffraction," in preparation for possible submission to *Earth & Planetary S. Lett*.

Oral presentations

M. Kunz, C. Dejoie, N. Tamura, K. Chen, S. Teat, C. Beavers, L. McCusker, C. Baerlocher; "Towards the use of Laue microdiffraction intensities for structural studies at extreme conditions," *Workshop on Dynamic X-ray Diffraction/Spectroscopy at Extreme Conditions*, DESY / XFEL, Hamburg, (Germany).

C. Dejoie, M. Kunz, N. Tamura, K. Chen, S. Teat, C. Beavers, L. McCusker, C. Baerlocher; "Towards the use of Laue microdiffraction intensities for structural studies at extreme conditions," *IUCr 2011*, Madrid (Spain).

ALS-MacDowell LB11020 X-ray Fluorescence Tomography-3D elemental mapping.

H.A. Bale, A. Haboub, A. A. MacDowell, et al; "A First Three-Dimensional Glimpse into Damage of Materials under *In Situ* Loading at Ultrahigh Temperatures," in preparation for submission to *Science*.

A. Haboub, H.A. Bale, J. R. Nasiatka, et al; "A micro-tomography load cell for operation at 1500 C," in preparation for submission to *Rev Sci. Instrum.*

ALS-Marchesini LB10014 Nanoscale Surveyor

"Interferometer encoded stage assembly for nano-cryo-scanning-tomography to simultaneously monitor rotational accuracy (to 300nm), scan precision (to10nm) and thermal expansion effects (to10nm)," draft LBNL ROI –XXX.

C. Yang, J. Qian, A. Schirotzek, F. Maia, S. Marchesini; "Iterative Algorithms for Ptychographic Phase Retrieval," submitted to *New Journal of Physics*.

A. Schirotzek, C. Yang, F. Maia, S. Marchesini; "Vibration deconvolution in Ptychography," in preparation for submission to *Optics Express*.

F. R. N. C. Maia, A. Schirotzek, C. Yang, S. Marchesini; "Scalable software for high thruput ptychographic imaging," in preparation for submission to *International J. of High Performance Computing Applications*.

Z. Wen, X. Liu, C. Yang, S. Marchesini; "Phase retrieval via the ADM algorithm," in preparation for *Inverse Problems*, 2011.

F. R. N. C. Maia, C. Yang, A. Schiroztek, S. Marchesini; "Parallel real-time ptychographic image reconstruction using GPUs," poster at: *SciDAC 2011*, Denver, CO, 2011.

F. R. N. C. Maia, A. Schirotzek, C. Yang, S. Marchesini' "Multi-GPU Real-time Ptychographic X-ray Image Reconstruction," invited talk, *GTC conference*.

ALS-Padmore LB09036 High quantum Yield Multi-Alkali Cathodes for psec Pulsed Electron Sources

T. Vecchione, I. Ben-Zvi, D. H. Dowell, J. Feng, T. Rao, J. Smedley, W. Wan, H, A. Padmore; "High QE low emittance green sensitive FEL photocathodes using K2CsSb," *FEL 2011*, Shanghai.

T. Vecchione, I. Ben-Zvi, D. H. Dowell, J. Feng, T. Rao, J. Smedley, W. Wan, H, A. Padmore; "A low emittance and high efficiency visible light photocathode for high brightness accelerator-based X-ray light sources," *Appl. Phys. Lett.* **99**, 034103 (2011).

ALS-Warwick LB10026 Test Monochromator-Spectrometer Systems with Prototype High Density Gratings for High Resolution X-Ray Scattering

D. L. Voronov, E. H. Anderson, R. Cambie, et al; "A 10,000 groove/mm multilayer coated grating for EUV spectroscopy," *Optics Express* **19** (7), 6320-6325 (2011). LBNL 4524E

D. L. Voronov, M. Ahn, E. H. Anderson, et al; "High efficiency multilayer blazed gratings for EUV and soft X-rays: Recent developments," *Proc. SPIE* **7802,** 780207-1 - 780207-13 (2010). LBNL 3095E

ALS-Yang-W LB11039 Soft X-ray Spectroscopy of Lithium and Conductive Polymers for Li-Ion Batteries

P. Olalde-Velasco, J. Jiménez-Mier, J.D. Denlinger, Z. Hussain, W.L. Yang; "Direct probe of Mott-Hubbard to charge-transfer insulator transition and electronic structure evolution in transition-metal systems," *Phys. Rev. B* **83**, 241102(R) (Jun. 24, 2011). url: http://prb.aps.org/abstract/PRB/v83/i24/e241102

G. Liu, S. Xun, V. Nenad, et al; "Polymers with Tailored Electronic Structure for High Capacity Lithium Battery Electrodes," *Advanced Materials* **23**, 4679 (Sep. 23, 2011). url: http://onlinelibrary.wiley.com/doi/10.1002/adma.201102421/abstract

X.S. Liu, J. Liu, T. Richardson, H. Li, F.C. Chou, Y.D. Chuang, R.M. Qiao, W.L. Yang; "Lithiation effect on electronic structure of Li_xFePO_4: a complete study by x-ray spectroscopy," submitted to *J. of American Chemical Society*.

W.L. Yang, Y.D. Chuang, D. Prendergast; "Soft x-ray absorption of lithium," in preparation for submission to *Physical Review Letters*.

ALS-Yashchuk LB09030 X-Ray Optical Metrology for Coherence-Preserving Adaptive Optics

S. Yuan, K. A Goldberg, V. V Yashchuk, R., Celestre; T. Warwick; W. R McKinney; "Cross-check of ex-situ and in-situ metrology of a bendable temperature stabilized KB mirror," *Nucl. Instr. and Meth.* A **635** (1-S1), S58-S63 (2011). url: http://dx.doi.org/10.1016/j.nima.2010.09.120

S. Yuan, V. V. Yashchuk, K. A. Goldberg, et al: "Development of in situ, at-wavelength metrology for soft x-ray nano-focusing," *Nucl. Instr. and Meth*. **A 649**(1), 160-162 (2011). url:http://www.sciencedirect.com/science/article/pii/S0168900210024198

D. J. Merthe, K. A. Goldberg, V. V. Yashchuk, et al; "An experimental apparatus for diffraction-limited soft x-ray nano-focusing," *Proc. SPIE* **8139**, 813907 (2011). url: http://dx.doi.org/10.1117/12.894116

W. R. McKinney, V. V. Yashchuk, K. A. Goldberg, M. Howells, N. A. Artemiev, D. J. Merthe, S. Yuan; "Design optimization of bendable x-ray mirrors," *Proc. SPIE* **8141**, 81410K (2011). url: http://dx.doi.org/10.1117/12.894175

D. J. Merthe, K. A. Goldberg, V. V. Yashchuk, et al; "An experimental apparatus for diffraction-limited soft x-ray nano-focusing," submitted to *Opt. Eng.*

CH-Budker, Mueller LB10002 Direct Comb Spectroscopy and Atom Interferometry of Lithium

G. Kim, P. Hamilton, D. Schlippert, H. Müller; "Progress towards a test of the universality of free fall using a ^{6}Li-^{7}Li atom interferometer," *42nd Annual Meeting of the APS Division of Atomic, Molecular and Optical*, Atlanta, GA (June 13-17, 2011). url: http://meetings.aps.org/link/BAPS.2011.DAMOP.U2.6

D. Schlippert, G. Kim, P. Hamilton, H. Müller; "Towards a test of the universality of free fall using a 6Li-7Li atom interferometer," *42nd Annual Meeting of the APS Division of Atomic, Molecular and Optical*, Atlanta, GA (June 13-17, 2011). url: http://meetings.aps.org/link/BAPS.2011.DAMOP.E1.131

P. Hamilton, G. Kim, D. Schlippert, H. Müller; "Test of the equivalence principle using lithium-6 and lithium-7," *2011 Atomic Physics Gordon Conference*, Mt. Snow, VT (June 26, 2011).

D. Schlippert, "Towards a test of the universality of free fall using a 6Li-7Li atom interferometer," Thyboron, Denmark (September 2011).

CH-Harris LB09011 Dynamics of Homogeneous Catalysis Reactions Investigated with Transient Two-Dimensional Infrared Spectroscopy

S. C. Nguyen, J. P. Lomont, M. C. Zoerb, A. D. Hill, J. P. Schlegel, C. B. Harris; "Chemistry of the triplet 14-electron complex Fe(CO)3 in solution studied by ultrafast time-resolved IR spectroscopy," submitted to *J.Am.Chem. Soc*.

S. C. Nguyen, J. P. Lomont, M. C. Zoerb, A. D. Hill, J. P. Schlegel, C. B. Harris; "Rotational diffusion time of organometallic complexes in solution," in preparation for submission to *J. Chem. Phys*.

CH-Lukens LB10037 Investigating f-electron Exchange Coupling in Actinide and Lanthanide Complexes

W. Lukens, N. Magnani, C. Booth; "Application of the Hubbard model to Cp^*_2Yb(bipy), a model system for exchange-coupled lanthanide single molecule magnets," in preparation to be submitted to *Inorg Chem.*

CH-Weber LB10027 Double-Auger Emission of small Molecules following Core-Excitation and Ionization

M. P. Jones, M.S. Schoeffler, C. B. Stuck, et al; "Double Auger Emission of Neon following Core-Excitation and Ionization," in preparation for submission to *Phys. Rev. A*.

F. Trinter, I. A. Bocharova, F. P. Sturm, et al; "Double Auger Emission of Carbon Monoxide following Core-Excitation and Ionization," in preparation for submission to *Phys. Rev. A*.

CS-Agarwal LB10001 Enabling High Performance Computing (HPC) Workflows on Clouds

M. Humphrey, Z. Hill, C. van Ingen, K. Jackson, and Y. Ryu; "Assessing the Value of Cloudbursting: A Case Study of Satellite Image Processing on Windows Azure," *IEEE e-Science 2011 Conference*. Stockholm, Sweden (Dec. 5-8, 2011).

CS-Canon LB11043 Defining an Ecosystem to Support Data-Intensive Science

Z. Fadika, R. Canon, M.Govindaraju, L. Ramakrishnan; "Evaluating Hadoop for Scientific Applications," in preparation for upcoming *High-Performance Parallel and Distributed Computing (HPDC)* Conference. url: http://www.hpdc.org/

CS-Li LB11018 Next Generation Computing for X-Ray Science

E. Chan, D. H. Lee, D. Voronov, H. Padmore, T. Xu, Ting, T. Russell, A. Hexemer; "Structural Characterization of Nanopatterned Surface Gratings with Grazing Incidence X-Ray Scattering," American Physical Society, *APS March Meeting 2011* (March 21-25, 2011), abstract #C1.037.

A. K. Scholz, H. Zhang, E. Chan, A. Hexemer, E. J. Kramer; "Real Time Small Angle X-ray Scattering from Cyclically Stretched Nanoparticle-filled Siloxane Elastomers," American Physical Society, *APS March Meeting 2011* (March 21-25, 2011), abstract #S1.053

M. A. Modestino, E. R. Chan, A. Hexemer, J. J. Urban, R. A. Segalman; "Controlling Nanorod Self-Assembly in Polymer Thin Films," *Macromolecules*, **44** (18), 7364–7371 (Web: September 6, 2011). doi: 10.1021/ma201252d

S. Chourou, A. Sarje, X. Li, E. Chan, A. Hexemer; "GISAXS Simulation and Analysis on GPU Clusters," submitted to *MAR12 Meeting of the American Physical Society* (May 2012).

A. Sarje, X. Li; "GPUs for Analyzing X-ray Scattering Data," submitted to *NVIDIA GPU Technology Conference* (May 2012).

A. Sarje, J. Pien, X. Li, E. Chan, S. Chourou, A. Hexemer, A. Scholz; "Large-scale Nanostructure Simulations from the X-ray Scattering Data Using Graphics Processors," submitted to *International Conference on Supercomputing (ICS2012*) (June, 2012).

CS-Nugent LB11025 The Lyman Alpha Forest Cosmology Simulator

A. Almgren et al; "Nyx: A New Cosmology Code," submitted to *Astrophysical Journal*.

Z. Lukic et al; "Nyx: First Lyman-Alpha Forest Science Results," in preparation for submission to *Astrophysical Journal*.

CS-Yang-C LB10029 Computational Techniques for Non-crystalline X-ray Diffraction Imaging

C. Yang, F. Maia, S. Marchesini; "A Comparative Study of Iterative Refinement Algorithms for Single-particle Diffractive Imaging," in preparation for submission to *IEEE Transactions on Image Processing*.

C. Frogner, C. Yang, S. Marchesini; "Angular Synchronization, Spectral Clustering and K-means: Imaging Classification for Single-particle Diffractive Imaging," in preparation for submission to *SIAM J. on Scientific Computing* or *SIAM J. on Imaging Sciences*.

Z. Wen, C. Yang, X. Liu, S. Marchesini; "Alternating Direction methods for Classical and Ptychographic Phase Retrieval," submitted to *Inverse Problems*.

ESD-Brodie LB09035 Uncovering the Mechanistic Basis for Soil Microbial Community Response to Altered Precipitation Patterns

N. J. Bouskill, H. C. Lim, U. Karaoz, S. Borglin, R. Salve, T. Wood, W. Silver, E.L. Brodie; "Pre-exposure to short-term drought increases the resilience of sub-tropical forest soil bacterial communities to extended drought," in preparation.

N. J. Bouskill, R. Baren, B. P. Bowen, J. D. Van Nostrand, J. Z. Zhao, T. R. Northen, E.L. Brodie; "The functional response of microbial communities to extended drought: A comparison of genomic and metabolomic data," in preparation.

N. J. Bouskill, T. Wood, H. C. Lim, T. Kwak, W. Silver, E.L. Brodie; "Elevated nitrous oxide efflux following wet-up in a sub-tropical rainforest exposed to extended drought, in preparation.

N. J. Bouskill, E. A. Sudderth, E. A. Wood, et al; "Consistent patterns in the response of soil microbial communities from divergent biomes to decreased precipitation," in preparation.

ESD-Commer LB10033 Enhanced Subsurface Fluid Characterization Using Joint Hydrological and Geophysical Data Inversion

M. Commer, M. B. Kowalsky, S. A. Finsterle, G. A. Newman; "MPiTOUGH2-EMGeo – A massively parallel data inversion framework for joint hydrogeophysical real-world applications," submitted to *Computational Methods in Water Resources 2012 International Conference*.

M. B. Kowalsky, S. A. Finsterle, M. Commer, et al; "On parameterization of the inverse problem for estimating aquifer properties using tracer data," accepted for publication in *Water Resources Research*.

M. Commer, M. B. Kowalsky, S. A. Finsterle, G. A. Newman; "MPiTOUGH2-EMGeo – A massively parallel data inversion framework for joint hydrogeophysical real-world applications," in preparation to be submitted to *Computational Geosciences*.

M. Commer, M. B. Kowalsky, S. A. Finsterle, G. A. Newman; "Joint hydrogeophysical data inversion using structural similarity constraints," in preparation to be submitted to *Water Resources Research*.

ESD-Davis LB11007 Effect of Secondary Mineral Coatings on Biogeochemical Processes

J. Davis, P. Fox, D. Singer, H. Guo; "Reactivity of U(VI) with secondary mineral coatings on sand grains from a fine sand aquifer," in preparation for submission to *Environmental Science and Technology*.

H. Guo, D. Singer, J. Davis, P. Fox; "Comparison of secondary mineral phases in coatings of quartz grains from two Atlantic coastal plain aquifers," in preparation for for submission to *Clays and Clay Mineralogy*.

P. Fox, J. Davis, D. Singer, H. Guo; "Reactivity of As(V) and As(III) with secondary mineral coatings on sand grains from a sand and gravel aquifer," in preparation for submission to *Geochimica et Cosmochimica Acta*.

ESD-Jansson LB11011 CYANOALKANES: Exploiting the Vast Diversity of Cyanobacterial Alkanes for Production of Biojetfuel

P. Hu, H.-Y. Holman, L. Mahoney, K. L. Chavarria, C. Zhang, N.W.T. Quinn, C. Jansson; "Single-Cell Metabolic Fingerprinting of the Cyanobacterium *Synechocystis* PCC6803 Engineered for Production of free Fatty Acids using Synchrotron Infrared Spectromicroscopy and Multivariate Analysis," under revision for *Applied Energy*.

C. Jansson, "Metabolic Engineering of cCanobacteria for Direct cCnversion of CO_2 to Hydrocarbon bBofuels." in press *Progress in Botany* **73** (2011).

C. Jansson, "Employing cCobacteria for Biofuel sSthesis and CCS," in press *Solar Energy* (Radu, R., Ed), InTech (2011).

ESD-Oldenburg LB10017 CO2 as Cushion Gas for Compressed Air Energy Storage in Subsurface Reservoirs

C. M. Oldenburg, L. Pan; "Utilization of CO2 as a Cushion Gas for Compressed Air Energy Storage," *10th Annual Conference on Carbon Capture and Sequestration* (May 2-5, 2011, Pittsburgh, PA).

ESD-Romps LB11044 Interactions Among Cloud Processes, Convection, and Climate Change

D. Romps, Z. Kuang; "A transilient matrix for moist convection," *J. of the Atmospheric Sciences* **68** (9), 2009-2025 (September 2011). doi: http://dx.doi.org/10.1175/2011JAS3712.1

D. Romps, "Convective momentum transport and its parameterization," in revision for *J. of the Atmospheric Sciences*.

J. Molinari, D. Romps, D. Vollaro, L. Nguyen, "CAPE in tropical cyclones," in revision for *J. of the Atmospheric Sciences*.

ESD-Salve LB09023 Identifying and Predicting Climate Change Impacts on the Land-Based Components of the Water Cycle

R. Salve, "A sensor array system for profiling moisture in unsaturated rock and soil," *Hydrological Processes* **25** (18), 2907-2915 (30 August 2011). doi: 10.1002/hyp.8053.

R. Salve, "Backfill Impacts on Moisture Measurements in Fractured Rock," submitted to *Ground Water Monitoring & Remediation*.

R. Salve, E. Gasperikova, D.M. Rempe, J. Peterson; "Application of Electrical Resistivity Tomography for Hillslope Hydrology Studies," in preparation for submission to *Water Resources Research*.

R. Salve, D.M. Rempe, J. Oshun, W.E. Dietrich; "Spatial and Temporal Dynamics of Vertical Unsaturated Flow and Groundwater Response along a Hillslope Underlain by Weathered Fractured Bedrock," in preparation for submission to *Water Resources Research*.

R. Salve, D. Rempe, W. E. Dietrich; "Dryout of a Steep Hillslope During Periods of Extended Seasonal Drought," American Geological Union, Fall Meeting, San Francisco CA (December 2011).

D. M. Rempe, E. Gasperikova, R. Salve, J. Peterson; "Time-lapse electrical resistivity tomography study of unsaturated moisture in fractured, weathered argillite," American Geological Union, Fall Meeting, San Francisco CA (December 2011).

R. Salve, "The role of the *unsaturated* fractured rock zone in transforming rainfall to runoff along a steep hillslope," invited talk to the Department of Geology and Geophysics University of Wyoming, Laramie WY (September 2011).

R. Salve; "Why it may be important to link flow in fractured bedrock to ecologic and atmospheric processes," Carbon Cycle 2.0 Seminar, Lawrence Berkeley National Laboratory (April 21, 2011).

R. Salve, "Flow through fractured bedrock along a hillslope," invited talk to College of Agriculture and Life Sciences, University of Arizona, Tucscon AZ (March, 2011).

ESD-Tokunaga LB11034 Testing a New Carbon Sequestration Strategy by Accelerating Calcite Precipitation in Soils

Y.-S. Han, T. Tokunaga**,** J. Wan, M. Conrad, R. Salve; "Testing Carbon Sequestration in Soil Through the Addition of Gypsum," poster presentation at American Geophysical Union, Fall meeting, San Francisco CA (Dec. 7th, 2011).

ESD-Torn LB10022 Biological Carbon Sequestration: Fundamental Research on Biological Carbon Capture and Soil Carbon Stabilization

K. Chourey, J.K. Jansson, N. VerBerkmoes, et al; A direct cellular lysis/protein extraction protocol for soil metaproteomics. *J. Proteome Res.* **9**, 6615-6622 (2010).

N. Kamennaya, C. Jansson, "Biomineralization; in 'Calcifying Cyanobacteria as a Potential Means for Biological Carbon Capture and Storage,'" invited review in preparation for *Advances in Biomenerals*.

N. Tas, C. Castanha, K. Reichl, M. Fischer, E. Brodie, M.S. Torn, J.K. Jansson; "Impact of pyrolized carbon on microbial diversity and C-stabilization potential in soils," in preparation for submission to *Global Change Biology*.

E. L. Brodie, H. C. Lim, C. Castanha, U. Karaoz, M. Bill, M.E. Conrad, M. S. Torn, J. K. Jansson; "Biochar addition to grassland soils stimulates hydrolytic enzyme activity and Actinomycetes capable of pyrolized C mineralization," in preparation for submission to *ISME Journal*.

N. Kamennaya, L. Mahoney, E. Holman, et al; "Exposure to Elevated CO_2 Concentrations Alters the Biologically Induced Carbonate Mineralization Pattern in the Marine Cyanobacterium *Synechococcus* PCC8806," in preparation to be submitted to *PNAS*.

C. Jansson, "Employing Cyanobacteria for Biofuel Synthesis and CCS," in press for *Solar Energy* (Radu, R., Ed), InTech.

C. Jansson, S. Wullschleger, U. Kalluri, G.T. Tuskan; "Phytosequestration: Carbon Biosequestration by Plants and the Prospects for Genetic Engineering," *BioScience* **60**, 685-696 (2010). url: http://www.aibs.org/bioscience-press-releases/resources/Jansson%20et%20al.pdf.

M.W.I.S. Schmidt, M. S. Torn, S. Abiven, et al; "Soil organic matter persistence as an ecosystem property," *Nature* **477**, 49-56 (2011). (Schmidt and Torn are equal co-authors)

R. Mackelprang, M. P. Waldrop, K. M. DeAngelis, et al; "Metagenome analysis of a permafrost microbial community reveals a rapid response to thaw," *Nature* **480**, 368-371 (15 December 2011). doi: 10.1038/nature10576

J. K. Jansson, "Towards 'Tera-Terra': Terabase sequencing of terrestrial metagenomes," *Microbe* **6**, 309-315 (2011).

ESD-Quanlin Zhou LB11041 Collaboration with China on Geologic Carbon Sequestration: Novel Field Tests to Characterize Heterogeneity for China's First Pilot Test

C. Chang, L. Xia, Q. Zhou, X. Li, Q. Yu; "Experimental study of residual water and CO_2 saturation of reservoir rocks in the Erdos Basin in China," submitted to *Acta Geologica Sinica* (English Edition).

EG-Arbelaez LB10018 Investigation of Image Current and Magnetic Field Tolerance Effects on High-Temperature Superconductor Undulators for Soft X-Ray FELs

S. Prestemon, D. Arbelaez, S. Davies, D. Dietderich, D. Lee, F. Minervini, R. Schlueter; "Development and analysis of HTS-undulator components for FEL applications," *IEEE Transactions on Applied Superconductivity*, Issue 99. ISSN: 1051-8223 (2011).

D. Arbelaez, T. Wilks, S. Prestemon; "A dispersion and pulse width correction algorithm for the pulsed wire method," in preparation for submission to *Nuclear Instruments and Methods*.

EETD-Coughlin, Fridley LB10004 Physically-Based Accounting for Resource Use in New Energy Pathways

K. Coughlin, "A Mathematical Analysis of Full Fuel Cycle Energy Use," in Press in *Energy* (Elsevier).

K. Coughlin, A. Sturges and D. Fridley; "Estimating the production potential of truly carbon-neutral biomass-based energy," in preparation for submission to *Energy* or *Biomass and Bioenergy*.

EETD-Fischer LB10044 Toward a US Greenhouse Gas Information System (GHGIS)

M.L. Fischer, S. Jeong, Y. Hsu, et al; "Top-Down Constraints on Fossil Fuel CO2 Emissions for Three Urban Areas of California," presented (abstract online) at *American Geophysical Union 2011 Fall Meeting* (Dec, 2011). url, http://www.agu.org/meetings/pdf/2011_FM_Program_Book.pdf

S. Jeong, Y. Hsu, A. E. Andrews, et al; "Estimating CH4 and N2O Emissions Using Tower Measurements in California, presented (abstract online) at *American Geophysical Union 2011 Fall Meeting* (Dec, 2011). url, http://www.agu.org/meetings/pdf/2011_FM_Program_Book.pdf

EETD-Gadgil LB10041 Developing a Fuel-Efficient Cookstove for Haiti

K. Lask, K. Booker, C Ceballos, J. Jones, N. Yang, A. Gadgil; "Performance of charcoal cookstoves for Haiti: Part 2: Results from Controlled Cooking Test," in review *LBNL Report (*December 2011).

K. Booker, T. W. Han, J. Granderson, J. Jones, K. Lask, N. Yang, A. Gadgil; "Performance of charcoal cookstoves for Haiti, Part 1: Results from Water Boiling Test," *LBNL Report: LBNL-5021E* (June 2011).

EETD- Masanet et al LB11021 Developing Analytical and Communications Frameworks to Enable Breakthrough Low-Carbon Technologies

Conference abstracts and presentations

W. Morrow, A. Gopal, E. Masanet, T. McKone, L. Dale, J. E. McMahon; "Early-Stage Economic and Life-Cycle Analysis for Salt- and Drought-Tolerant Switchgrass Derived Biofuels," *LCA XI Conference*. Chicago IL (October 4, 2011). url: http://lcacenter.org/lcaxi/final/434.pdf

P. Zhai, P. Larsen, E. Masanet, D. Millstein, S. Menon; "Modeling Emission Changes of U.S. Power Grid with High Penetration of Photovoltaics," *LCA XI Conference*, Chicago IL (October 4, 2011). url: http://lcacenter.org/lcaxi/final/454.pdf

Articles in preparation

W. Morrow, A. Gopal, E. Masanet, T McKone, L. Dale, J. E. McMahon; "Economic and Life-Cycle Analysis of Drought Tolerant Switch Grass for Biofuels," in preparation for submission to *Environmental Science & Technology*.

P. Zhai, P. Larsen, M. Millstein, S. Menon, E. Masanet; "Avoided Emissions from High Penetration of Photovoltaic Electricity in the United States," in preparation for submission to *Energy - The International Journal*.

R. Sathre, E. Masanet; "Energy and Climate Implications of CCS Deployment Strategies in the US Coal-fired Electricity Fleet Through 2100," in preparation for submission to *Environmental Science & Technology*.

E. Masanet, R. Sathre, P. Larsen, W. Morrow, A. Gopal, A. Shehabi, P. Zhai; "Life Cycle Assessment of Renewable Energy Systems," invited paper in preparation for *Annual Review of Environment and Resources*, Volume 37 (2012).

N. DeForest, S. Shehabi, E. Masanet, D. Milliron, G. Garcia, S. Selkowitz, E. Lee; "A Regional Assessment of Solar Heat Management via Dynamic Window Coatings," under review for *Proceedings of the 201 2012 ACEEE Summer Study on Energy Efficiency in Buildings*.

EETD-McKone LB11022 Life-Cycle Analysis of Geologic Carbon Sequestration

H Breunig, J Birkholzer, A Borgia, P Price, C Oldenburg, T McKone; "Life Cycle Assessment of Pressure Management for Geologic Carbon Sequestration using Brine Extraction," final draft of LBNL Technical Report in review.

EETD-McMahon/Dale LB11023 Mapping Genes to Salty Acres: Engineering Salt-Tolerant Switchgrass Lines for Cost-Effective, Large-Scale Production of Sustainable Low-Carbon Biofuels

W. Morrow, A. Gopal, G. Fitts, L. Dale, E. Masanet, T. Mckone, J. McMahon; "Effect of Drought on Cellulosic Biofuel Costs," in preparation for submission to *Energy Policy Journal*.

S. Lewis, L. Dale, G. Fitts, K. Koy, M. Kelly; "Spatial Suitability Model for Drought-tolerant Switchgrass," poster presented at the *American Geophysical Union* (December 2012).

EETD-Menon LB11024 From Fossil Fuel to Photovoltaics: Economic, Environmental, and Health Impacts for Policy Considerations

Millstein, D., S. Menon; "Regional Climate Consequences of Large-Scale Cool Roof and Photovoltaic Array Deployment," *Environ. Res. Lett.* **6**, 034001 (2011). url: http://dx.doi.org/10.1088/1748-9326/6/3/034001

P. Zhai, P. Larson, D. Millstein, S. Menon, E. Massanet; "Avoided Emissions from High Penetration of Photovoltaic Electricity in the United States," in preparation to be submitted to *Energy Journal.*

EETD-Persson LB11027 Accelerated Materials Design through First-Principles Calculations and Data Mining

A. Jain, G. Hautier, C. J. Moore, S. P. Ong, C. C. Fischer, T. Mueller, K. A. Persson, G. Ceder; "A High-Throughput Infrastructure for Density Functional Theory Calculations," *Comp. Mat. Sci.* **50**, 2295 (2011).

Website for The Materials Project: *www.materialsproject.org*

EETD-Selkowitz LB11032 Dynamic Light Redirection by Optical Metamaterial Coatings

G. Masson, R. Mendelsberg, I. Fernandez-Cuesta S. Cabrini, D. Milliron, B. Helms; "Nanostructured Electro-Actuated Polymer Glazings For Dynamic Daylighting Control," in preparation for submission to *Advanced Materials*.

G. Masson, R. Mendelsberg, I. Fernandez-Cuesta S. Cabrini, D. Milliron, B. Helms; "Stimuli Responsive Glazings With Dynamic Daylight Control," submitted for Spring Meeting 2012 of *Materials Research Society*.

EETD-Wetter LB10028 Building Systems for Net Zero Energy Buildings

M. Wetter, W. Zuo, T. S. Nouidui; "Modeling of Heat Transfer in Rooms in the Modelica 'Buildings' library," in the *12th International Conference of the International Building Performance Simulation Association*, Sydney, Australia (Building Simulation 2011).

W. Zuo, M. Wetter; "Advanced Simulations of Building Energy and Control Systems with An Example of Chilled Water Plant Modeling," in the *8th International Forum and Workshop on Combined Heat, Air, Moisture and Pollutant Simulations,* Nanjing, China (CHAMPS 2011).

M. Wetter, W. Zuo, T. S. Nouidui; "Recent Developments of the Modelica Buildings Library for Building Heating, Ventilation and Air-Conditioning Systems," in the *8th International Modelica Conference*. Dresden, Germany (2011).

M. Wetter, W. Zuo; "Modeling of Thermofluid Networks Near Zero Mass Flow Rate with Feedback Control using an Equation-based Language," in preparation.

Y. Yang, A. Pinto, A. Sangiovanni-Vincentelli; Q. Zhu; "A Design Flow for Building Automation and Control Systems," *Proceedings of the IEEE Real-Time Systems Symposium (RTSS)*, 105-116 (Nov. 30 2010-Dec. 3 2010).

M. Maasoumy, A. Pinto, A. Sangiovanni-Vincentelli, "Model-based Hierarchical Optimal Control Design for HVAC Systems," *Proceedings of the Dynamic System and Control Conference*, Arlington VA (2011).

A. Puggelli, M. Mozumdar, L. Lavagno, A. Sangiovanni-Vincentelli; "A Routing-Algorithm-Aware Design Tool for Indoor Wireless Sensor Networks," to appear in *Proceedings of the IEEE International Conference on Computing, Networking and Communications (ICNC)*, Maui, HI (2012).

GN-Deutsch, Rubin LB11030 Highly Parallelized, Low-Cost Synthesis of Microbial Genes Using High-Density Oligonucleotide Arrays

S, Deutsch, "Rational Engineering of Glycosyl Hydrolases Through Synthetic Metagemonics," in preparation for possible submission to *Nature Biotech*.

LSD-Blakely LB10040 Synchrotron-Based Microtomography for Functional Analysis of Normal Tissue and Tumor Molecular Markers, and their Perturbation by Low Dose Radiation Exposure.

E. Blakely, K. Bjornstad, C. Rosen, et al; "High-resolution tomographic imaging of murine tumors and organs," in preparation for submission to *Nature Methods.*

LSD-LaBarge LB11016 Determination of Impact of the Micro-Environment and Tissue-Level Self-Organization on Cell Fate Decisions and Homeostasis …

L. Chanson, D. Brownfield, J. C. Garbe, I. Kuhn, M. R. Stampfer, M. J. Bissell, M. A. LaBarge; "Self-organization is a dynamic and lineage-intrinsic property of mammary epithelial cells," *PNAS* **108** (8), 3264-9 (2011 Feb 22, Epub 2011 Feb 7).

C. H. Lin, J. K. Lee, M. A. LaBarge; "Fabrication and use of MicroEnvironment microarrays (MEArrays)," in press at *J. of Visual Experimentation*.

C. H. Lin, F. Pelissier, K. Sputova, J. Gray, M. A. LaBarge; "Dissecting the role of microenvironment in therapeutic response," in preparation for submission to *Nature Biotech*.

F. Pelissier, C. H. Lin, K. Sputova, M. R. Stampfer, M. A. LaBarge MA; "Age-associated changes in mechanosensing in human mammary epithelia," in preparation for submission to *Aging Cell*.

LSD-Mao LB10013 Identification of Genetic Networks Controlling Susceptibility to Radiation-Induced Carcinogenesis

T. Li, H. S. Hung, Y. C. Wang, et al; "Transgenic Mice for Cre-Inducible Overexpression of the Cul4A Gene," *Genesis* **49**, 134-41 (2011).

J. Pérez-Losada, A. Castellanos-Martín, J. H. and Mao; "Cancer Evolution and Individual Susceptibility," *Integrative Biology* **3**, 316-328 (2011).

R. Xu, J. H. Mao; "Gene transcriptional networks integrate microenvironmental signals in human breast cancer," *Integrative Biology* **3**, 368-374 (2011).

D. H. Nguyen, H. A. Oketch-Rabah, I. Illa-Bochaca, et al; "Radiation acts on the microenvironment to affect Breast carcinogenesis by distinct mechanisms that decrease breast cancer latency and affect tumor type," *Cancer Cell* **19**, 640-651 (2011).

Y. V. Wang, M. Leblanc, N. Fox, et al; "Fine-tuning p53 activity through C-terminal modification significantly contributes to HSC homeostasis and mouse radiosensitivity," *Genes & Development* **25**, 1426-1438 (2011).

M. D. To, D. A. Quigley, J. H. Mao, et al; "Progressive genomic instability in the FVB/Kras^{LA2} mouse model of lung cancer," *Molecular Cancer Research* **9**, 1339-45 (2011).

J. H. Mao, D. Wu, I. J. Kim, et al; "*Hipk2* cooperates with *p53* to suppress g-ray radiation-induced mouse thymic lymphoma," *Oncogene* (2011 Jul 25). doi: 10.1038/onc.2011.306 [Epub ahead of print].

LSD-McMurray LB09016 SPARKLE-A Fluorescence Energy Transfer (FRET) Methodology for Visualization of Simultaneous and Reversible Interactions

J. Majka, B. Alford, J. Ausio, R. M. Finn, C. T. McMurray; "ATP hydrolysis by RAd50 switches MRE11 form an endonucelase to an exonucelase," *J Biol. Chem.* **287**, 2328-2341 (2011 Nov 18).

W. H. Lang, J. E. Coats, J. Majka, G. L. Hura, Y. Lin, I. Rasnik, C. T. McMurray; "Conformational trapping of mismatch recognition complex MSH2/MSH3 on repair-resistant DNA loops," *Proc Natl Acad Sci U S A.* 108 (42), E837-44 (2011).

I. V. Kovtun, K. O. Johnson, C. T. McMurray, "Cockayne syndrome B protein antagonizes OGG1 in modulating CAG repeat length *in vivo*," *Aging* (Albany NY) **3** (5), 509-14 (2011).

C. T. McMurray; “Mechanisms of trinucleotide repeat instability during human development,” *Nat. Rev. Genet.* **11** (11), 786-99 (2010).

Z. Xun, D. D.-Y. Lee, J. Lim, C. A. Canaria, A. Barnebey, S. M. Yanonne, C. T. McMurray; “Retinoic acid-induced differentiation increases the rate of oxygen consumption and enhances the spare respiratory capacity of mitochondria in SH-SY5Y cells,” in revision for *Molecular Aging and Development*.

D.-Y. Lee, V. Platt, B. Bowen, K. Louie, C. Canaria, C. T. McMurray, T. Northen; **“**Resolving brain regions using nanostructure initiator mass spectrometry imaging of phospholipids,” submitted to *Integrative Biology.*

LSD-Wang-D LB10035 Multinozzle Arrays for Single Cell Metabolomics

P. Mao, H. T. Wang, P. Yang, D. Wang; "Multinozzle Emitter Arrays for Nanoelectrospray Mass Spectrometry," *Analytical Chemistry* **83** (15), 6282-6289 (2011). PMCID: PMC3146565

LSD-Wiese LB10039 Functional Characterization of NUCKS- a Potential Cancer Susceptibility Locus Required for Recombination

C. Wiese, E. Dray, T. Groesser, S.B. Seidler, A.C. Østvold, P. Sung, D. Schild; “NUCKS is a RAD51AP1 Paralog and Required for DNA Repair and Genomic Stability,” close to being submitted to *JBC* or *PNAS*.

Y. Yue, D. Schild, A.C. Østvold, J.-H. Mao, C. Wiese; “*Nucks* suppresses radiation-induced tumors in mice,” in preparation for submission to *Oncogene*.

MSD-Ager LB11002 Induced Bucket Brigade Photovoltaic Effect

J. Seidel, D. Fu, S.-Y. Yang, E. Alarcón-Lladó, J. Wu, R. Ramesh, J. W. Ager III; “Efficient photovoltaic current generation at ferroelectric domain walls,” *Phys. Rev. Lett.* **107**, 126805 (2011).

J. W. Ager, “Bucket Brigade Photovoltaic Effect in Ferroelectrics,” in press *SPIE Newsroom*.

MSD-Clarke Haeffner LB10003 Heating Rates of Planar Ion Traps for Quantum Information

N. Daniilidis, S. Narayanan, S. A. Möller, et al; “Fabrication and heating rate study of microscopic surface electrode ion traps,” *New J. Phys.* **13**, 013032 (2011).

T. Karin, I. Le Bras, A. Kehlberger, K. Singer, N. Daniilidis, H. Häffner; “Transport of charged particlesn by adjusting rf voltage amplitudes,” *Appl. Phys. B* **106**, 117 (2012).

MSD-Kaindl LB11013 Attosecond XUV Condensed-Matter Science: Electronic Wavefunction Coherence and Correlated Dynamics

J. Robinson, P. Ranitovic, Z. Hussain, R. A. Kaindl; “Multicolor Streaking Setup for Attosecond Condensed Matter Spectroscopy,” in preparation for submission to *Rev. Sci. Instr*.

MSD-Kaindl LB11014 Ultrafast 2D Fourier-Transform Spectroscopy of Electronic Dynamics in Photovoltaic Nanomaterials

G. Coslovich, H. Y. Choi, J. Urban, E. Chan, R. W. Schoenlein, R. A. Kaindl; "Broadband interferometer for ultrafast 2D Fourier-transform spectroscopy of nanoscale materials," in preparation for submission to *Optics Express*.

MSD-Orenstein LB11026 Probing and Controlling Spin and Charge in Strong Spin-Orbit Materials

X. Wan, Ari M. Turner, A. Vishwanath, S. Y. Savrasov; "Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates," *Phys. Rev. B* **83**, 205101 (2011).

P. Hosur, S. Parameswaran, and A. Vishwanath; "Charge Transport in Weyl semimetals," to appear in *Phys. Rev. Lett.* arXiv:1109.6330.

Y. Z. You, I. Kimchi, A. Vishwanath, "Topological Superconductivity on doping a Spin Orbit Mott Insulator," submitted to *Phys. Rev. Lett*. arXiv:1109.4155.

MSD-Smit LB09029 Tuning the Self-Assembly of Membrane Proteins

J. M Rodgers, M. Webb, B. Smit; "Understanding the Phase Behavior of Coarse-Grained Model Lipid Bilayers Through Computational Calorimetry," *J. Phys. Chem B*, Article ASAP doi: 10.1021/jp207837v.

MSD-Tirrell LB10021 Structured Charged Polymers

R. Chollakup, D. J. Audus, J. B. Beck, et al; "Polyelectrolyte Molecular Weight and Salt Effects on the Phase Behavior and Coacervation of Aqueous Solutions of Poly(acrylic acid) Sodium Salt and Poly(allylamine) Hydrochloride," in press for *Macromolecules*.

R. Farina, N. Laugel, P. Pincus, M. Tirrell; "Strong Polyelectrolyte Brushes in Mixed Mono- and Tri-Valent Ionic Media at Fixed Total Ionic Strengths," submitted to *Macromolecules*.

D. Priftis, R. Farina, M. Tirrell; "Interfacial Energy of Polypeptide Complex Coacervates Measured via Capillary Adhesion, submitted to *Langmuir*.

MSD-Walukiewicz LB11046 Intermediate Band Solar Cell-Proof of Concept and Search for New Materials

N. López, L. A. Reichertz, K. M. Yu, K. Campman, W. Walukiewicz; "Multiband solar cell," presented at the *26th European Photovoltaic Solar Energy Conference and Exhibition*, Hamburg, Germany, paper to be published in the conference proceeding (5-9 September, 2011).

N. López, L. A. Reichertz, K. M. Yu, K. Campman, W. Walukiewicz; "Demonstration of a Multiband Solar Cell," invited paper, *SPIE Photonic West, Conference OE102: Physics, Simulation, and Photonic Engineering of Photovoltaic Devices*, San Francisco CA (21-26 January 2012).

MSD-Wang-F LB10025 Integrated Optoelectronic Devices Based on Graphene

J. Horgn, C.F. Chen, B Geng, et al; "Crude Conductivity of Dirac Fermions in Graphene," *Phys. Rev. B* **83**, 165113 (2011).

C.F. Chen, C.H. Park, B. Geng, et al; "Control Inelastic Light Scattering Quantum Pathways in Graphene," *Nature* **471**, 617 (2011).

MSD-Yang-P LB10030 Design and Surface Properties of Semiconductor Nanowires

D. Fu, J. Zou, K. Wang, R. Zhang, D. Yu, J. Wu; "Electrothermal Dynamics of Semiconductor Nanowires under Local Carrier Modulation," *Nano Lett*. **11**, 3809 (2011). url: http://www.mse.berkeley.edu/~jwu/publications/Fu-NanoLett-11.pdf

J. Seidel, D. Fu, S.-Y. Yang, E. Alarcon-Llado, J. Wu, R. Ramesh, J. W. Ager III; "Efficient photovoltaic current generation at ferroelectric domain walls," *Phys. Rev. Lett*. **107**, 126805 (2011). url: http://www.mse.berkeley.edu/~jwu/publications/Seidel-PRL-11.pdf

W. Fan, J. Cao, J. Seidel, et al; "Large Kinetic Asymmetry in Twin Wall-Mediated Metal-Insulator Phase Transition," *Phys. Rev. B* **83**, 235102 (2011). Highlighted by *PRB* as "Editor's Suggestion". url: http://www.mse.berkeley.edu/~jwu/publications/Fan-PRB-11.pdf

A. C. Ford, C. W. Yeung, S. Chuang, H. S. Kim, E. Plis, S. Krishna, C. Hu, A. Javey; "Ultrathin body InAs tunneling field-effect transistors on Si substrates," *Appl. Phys. Lett.* **98**, 113105 (2011).

K. Cho, D. J. Ruebusch, M. H. Lee, et al; "Molecular monolayers for conformal, nanoscale doping of InP nanopillar photovoltaics," *Appl. Phys. Lett.* **98**, 203101 (2011).

MSD-Zheng LB11040 Imaging Through Liquids using a TEM

H. Xin, H. Zheng; "In situ observation of oscillatory growth of bismuth nanoparticles," submitted to *Nano Lett*.

H. Zheng, J. Park, U. Dahmen, P. Alivisatos; "In situ study of bismuth oxide hollow nanoparticle formation," in preparation for submission to *Nano Lett*.

H. Zheng, J. B. Rivest, T. Miller, et al; "Observation of transient structural transformation dynamics of a single Cu_2S nanorod," *Science* **333**, 206 (2011).

U. Mirsaidov, H. Zheng, Y. Casana, P. Matsudaira; "Imaging protein structure in water with 2.7 nm resolution," in review for *Biophysical Journal*.

H. Zheng, J. B. Rivest, T. Miller et al; "Observation of dynamic structural transformations in a copper sulfide nanorod by TEM," *Microscopy and Microanalysis Meeting*, Nashwille TN (Aug. 2011).

H. Zheng, H. Liao, J. Park, U. Dahmen, P. Alivisatos; "Observation of single nanocrystal growth trajectories in solution using liquid cell TEM," *Microscopy and Microanalysis Meeting*, Nashwille TN (Aug. 2011).

U. Mirsaidov, H. Zheng, Y. Casana, P. Matsudaira; "Nanometer-scale electron microscopy of proteins in liquid," *Microscopy and Microanalysis Meeting*, Nashwille TN (Aug. 2011).

J. Park, H. Zheng, W.C. Lee, P.L. Geissler, E. Rabani, A.P. Alivisatos; "*In situ* Observation of Oscillatory Growth of Bismuth Nanoparticles," *ACS Nano* (in press).

NSD-Haxton LB11010 Lattice QCD Codes by Discretizing Time and Space

A. Walker Loud (with NPLQCD), ``Present Constraints on the H-dibaryon at the Physical Point from Lattice QCD," *arXiv*: 1103.2821.

A. Walker-Loud (with NPLQCD), ``High Statistics Analysis using Anisotropic Clover Lattices (IV): The Volume Dependence of Light Hadron Masses," *Phys. Rev. D* **84**, 014507 (2011).

A. Walker-Loud (with NPLQCD), ``the I=2 pi-pi S-wave Scattering Phase Shift from Lattice QCD," *arXiv*: 1107.5023.

A. Walker Loud (with NPLQCD), ``SU(2) Low Energy Constants from Mixed-Action Lattice QCD," *arXiv*: 1108.1380.

A. Walker-Loud (with NPLQCD), ``Evidence for Non-Analytic Light Quark Mass Dependence in the Baryon Spectrum," *NT-LBNL-011-014*.

W. Detmold, B. Tiburzi, and A. Walker-Loud, ``Electromagnetic Polarizabilities: Lattice QCD in Background Fields," *arXiv*: 1108.1698 (conference proceedings).

S. Syritsyn, ``Calculation of Nucleon Structure in Lattice QCD with almost-Physical Light Quarks," *NT-LNBL-11-016* (conference proceedings).

A. Walker-Loud with NPLQCD, ``The Deuteron and Exotic Two-Body Bound States," *arXiv*: 1109.2889.

S. Syritsyn (with LHP Collaboration), ``Quark Contributions to Nucleon Momentum and Spin from Domain-Wall Fermion Calculations," *NT-LBNL-11-020* (conference proceedings).

S. Syritsyn (with LHP Collaboration), ``Excited-State Contamination in Nucleon Structure Calculations," *arXiv*: 1111.0255 (conference proceedings).

PBD-Hillson LB10042 Advances in Standardized, Scar-less, Sequence-Independent Cloning Methods.

N. J. Hillson, R. D. Rosengarten, J. D. Keasling; "j5 DNA assembly design automation software," under revision for *ACS Synthetic Biology* (submitted Oct. 4, 2011).

J. Chen, D. Densmore, T. S. Ham, J. D. Keasling, N. J. Hillson, "DeviceEditor biological CAD canvas," under revision for *J. of Biological Engineering* (submitted Nov 15, 2011).

PBD-Lee LB11017 Piezoelectric Biomaterials for Novel Energy Conversion

W.-C. Chung; J.-W. Oh, K. Kwak , B.-Y. Lee, J. Meyer, E. Wang, A. Hexemer, S.-W. Lee; "Biomimetic self-templating supramolecular structures," *Nature* **478**, 364-368 (2011). url: http://www.nature.com/nature/journal/v478/n7369/full/nature10513.html

B.-Y. Lee, J. Zhang, C. Zueger, W. Chung, J. Meyer, S. Y. Yoo, D. S. Choi, R. Rames, S.-W. Lee; "Phage-Based Piezoelectric Thin Films for Energy Generation," Material Research Society 2011 Fall Meeting, 2011 Boston MA. url: http://www.mrs.org/f11-program-hh/

PBD-Scheller LB10019 Engineering of Drought and Heat Tolerance in Bioenergy Crops.

U. Christensen, A. Zygadlo-Nielsen, J. Harholt, P. Ulvskov, P. Canlas, P. Ronald, H. V. Scheller; "Characterization and biological function of mannosylglycerate synthase in *S. moellendorfii*," in preparation for possible submission to *Plant Journal*.

J. Harholt, I. Sørensen, A. Roberts, W. Willats, H. V. Scheller, B. L. Petersen, J. A. Banks, P. Ulvskov, "A comparative study of cell wall structure and glycosyltransferase repertoire of the spike moss *Selaginella moellendorffii*," submitted to *Plos One*.

J. A. Banks, T. Nishiyama, M. Hasebe M, et al; "The compact *Selaginella* genome identifies changes in gene content associated with the evolution of vascular plants," *Science* **332**: 960-963.

H. V. Scheller, J. Harholt, P. Ulvskov; "Stress-tolerant plants expressing mannosylglycerate-producing enzyme," *PCT patent application*, WO2010129574 (2010).

U. Christensen, P. Benke, A. Z. Nielsen, et al; "Engineering bioenergy crops to accumulate mannosylglycerate a compatible solute produced by thermophilic bacteria in response to stress- 'A Bio-Based Future'," August 29 - 31, 2011, Berkeley, CA.

U. Christensen, P. Benke, A. Z. Nielsen, et al; "Engineering bioenergy crops to accumulate mannosylglycerate – a compatible solute produced by thermophilic bacteria in response to stress," *6th Annual DOE JGI User Meeting*, Walnut Creek CA (March 22-24, 2011).

U. Christensen, P. Benke, A. Z. Nielsen, et al; "Engineering of stress tolerant bioenergy crops by accumulation of mannosylglycerate," 6th Frontiers in Bioenergy Symposium, West Lafayette IN (May 15-18, 2011).

PBD-Voigt LB11037 Engineering Thermophilic Bacteria For Converting Hydrocarbon To Valuable Chemicals, Methyl Halides

Two (2) publications are planned for peer reviewed journal(s) but are not yet drafted.

PBD-Zwart LB09001 Development of Reusable Software Modules for the Analyses of bioSAXS Data

H. Liu, P. Zwart; "Computation of Small Angle Scattering pro_les with 3D Zernike Polynomials," accepted for publication in *Acta Cryst A*.

H. Liu, P. Zwart; "The Small Angle scattering toolbox," accepted for publication in *J. of Applied Crystallography*.

H. Liu, P. Zwart; "Accelerated Macromolecular solution structure determination," in preparation for submission to *PNAS*.

H. Liu, P. Zwart; "Zalign: multi-resolution structural alignment," in preparation to be submitted to *Acta Cryst D*.

PBD-Zwart LB11042 Feasibility and Development of Fluctuation X-ray Scattering at the NGLS

G. Chen, M. Modestino, B. Poon, A. Schirotzek, S. Marchesini, R. Segalman, A. Hexemer P. Zwart; "Structure determination of Pt-coated Au dumbbells via Fluctuation X-ray Scattering," in preparation to be submitted to *J. of Synchrotron Radiation*.

H. Liu, A Janssen, P. Zwart; "Computation of Fluctuation Scattering profiles via 3D Zernike Polynomials," in preparation for submission to *Acta Cryst A*.

PH-Muller LB10043 Gathering and Analysis of Worldwide Land Temperature Data

R. Rohde, J. Curry, D. Groom, R. Jacobsen, R. Muller, S. Perlmutter, A. Rosenfeld, C. Wickham, J. Wurtele; "Berkeley Earth Temperature Averaging Process," submitted for publication in *JGR Atmospheres*. url: http://berkeleyearth.org/pdf/berkeley-earth-averaging-process.pdf

C. Wickham, J. Curry, D. Groom, R. Jacobsen, R. Muller, S. Perlmutter, R. Rohde, A. Rosenfeld, J. Wurtele; "Influence of Urban Heating on the Global Temperature Land

Average Using Rural Sites Identified from MODIS Classifications," submitted for publication in *JGR Atmospheres*. url: http://berkeleyearth.org/pdf/berkeley-earth-uhi.pdf

R. Muller, J. Curry, D. Groom, R. Jacobsen, S. Perlmutter, R. Rohde, A. Rosenfeld, C. Wickham, J. Wurtele; "Earth Atmospheric Land Surface Temperature and Station Quality in the United States," submitted for publication in *JGR Atmospheres*. url: http://berkeleyearth.org/pdf/berkeley-earth-station-quality.pdf

R. Muller, J. Curry, D. Groom, R. Jacobsen, S. Perlmutter, R. Rohde, A. Rosenfeld, C. Wickham, J. Wurtele; "Decadal Variations in the Global Atmospheric Land Temperatures,"sSubmitted for publication in *JGR Atmospheres*. url: http://berkeleyearth.org/pdf/berkeley-earth-decadal-variations.pdf

PH-Nomura LB10016 Theoretical Studies of Dark Matter Beyond the Standard Model

C. Cheung, Y. Nomura; "Singlet Portal to the Hidden Sector," *JHEP* **11**, 103 (2010).

Y. Nomura, "Physical Theories, Eternal Inflation, and the Quantum Universe," *JHEP* **11**, 063 (2011).

G. Larsen, Y. Nomura, H. L. L. Roberts; "The Cosmological Constant in the Quantum Multiverse," *Phys. Rev. D* **84**, 123512 (2011).

Cross-Div.-Milliron LB10015 Multifunctional Window Coatings for High-Performance Buildings

E. L. Rosen, R. Buonsanti, A. Llordes, A. M. Sawvel, D. J. Milliron, B. A. Helms; "Exceptionally mild reactive stripping of native ligands from nanocrystal surfaces using Meerwein's salt," *Angew. Chem. Int. Ed.* **51**, 684 (2012).

R. Buonsanti, A. Llordes, S. Aloni, B. A. Helms, D. J. Milliron; "Tunable infrared absorption and visible transparency of colloidal aluminum-doped zinc oxide nanocrystals," *Nano Lett*. **11**, 4706 (2011).

G. Garcia, R. Buonsanti, E. L. Runnerstrom, et al; "Dynamically modulating the surface plasmon resonance of doped semiconductor nanocrystals," *Nano Lett.* **11**, 4415 (2011).

A. Llodes, A. T. Hammack, R. Buonsanti, R. Tangirala, S. Aloni, B. A. Helms, D. J. Milliron; "Polyoxometalates and colloidal nanocrystals as building blocks for metal oxide nanocomposite films," *J. Mater. Chem.* **21**, 11631 (2011).

R. J. Mendelsberg, S.H.N. Lim, Y. K. Zhu, J. Wallig, D. J. Milliron, A. Anders; "Achieving high mobility ZnO:Al at very high growth rates by dc filtered cathodic arc deposition," *J. Phys. D* **44**, 232003 (2011).

A. Anders, J. Brown, S. Lim, R. Mendelsberg, L. Gontijo, K. M. Yu, M. Field; "Improving aluminum doped zinc oxide films by minimizing negative ion damage," *8th Int. Conf. Coatings on Glass and Plastics*, Braunschweig, Germany, pp. 33-34 (June 2010).

A. Anders, R. Mendelsberg, S. Lim, Y. Zhu' "Hitting the energy sweet spot: How to make high quality aluminum doped zinc oxide films," *Proc. Ann. Tech. Conf. Soc. Vacuum Coaters,* Chicago IL, paper H4 (April 2011).

R.J. Mendelsberg, S.H.N. Lim, Y. Zhu, D. J. Milliron, A. Anders; "Effects of oxygen plasma treatment before, during, and after growth of ZnO:Al by dc cathodic arc deposition," *2011 MRS Spring Meeting*, San Francisco CA, paper G9.8/S8.8 (2011).

R. J. Mendelsberg, G. Garcia, D. J. Milliron; "Extracting reliable electronic properties from transmission spectra of metal oxide thin films and nanocrystal films by careful application of Drude theory," submitted to *J. of Applied Physics*.