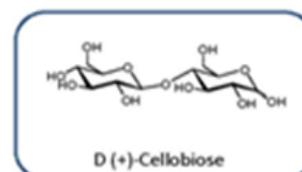
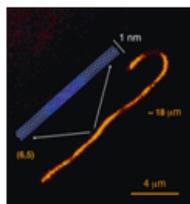
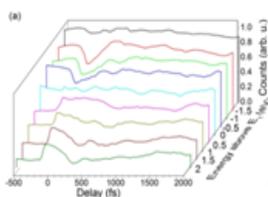
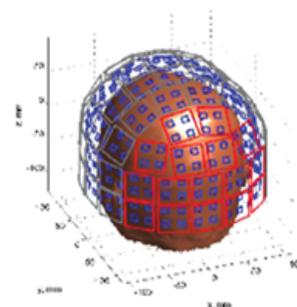
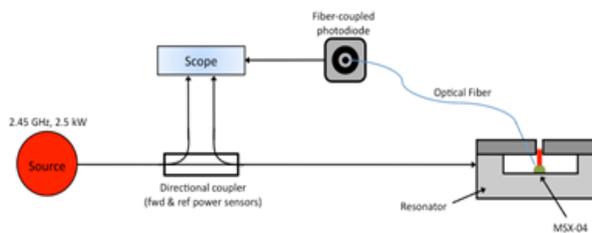
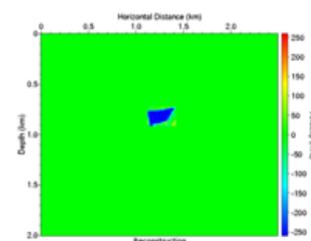
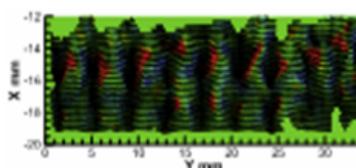
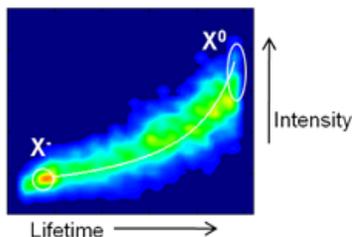


# Los Alamos Postdoc Research Day

**June 16, 2011**



## Abstract Book



**Cover images courtesy of:**

Jin Kyung Kim, B-8

Christophe Galland, C-PCS

Youzuo Lin, EES-17

David Mascarenas, INST-OFF

Jared Crochet, MPA-CINT/C-PCS

Steve Gilbertson, MPA-CINT

Evgeny Burmistrov, P-21

Sridhar Balasubramanian, P-23

Amanda Duque, WX-7

# Table of Contents

Page

---

## ACCELERATOR OPERATIONS AND TECHNOLOGY DIVISION

### AOT-ABS Accelerator and Beam Science

Kolski, Jeff

- 01** Application of Independent Component Analysis (ICA) to Long Bunch Beams in the Los Alamos Proton Storage Ring 1

## BIOSCIENCE DIVISION

### B-6 Genome Science

Beckloff, Nicholas

- 02** Discovery of Novel sRNAs from Yersinia Pestis 2

Dichosa, Armand

- 03** Inducing Artificial Polyploidy in Bacillus Subtilis: Implications to Advance Single Cell Genomics 3

### B-7 Biosecurity and Public Health

Li, Nan

- 04** Functional Discovery of Host Small RNAs in Infectious Disease 4

Micheva-Viteva, Sofiya

- 05** RNAi-based HTS to Identify Human Host Factors Involved in Yersinia Virulence 5

Nagy, Amber

- 06** Cytotoxicity of Quantum Dots in Normal Human Bronchial Epithelial Cells: Comparisons of Core Type and Functionalization 6

Wolfenden, Mark

- 07** Siderophores for Pathogen Capture and Radioisotope Assisted Diagnostics 7

### B-8 Bioenergy and Environmental Science

Blum, Marc-Michael

- 08** Engineering of Diisopropyl Fluorophosphatase for Enhanced Activity Against V-type Nerve Agents 8

Kim, Jin Kyung

- 09** Model System Studies of Cellulose Conversion to Biofuel via Garcia-Gonzalez Reaction 9

Koglin, Alex

- 10** Novel Methods to Investigate Structures and Structural Dynamics of Very Large Proteins by NMR Spectroscopy: Assembly and Alteration of Antibiotic Biosynthesis 10

Marti-Arbona, Ricardo

- 11** A Systematic Approach to Transcriptional Regulator Function Discovery: Novel Effectors for an Old Regulator (MetJ) and Function Discovery for Bxe\_B3018 and Bxe\_A0425 11

# Table of Contents

Page

---

## B-9 Advanced Measurement Science

Nguyen, Hau

- 12** Protein Domain Trapping Method: In Search of Compact, Soluble Protein Fragments for Structural Biology 12

## CHEMISTRY DIVISION

### C-IIAC Inorganic, Isotope, and Actinide Chemistry

Ballard, Beau

- 13** Bulk Production of Generator Parent  $^{72}\text{Se}$  at the Los Alamos IPF using a NaBr Target 13

Daly, Scott R.

- 14** Insights into the Selectivity of Minor Actinide Extractants: Sulfur K-edge X-ray Absorption Spectroscopy and Time Dependent-Density Functional Theory of Dithiophosphinates 14

### C-PCS Physical Chemistry and Applied Spectroscopy

Galland, Christophe

- 15** Single Quantum Dot Spectroelectrochemistry Reveals the Role of Charging in Photoluminescence Blinking 15

Kumar, Sandeep

- 16** High-Throughput Screening of Antibodies against Mycobacterium Tuberculosis Biomarkers 16

Mohite, Aditya

- 17** Observation of Exceptionally Long Minority Carrier Diffusion Lengths in VLS-grown In-Situ Doped Axial Si Nanowire p-n Junctions 17

Park, Young-Shin

- 18** Controlling Radiative and Nonradiative Recombination Pathways of Multi-Excitonic States in Colloidal Nanocrystal Quantum Dots 18

Sakamuri, Rama Murthy

- 19** Binding Of Lipoarabinomannan to Serum High-Density Lipoproteins Decreases its Bioavailability in the Serum of Tuberculosis Patients 19

## COMPUTER, COMPUTATIONAL, AND STATISTICAL SCIENCES DIVISION

### CCS-2 Computational Physics and Methods

Simon, Guillaume

- 20** Interactions between Balanced and Unbalanced Turbulent Cascades; or how Ocean Circulation Equilibrates 20

Wei, Tie

- 21** Effects of Initial Conditions on Single and Two-Mode Rayleigh-Taylor Instability 21

# Table of Contents

Page

---

## DECISION APPLICATIONS DIVISION

### D-5 Nuclear Design and Risk Analysis

Zhou, Wenzhong

- 22 Model and Simulation Code Development for Actinide-Containing Fuels 22

## EARTH AND ENVIRONMENTAL SCIENCES DIVISION

### EES-14 Earth Systems Observations

Aiken, Allison

- 23 Laboratory Studies of the Optical Properties of Warming Aerosols with the SP2 and Photoacoustic Spectrometer: Soot and Hematite 23

Derseh, Rebeka

- 24 Isotopic Tracer for Climate Relevant Secondary Organic Aerosol 24

Flowers, Bradley

- 25 Wavelength-Dependent Optical Properties, Mass Absorption Coefficients, and Closure Studies for Carbonaceous Aerosols: Quantifying Absorption Enhancements of Absorptive and Non-Absorptive Coatings on Black Carbon Particles 25

Gangodagamage, Chandana

- 26 Scaling Laws in Arctic Permafrost River Basins: Statistical Signature in Transition 26

Han, Jiabin

- 27 Effect of Carbonated or Leached Cement on Corrosion of Mild Steel in Simulated Wellbore Systems 27

Xu, Chonggang

- 28 Simulating the Shrub Abundance Increase in the Arctic 28

### EES-16 Computational Earth Sciences

Chen, Min

- 29 Understanding Seasonal and Inter-Annual Lake Area Change Dynamics in Yukon Flats, Alaska 29

Deng, Hailin

- 30 Assessment of Storage Capacity, Injectivity, and Leakage Using Multiscale Reservoir Simulation of CO<sub>2</sub> Sequestration at Rock Springs Uplift, Wyoming 30

Harp, Dylan

- 31 An Agent-Based Approach to Global Uncertainty and Sensitivity Analysis (ABAGUS) 31

Lewis, Kayla

- 32 Soil Subsidence Associated with Permafrost Degradation in the Arctic 32

# Table of Contents

Page

---

## **EES-17 Geophysics**

Lin, Youzuo

- 33** Double-Difference Waveform Inversion with Spatially-Variant Regularization for Quantitative Reservoir Monitoring 33

MacCarthy, Jonathan

- 34** Imaging Lithospheric Structure of Intercontinental Mountains through Simultaneous Inversion of Disparate Geophysical Data Types 34

## **HIGH PERFORMANCE COMPUTING DIVISION**

### **HPC-5 High-Performance Systems Integration**

Manzanares, Adam

- 35** Reducing Concurrency Bottlenecks in Parallel I/O Workloads 35

## **LANL INSTITUTES OFFICE**

Mascarenas, David

- 36** The Development of Active Self-Preservation Policies for Ensuring the Cyber-Physical Security of Unattended, Car-Like, Mobile Sensor Nodes 36

Stull, Christopher

- 37** Toward Quantifying the Predictive Maturity of Computer Codes 38

## **INTERNATIONAL, SPACE, AND RESPONSE DIVISION**

### **ISR-1 Space Science and Applications**

Lasue, Jeremie

- 38** Mars Science Laboratory ChemCam Fast Motion Field Test Results 39

### **ISR-6 High Power Electrodynamics**

Pavlenko, Vitaly

- 39** Superconducting Tunable THz Sources 40

## **LOS ALAMOS NEUTRON SCIENCE CENTER**

### **LANSCE -LC Lujan Center**

Wang, Peng

- 40** High Pressure and High Temperature Neutron Reflectometer Cell for Solid-Fluid Interface Research 41

# Table of Contents

Page

---

## MATERIALS PHYSICS AND APPLICATIONS DIVISION

### MPA-11 Sensors and Electrochemical Devices

|                   |  |    |
|-------------------|--|----|
| Brady, John       |  |    |
| 41                | Acoustic Imaging System for Oil Well Downhole Applications                               | 42 |
| Sturtevant, Blake |  |    |
| 42                | Coupling Layer Corrections in Pulse-Echo Time-of-Flight Measurements in Solids Revisited | 43 |

### MPA-CINT Center for Integrated Nanotechnologies

|                        |   |    |
|------------------------|---|----|
| Cho, Jeong-Hyun        |   |    |
| 43                     | Silicon NW Growth on Metal Substrates for a High Performance Lithium-Ion Battery Anode  | 44 |
| Crochet, Jared         |   |    |
| 44                     | Advanced Microscopic Imaging of Single-Wall Carbon Nanotubes: From One-Dimensional Surface Science to Nano-Scale Rheology             | 45 |
| Dayeh, Shadi           |   |    |
| 45                     | An Atomic Scale Understanding of Defect Nucleation and Propagation in Heterostructure Nanowires                                       | 46 |
| Ghosh, Yagnaseni       |   |    |
| 46                     | Understanding “Giant” Nanocrystal Quantum Dots by Synthetic Manipulations and Spectroscopic Methods                                   | 47 |
| Gilbertson, Steve      |   |    |
| 47                     | Quasiparticle Lifetime Near the Dirac Point in Graphene   | 48 |
| Jung, Jaemyeong        |   |    |
| 48                     | Molecular Level Understanding of Cellulase-Catalyzed Hydrolysis of Cellulose: A Single-Molecule Approach                              | 50 |
| Laocharoensuk, Rawiwan |   |    |
| 49                     | Flow Solution-Liquid-Solid Growth: Novel Solution-Phase Technique for Fabrication of Axially Heterostructured Semiconductor Nanowires | 51 |
| Perea, Daniel          |   |    |
| 50                     | Synthesis of Abrupt Interfaces without Kinking in VLS-Grown Si-Ge Axial Nanowire Heterostructures by Novel In Situ Catalyst Alloying  | 52 |
| Seo, Minah             |   |    |
| 51                     | Polarization Anisotropy of Transient Carrier Dynamics in Single Silicon Nanowire  | 53 |
| Yoo, Jinkyong          |   |    |
| 52                     | Si Nanopillar-Based Radial <i>p-n</i> Junction Photovoltaic Cells   | 54 |

# Table of Contents

Page

---

## MPA-CMMS Condensed Matter and Magnet Science

Beaux, Miles

- 53** Hard X-Ray Photoelectron Spectroscopy and Electronic Structure of Single Crystal UPd<sub>3</sub>, UGe<sub>2</sub>, and USb<sub>2</sub> 55

## MPA-MC Materials Chemistry

Cape, Jonathan

- 54** DNA Aptamer Based Detection of O,O-Dialkyl Halophosphates 56

Jilek, Robert

- 55** New Frontiers in Actinide Imido Chemistry: Preparation and Reactivity of Uranium(IV) Imido Dihalides 57

Lovejoy, Katherine

- 56** Materials Designed for Identification of Forensic Analytes 57

Travia, Nicholas

- 57** Snapshots of Thorium-Mediated THF Ring-Opening Reactions Using bis(pentamethylcyclopentadieny) 58

## MATERIALS SCIENCE AND TECHNOLOGY DIVISION

### MST-7 Polymers and Coatings

Gandham, Lakshminarayana

- 58** Structural, Thermal, and Optical Characterization of Transparent Glass Ceramics Containing LaF<sub>3</sub>: Ce<sup>3+</sup> Nanocrystals for Scintillation Applications 59

### MST-8 Structure/Property Relations

Balogh, Levente

- 59** The Nature of Dislocations in Irradiated Zirconium Determined by Diffraction Line Profile Analysis 60

Escobedo, Juan

- 60** Effects of Grain Size and Boundary Structure on the Dynamic Tensile Response of Copper 61

Fensin, Saryu

- 61** Structure and Shock Response of a Sigma 11 Asymmetric Tilt Grain Boundary in Copper at Finite Temperature 62

Lee, Tongsik

- 62** Atomistic Modeling of the Thermodynamic Equilibrium and Phase Transitions in Solids 63

Martinez Saez, Enrique

- 63** Synchronous Parallel Kinetic Monte Carlo: Diffusion in Heterogeneous Systems 64

Perez-Bergquist, Alejandro

- 64** Grain Boundary Response in Shocked Copper Multicrystals: TEM Characterization and Atomistic Modeling 65

# Table of Contents

Page

---

## NUCLEAR NONPROLIFERATION DIVISION

### N-4 Safeguards and Security Systems

Kutchesfahani, Sara

- 65 How to Strengthen International Safeguards: Moving Forward with the Additional Protocol 66

## PHYSICS DIVISION

### P-21 Applied Modern Physics

Burmistrov, Evgeny

- 66 Helmet Shaped SQUIDS Array for Ultra-Low Field MRI and MEG 67

Chandrana, Chaitanya

- 67 'Shim-a-Ring' Magnets: Coaxial Shimming of Ring Magnets for Nuclear Magnetic Resonance (NMR) and Magnetic Separations 69

Guthormsen, Amy

- 68 Using ERPs to Track the Timecourse of Visual Object Recognition 70

Karaulanov, Todor

- 69 Demonstration of Anatomical Imaging with a Portable Non-Cryogenic Ultra-Low Field MRI System 71

Lybarger, Jr., Warren

- 70 Single-Ion Heisenberg-Limited Quantum Phase Sensors 72

### P-23 Neutron Science and Technology

Balasubramanian, Sridhar

- 71 Initial Condition Effects on Richtmyer-Meshkov Mixing and Turbulence 73

Leftwich, Megan

- 72 Motivation, Design, and Fabrication of the Vertical Shock Tube 74

Pol, Suhas

- 73 Understanding Wind Turbine Fatigue Using Advanced Fluid Diagnostics 75

## THEORETICAL DIVISION

### T-1 Physics and Chemistry of Materials

Borovikov, Valery

- 74 Influence of Interstitials or Vacancies Introduced into Grain Boundary on Sliding Process in bcc Tungsten 76

Matanovic, Ivana

- 75 Theoretical Study of Electrochemical Processes on Novel Platinum Group Metal Catalysts 77

Pierpont, Aaron

- 76 DFT Study of  $\text{Cp}_2\text{Th}$  and  $\text{Cp}_2\text{U}$  Catalysts for Hydrodenitrogenation (HDN) and Hydrodesulfurization (HDS) 78

Wen, Xiaodong

- 77 The High Temperature UC<sub>2</sub> Phase - A Rotational Solid 79

# Table of Contents

---

|  | Page |
|--|------|
| <b>T-4 Physics of Condensed Matter and Complex Systems</b>   |      |
| Haraldsen, Jason   |      |
| 78 Emergent States in Paraelectric and Superconducting Interfaces  | 80   |
| <b>T-5 Applied Mathematics and Plasma Physics</b>  |      |
| Achler, Tsvi   |      |
| 79 Processing Mixtures of Patterns Using Generative Models   | 81   |
| Gutfraind, Alexander   |      |
| 80 The Sendai Network Problem: Optimizing Network Deployment and Recovery  | 81   |
| Ji, Zhengpin   |      |
| 81 Deep Generative Networks as Systems Level Models of Primate Visual Cortex   | 82   |
| <b>T-6 Theoretical Biology and Biophysics</b>  |      |
| Ullah, Ghanim  |      |
| 82 A Data-Driven Model of a Modal Gated Ion Channel: The IP3 Receptor in Insect Sf9 Cells  | 83   |
| Zhang, Jingshan  |      |
| 83 Quantifying the Role of FDC as a Long Term Reservoir of HIV-1 Virus   | 83   |
| <b>WEAPONS EXPERIMENTS DIVISION</b>  |      |
| <b>WX-7 High Explosives Science and Technology</b>   |      |
| Duque, Amanda  |      |
| 84 Temperature Measurements of High Explosives Under Microwave Irradiation for Kinetic Analysis of Thermally Induced Transitions | 84   |
| <b>WX-9 Shock and Detonation Physics</b>   |      |
| Dang, Nhan   |      |
| 85 Picosecond Temperature Measurement in Condensed Phases  | 86   |
| Johnson, Carl  |      |
| 86 Revisiting the Munroe Effect, New Experiments and Applications  | 87   |

# Table of Contents

Page

---

## X-COMPUTATIONAL PHYSICS

### **XCP-4 Methods and Algorithms**

Lee, Amy

**87** Modeling the Response of Glazing to Blast Loading 88

### **XCP-5 Materials and Physical Data**

Starrett, Charles

**88** Many Body Correlations in a Variational Average Atom 89

### **XCP-6 Plasma Theory and Applications**

Huang, Chengkun

**89** A Double-Foil Target for Improving Beam Quality in Laser Ion Acceleration with Thin Foils 90



## Accelerator Operations and Technology Division AOT-ABS

|                 |   |                |
|-----------------|---|----------------|
| Name            | Jeff Kolski   | LA-UR 11-10015 |
| Group:          | AOT-ABS   |                |
| Mentor:         | Ken Johnson, Thomas Spickermann, and Rodney McCrady   |                |
| Field of Study: | Physics   |                |
| Discipline:     | Accelerator Physics   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Application of Independent Component Analysis (ICA) to Long Bunch Beams in the Los Alamos Proton Storage Ring |                |

### ABSTRACT

Independent component analysis (ICA) has been applied successfully in several accelerators as a means of measuring the transverse betatron phase and amplitude functions, dispersion function, linear coupling, and sextupole strength. The typical method for applying ICA in accelerators analyzes simultaneously measured turn-by-turn beam position data. However, this traditional method of ICA application is not feasible in the Los Alamos Proton Storage Ring (PSR) because the beam position measurement diagnostic system makes use of a matrix switch such that data may only be collected at one monitor at a time. A new method for applying ICA in the Proton Storage Ring is developed, which analyzes longitudinal beam signals digitized for an entire machine cycle. This new method for the application of ICA along the beam pulse is applied to real data and several of the independent modes are experimentally verified.

## Bioscience Division

### B-6

|                 |   |                |
|-----------------|---|----------------|
| Name            | Nicholas Beckloff                             | LA-UR 11-03048 |
| Group:          | B-6   |                |
| Mentor:         | Patrick Chain                                 |                |
| Field of Study: | Bioscience                                    |                |
| Discipline:     | Bioscience                                    |                |
| Appointment:    | Postdoctoral Research Associate               |                |
| Poster Title:   | Discovery of Novel sRNAs from Yersinia Pestis |                |

#### ABSTRACT

The discovery of small RNAs (sRNAs) and their important function in gene regulation has dramatically increased due in part to the implementation of next generation sequencing (NGS) technologies. sRNAs are widespread effectors of post-transcriptional gene regulation in bacteria. Currently minimal information exists on the expression of sRNAs in *Yersinia pestis*, the causative agent of plague. We are interested in their potential role in pathogenicity, thus are exploring their expression using RNA-Seq under conditions mimicking its natural lifecycle within human host (37°C and infection of macrophages) and within the flea vector (26°C). Illumina libraries were prepared from total RNA isolated from *Y. pestis* infected macrophages and sequenced using the Illumina HiSeq2000. Several of the libraries were prepared from enriched mRNA and size selected sRNA protocols. The reads were mapped to reference genomes and the effect of the various protocols ascertained based on mapping statistics. The sRNAs were predicted using a computational model consisting of analysis of intergenic read coverage and gene and transcript expression data. Here, we will describe the project, and resulting identification of putative novel sRNAs that are expressed under conditions mimicking mammalian host infection.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Armand Dichosa  | LA-UR 11-10700 |
| Group:          | B-6   |                |
| Mentor:         | Cliff Han and Chris Detter  |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Single Cell Genomics  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Inducing Artificial Polyploidy in <i>Bacillus Subtilis</i> : Implications to Advance Single Cell Genomics |                |

## ABSTRACT

Genomic amplification can be accomplished through multiple displacement amplification (MDA), an isothermal reaction involving the  $\Phi$ 29 DNA polymerase and a circular chromosomal template. This process has allowed researchers to yield micrograms of genomic amplicons from a single chromosome copy. As such, MDA with current approaches to single cell isolation and much sequencing efforts have made it possible to determine bacterial/archaeal phylotypes and metagenomic profiles from an environmental sample in situ without the need for cultivation. However, inherent issues surrounding MDA when using a single chromosomal template make it difficult to obtain an accurate genomic profile. In particular, low genomic coverage and gaps observed in the assembled genome are due to uneven amplification and biases. To complete the genomic assembly, additional genomic template and labor are needed.

Our prior investigations have shown that increasing the number of chromosomal template greatly reduces the observed gaps in the assembled genome, thereby producing a more complete genomic profile. However, isolating an adequate number of the exact species/strain from an environmental sample without cultivation is in itself difficult. Consequently, we hypothesized that simultaneously inhibiting bacterial cells from completing cytokinesis while maintaining viability will phenotypically result in cells that are larger-than-normal and possess at least two complete copies of its chromosome. To test our hypothesis, we used PC190723 to prevent *Bacillus subtilis* ATCC 6633 from completing cytokinesis. PC190723 is an antimicrobial compound known to inhibit FtsZ, the bacterial and euryarchaeal protein that is largely implicated in cell division. Cytographic data via flow cytometry have shown that *B. subtilis* responds to PC190723 treatment with increased cell size, while microscopy evidence verifies the treated cells to be at least double in size to the untreated controls. Our qPCR analyses of sorted cells quantified more genomic content and four times less amplification bias from the inhibited cells. Ultimately, de novo genomic assemblies suggest that a single polyploid *B. subtilis* cell contributes 17% more genomic coverage than an untreated cell. Our study implies that similar FtsZ-inhibitors, whether singly or in combination, can be used to induce artificial polyploidy in a microbial community, and, when utilized with high-throughput, FACS-based analyses, a more complete genomic and/or metagenomic profile can be achieved with greater efficiency.

## B-7

|                 |   |                |
|-----------------|---|----------------|
| Name            | Nan Li  | LA-UR 11-02971 |
| Group:          | B-7   |                |
| Mentor(s):      | Elizabeth Hong-Geller and Anu Chaudhary                       |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Molecular Biology   |                |
| Appointment:    | Postdoctoral Research Associate                               |                |
| Poster Title:   | Functional Discovery of Host Small RNAs in Infectious Disease |                |

### ABSTRACT

A major breakthrough in molecular biology during the last decade is the discovery of small RNAs, especially microRNAs (miRNAs), a novel class of RNAs that do not encode for proteins, but instead function as regulatory biomolecules to directly control gene expression. miRNAs are extensively conserved throughout evolution and are extremely critical for normal cell function. For example, human miRNAs have been implicated as major regulators in cancer and have been developed as biomarkers for cancer diagnosis and prognosis and as potential therapeutic targets for cancer treatment. However, miRNA function during host defense to biothreat pathogen infection has been poorly characterized. Given that conventional antibiotics that target conserved protein molecules have been continuously challenged by accelerated bacterial evolution to produce drug-resistant pathogens, RNA represents a largely unexploited category of potential targets for antimicrobial design. Here, our ultimate goal is, by fundamental analysis of miRNA function during host-pathogen interactions, to develop next-generation antibiotics using miRNA as therapeutic targets. In this work, we will investigate the expression and function of host miRNAs during infection by Select Agent pathogen *Yersinia pestis* and pathogen *Yersinia enterocolitica*, the causative agents of plague and yersiniosis, respectively. We will first interrogate expression levels of host miRNAs before and after infection using microRNA microarray analysis. Significantly altered miRNAs during pathogen infection will then be subject to functional characterization via loss of function strategy through high-throughput, high-content cellular analysis techniques. Candidate miRNAs that appear to play essential roles in host immune response will serve as targets for further design of small molecule therapeutic inhibitors. This work will advance not only our understanding of the molecular mechanism of host-pathogen interaction, but also the development of small RNAs as novel therapeutic targets for antibiotic discovery.

Name: Sofiya Micheva-Viteva

LA-UR 10-02021

Group: B-7

Mentor: Elizabeth Hong-Geller

Field of Study: Bioscience

Discipline: Biosecurity and Human Health

Appointment: Postdoctoral Research Associate

Poster Title: RNAi-Based HTS to Identify Human Host Factors Involved in Yersinia Virulence

## ABSTRACT

Microbial pathogens have developed intricate mechanisms for subversion of host immune defense system by direct interaction with specific host factors. Host proteins that are manipulated by pathogens for successful infection can be targeted for development of novel therapeutics. To identify host proteins essential for microbial pathogenicity, we have established a platform for genome-wide loss-of-function high-throughput screens (HTS) employing RNA interference (RNAi). We have focused our studies on *Yersinia* spp because of their high virulence and potential threat for social devastation in case of intentional release of weaponized multi-drug resistance strains. We have performed high throughput shRNA-based functional genomics studies applying two commercial sub-libraries covering about 8,000 human genes. To ensure a robust assay in 96-well HTS format, we have established cell-based model system using infection with whole, live pathogen. We have screened 2103 constructs targeting 757 human kinase genes and 20 genes from the human chaperone family and have identified 21 host factors as high confidence ‘hits’ in our *Y. enterocolitica*-based infectivity assays. Among the initial hits from the genomic screen were HSP90, HSPH1, and CK2 which downregulation improved viability of HeLa and HEK-based cell lines upon *Y. enterocolitica* and *Y. pestis* infection at MOI 50 and 100, respectively. Using small molecule inhibitor against HSP90 (17-AAG, Sigma) and CK2 (TBB, Sigma) we obtained significantly higher percentage primary human dendritic cells (HDC) surviving the impact of *Yersinia* infection. Additionally, we have identified host factors such as SGK1, WNK1, and c-KIT which downregulation in epithelial cells antagonized the inhibitory effect of *Yersinia* infection on NFκB signaling. Applying highly specific kinase inhibitors we have validated c-KIT and CK2 as host factors utilized by *Y. pestis* and *Y. enterocolitica* in order to downregulate cytokine and chemokine release by primary HDC. We have discovered host biomarkers that can be used as candidates for novel therapeutic strategies against *Yersinia pestis* infection. We are currently testing if the kinase inhibitors antagonizing *Yersinia* sp-driven downregulation of cytokine release by host immune cells can act as broad spectrum antimicrobials.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Amber Nagy   | LA-UR-11-10626 |
| Group:          | B-7  |                |
| Mentor(s):      | Rashi Iyer and Bob Williams  |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Nanotoxicology   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Cytotoxicity of Quantum Dots in Normal Human Bronchial Epithelial Cells:<br>Comparisons of Core Type and Functionalization |                |

## ABSTRACT

Quantum dots (QDs) are semiconductor nanocrystals possessing unique optical properties and can be used for a wide variety of applications, from photovoltaics to biomedicine. The physicochemical properties of QDs, such as size, charge, functionalization, composition and redox activity all impact their interactions with biological systems and eventually dictate their utility. In our project we attempt to understand and correlate the effect of each of these individual properties to specific or types of biological responses. Because inhalation is a key route of exposure and Cadmium (in bulk form) has been found to cause lung cancer, primary normal human bronchial epithelial (NHBE) cells were exposed to well-characterized QDs functionalized with either mercaptopropionic acid (MPA) or mercaptoundecanoic acid (MUA) to obtain negatively-charged QDs of varying compositions (CdSe, CdTe and InP) and sizes (3 nm and 5 nm). Cellular parameters including the generation of reactive oxygen species (ROS), necrosis, apoptosis and proliferation were examined.

Our studies demonstrate that at low concentrations CdSe-MUA QDs do not induce significant necrosis or apoptosis, but at higher concentrations a significant increase in apoptosis was observed with a simultaneous decrease in proliferation. Furthermore, the apoptotic response may be potentially correlated to the ability of the CdSe-MUA QDs to induce an intracellular ROS response. In contrast, the CdSe-MPA QDs treated cells demonstrated a size-dependent increase in proliferation with a concurrent but slight increase in ROS levels, suggesting that the nature of the ligand may impact cellular responses. Interestingly, CdTe QDs caused a size- and ligand-independent increase in cell proliferation. Finally, InP QDs did not induce any notable cellular cytotoxicity, irrespective of size, dose and surface ligand.

In summary, composition appears to be a deciding factor in the ability of QDs to induce cellular level toxic response; however, our proliferation results suggest that size and ligand nature might play a role in more subtle cellular responses, albeit this may very well be a function of dose.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Mark Wolfenden  | LA-UR 10-03060 |
| Group:          | B-7   |                |
| Mentor(s):      | Jurgen Schmidt and David Kimball  |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Bioorganic Chemistry  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Siderophores for Pathogen Capture and Radioisotope assisted Diagnostics |                |

## ABSTRACT

Long identified as important iron binding species, siderophores (SDPs) have recently gained popularity as key targets for identification and treatment of various pathogens. There are currently over 500 identified SDPs which are secreted by and specific to pathogens and bind iron, for acquisition, with dissociation constants as low as  $10^{-59}$  M<sup>-1</sup>. Siderophores are actively internalized and therefore allow selective interrogation of intact pathogens over pathogen debris. We present our recent results in syntheses towards siderophore mimetics that will allow the immobilization of bacteria on surfaces for sensors. Iron recruiting mechanisms can be exploited for delivering a radioisotope to intact pathogens. The potential of this approach for in vivo PET imaging of multi- and extended extensive drug resistant bacteria will be discussed. We will show how such delivery of isotopes can be deployed for theragnostic approaches to combat resistant, difficult to culture and detect pathogens of emerging concern for public health and biosecurity.

## B-8

|                 |  |                |
|-----------------|--|----------------|
| Name            | Marc-Michael Blum  | LA-UR 11-02687 |
| Group:          | B-7/B-8  |                |
| Mentor:         | Bob F. Williams and Cliff Unkefer  |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Protein Engineering  |                |
| Appointment:    | Director's Postdoctoral Fellow   |                |
| Poster Title:   | Engineering of Diisopropyl Fluorophosphatase for Enhanced Activity Against V-type Nerve Agents |                |

### ABSTRACT

Despite being banned under the Chemical Weapons Convention (CWC) highly toxic organophosphorus nerve agents like sarin (GB), soman (GD) or VX still pose a credible threat to military personnel and civilian populations. Therefore defensive research programs try to improve detection, protection and means of decontamination as well as medical therapies for the treatment of nerve agent poisoning. Current treatment of nerve agent poisoning include administration of atropine in combination with AChE-reactivating oximes and anticonvulsants like benzodiazepines. New forms of therapy are highly desirable as some agents are resistant to oxime reactivation. The enzyme DFPase from *Loligo vulgaris* is highly effective against G-type nerve agents and rational engineering efforts have recently lead to enzyme mutants with further enhanced activity and for the first time a small but distinct activity against V-type nerve agents (VX and two VX variants). Also the mutants show a preference for the more toxic enantiomers of the agents. Using these mutants as a starting point we aim to enhance activity against the V-agents as well as to reduce the  $K_M$  value of the mutants to ensure activity also at the comparably small agent concentrations found in vivo.

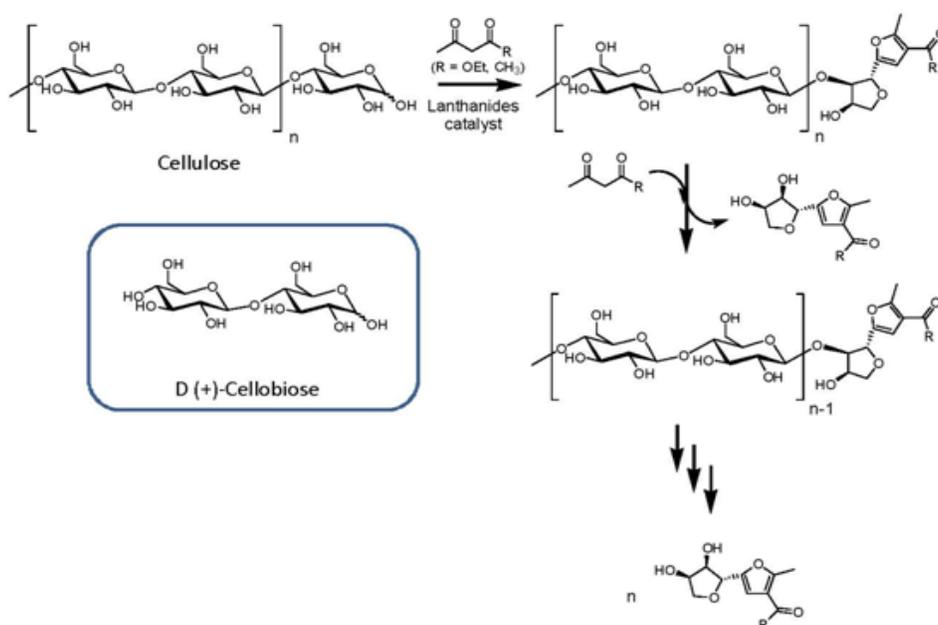
|                 |  |                |
|-----------------|--|----------------|
| Name            | Jin Kyung Kim  | LA-UR 11-10558 |
| Group:          | B-8  |                |
| Mentor:         | Pete Silks   |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Synthetic Organic Chemistry  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Model System Studies of Cellulose Conversion to Biofuel via Garcia-Gonzalez Reaction |                |

## ABSTRACT

The chemical conversion of cellulose to renewable fuel components has received attention worldwide, as a part of researches utilizing biomass for alternative energy resources. Direct catalytic conversion of cellulose (6 carbons in monomer unit, glucopyranose) into high density fuels (8-15 carbon chains) has a significant importance. This process will benefit cost reduction and environmental impacts of extensive treatments of cellulosic biomass to its monomer or other building block compounds.

We adopted Garcia-Gonzalez reaction, a Knoevenagel type carbon-carbon bond formation of unprotected sugars and dicarbonyl compounds, for catalytic carbon chain extension. Cellobiose (2 glucose units) was chosen for its good solubility and for the quantitative investigation. Various lanthanides (Lu, Gd, Eu, Ce) were tested as catalysts, as they can be used in aqueous media and are orally nontoxic. Reaction of cellobiose with dicarbonyl compounds (5 carbons) such as ethyl acetoacetate or 2,4-pentadione gave the (glucosyltetrahydrofuran)luran, followed by glycosidic bond cleavage generated the trisubstituted furan (11 carbons). The reactions can be completed either by prolonged heating at relatively mild temperature (90 °C) or conveniently by the microwave reactor.

We speculate that this process can be applied to the cellulose conversion directly, with the convenient methods of dissolving cellulose being established.



|                 |  |                |
|-----------------|--|----------------|
| Name            | Alex Koglin  | LA-UR 11-03048 |
| Group:          | B-8/B-7  |                |
| Mentor(s):      | Cliff Unkefer and Bob Williams   |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Structural Biology, Natural Product Biosynthesis, Organic Synthesis: Selective Isotopic Labeling   |                |
| Appointment:    | Oppenheimer Distinguished Postdoctoral Fellow  |                |
| Poster Title:   | Novel Methods to Investigate Structures and Structural Dynamics of Very Large Proteins by NMR Spectroscopy: Assembly and Alteration of Antibiotic Biosynthesis |                |

## ABSTRACT

Natural products or structural derivatives of those span a wide variety of medicinal activities and ranges from antibiotics, anti-tumor drugs, immunosuppressants, and chemotherapeutics to compounds with antipyretic and analgesic properties and further includes bacterial or fungal toxins, venoms and virulence factors. This includes the vast majority of established antibiotics such as erythromycin, tetracycline, penicillins, macrolide antibiotics and vancomycin; immunosuppressives such as rapamycin, ciclosporin and FK506, or anticancer agents such as taxol, bleomycin and the adriamycin/ daunomycin class of anthracyclines like doxorubicin.

In particular, the discovery of antibiotics transformed medicine dramatically by providing efficient treatment options against often fatal bacterial infections. The recent and accelerated emergence of multi-drug antibiotic resistance significantly reduces the availability of effective treatments. Bacterial infections have become once more major public health threats and our arsenal for fighting bacterial infections now has critical gaps and new antibiotics are urgently needed. In general, antibiotics are secondary metabolites and they derive from Non-Ribosomal Peptide Synthetases (NRPS). Their biosynthetic processing is accomplished on multi-functional enzymatic complexes as series biosynthetic steps along assembly line protein clusters that can reach the Mega-Dalton range. Today, only a marginal amount of those bioactive compounds produced by micro-organisms using this logic have been explored even though they provide an incredible arsenal for potential new drugs.

Understanding the general structural principles, the inter-protein communications and mechanisms by which substrates are specifically recognized and incorporated may allow the exploration of genetically encoded clusters for engineering of natural product assembly lines for the biosynthesis of novel bioactive compounds that could alleviate the emergence of multiple and extreme drug resistance against the majority of established antibiotics including last resort treatments.

Name: Ricardo Marti-Arbona LA-UR-11-10611  
Group: B-8  
Mentor: Pat Unkefer  
Field of Study: Bioscience  
Discipline: Protein Chemistry  
Appointment: Postdoctoral Research Associate  
Poster Title: A Systematic Approach to Transcriptional Regulator Function Discovery: Novel Effectors for an Old Regulator (MetJ) and Function Discovery for Bxe\_B3018 and Bxe\_A0425

## ABSTRACT

Transcriptional Regulators (TRs) have evolved to regulate and control the physiological processes that dictate phenotypic traits. Regulation occurs in response to stimuli, this response manifests itself in the binding of a Transcriptional Regulator Effector molecule (TRE) by the TR. This binding modulates the affinity of the TRE/TRs binary complex for its specific DNA Operator Sequence (DOS) in the promoter region normally upstream of genes to either facilitate or inhibit transcription. Previously, no systematic approach has been successfully applied to the discovery of TRE/TRs binary complexes. Utilizing Frontal Affinity Chromatography coupled to Mass Spectrometry detection (FAC-MS), we have developed a High-Throughput System (HTS) for the discovery and characterization of small-molecules that modulate TR binding to TR targets. In the FAC-MS-based approach, proteins are immobilized on liquid chromatography columns and a mixture of potential ligands is continuously infused through the column and into the electrospray mass spectrometer. We tested this approach using the transcriptional regulator MetJ. Consistent with previous studies, FAC-MS showed that S-adenosyl-L-methionine from our metabolite library bound to MetJ with the highest affinity. In addition, we have shown that adenine and 5'-deoxy-5'-(methylthio) adenosine bind to the effector binding-site on MetJ. We have demonstrated the ability of FAC-MS to screen complex mixtures of molecules and identify high-affinity binders to TRs.

Our results from the MetJ experiments validate the potential of FAC-MS as a high-throughput approach for the discovery of effector molecules and characterization of effector/TR binding for TRs of unknown function. Function prediction and possible effector library formulation are key factors in the discovery of the biological function of TRs. Potential effectors are predicted by the identification of functional patterns within the proteins found in the genomic proximity of the TR of interest. These patterns can suggest involvement of the TR on the regulation of specific metabolic pathways. Utilizing this approach, we have predicted the metabolic pathway regulated by the previously unknown function TR Bxe\_B3018 from *Burkholderia xenovorans*. FAC-MS has confirmed the prediction by identifying two TREs for Bxe\_B3018. Aminoacetone and Aminopropan-2-ol are tight binders to Bxe\_B3018 and a Protein Binding Microarray (PBM) has identified its DOS as 5'-AGAANNNNNTTCT-3'. Fluorescence Polarization (FP) experiments have shown that Aminoacetone and Methylglyoxal, as well as other Aminoacetone analogs disrupt the affinity of Bxe\_B3018 for its DOS, while Aminopropan-2-ol does not. There are also cases in where no functional prediction can be achieved with our comparative analysis of sequence and genomic functionality context. Bxe\_A0425 is a vivid example of these, by screening complex mixtures of metabolites with our FAC-MS HTS we have identified Choline as a tight binder ligand and PBM has identified its DOS as 5'-TGTTANNNNNNNNNNNTAACA-3'. These findings validate the effectiveness of our systematic approach to TRE discovery and open the door to a new era of protein function discovery and greater understanding of metabolic regulation.

## B-9

|                 |  |                |
|-----------------|--|----------------|
| Name            | Hau Nguyen   | LA-UR 11-03125 |
| Group:          | B-9/INST-OFF   |                |
| Mentor(s):      | Geoff Waldo and Tom Terwilliger  |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Protein Engineering  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Protein Domain Trapping Method: In Search of Compact, Soluble Protein Fragments for Structural Biology |                |

### ABSTRACT

Structural characterization of large, multi-domain proteins is still a challenge for both crystallography and solution NMR spectroscopy. While the big size of a full-length protein is not feasible for NMR, the solubility of the full length construct and the low expression level often are obstacles for crystallization. The individual domains of these proteins, however usually have interesting structures and functions. Their smaller sizes and better stability levels make them ideal candidates for structural characterization by both solution NMR and crystallography. We present here a robust, high-throughput method to screen for in-frame, compact soluble domains suitable for structural characterization from large, multi-domain proteins. Our domain trapping strategy was tested on a regulatory subunit p85 $\alpha$  of PI3K, an ideal benchmark considering its folded SH3 [1], BCR [2], N-SH2 [3], and C-SH2 [4,5] domains have been structurally-characterized. The method was also applied to identify sets of compact soluble domains for PpsC, a polyketide synthase containing 2188 residues from *Mycobacterium tuberculosis*.

Our screening strategy relies on two in-house technologies: a DHFR insertional vector that uses low concentrations of the inhibitor trimethoprim to select for in-frame fragments, and the split-GFP assay to select for clones expressing soluble fragments [6]. Clones displaying a wide range of fluorescence were picked from the agar plates and grown in 96 well liquid cultures. DNA sequencing was used to determine the boundaries of each fragment by aligning them to the parent gene and all fragment were color coded by their solubility levels. To test whether soluble protein fragments identified by this method are well folded in the absence of GFP11 tag, selected compact soluble fragments were sub-cloned into a His tag expression vector and prepared for 2D solution NMR experiments. <sup>1</sup>H-<sup>15</sup>N HSQC spectra of these compact soluble protein fragments are well dispersed indicating that these protein fragments are well folded and are good candidates for structural characterization by both NMR spectroscopy and crystallography.

### Acknowledgements

This work was supported by the NIH Protein Structure Initiative (U54 GM074946-01US)

### References

- [1] Booker, G.W. et al. *Cell* 73, 813-822 (1993)
- [2] Musacchio, A. et al. *Proc Natl Acad Sci U S A* 93, 14373-14378 (1996)
- [3] Booker, G.W. et al. *Nature* 358, 684-687 (1992)
- [4] Siegal, G. et al. *J Mol Biol* 276, 461-478 (1998)
- [5] Hoedemaeker, F.J. et al. *J Mol Biol* 292, 763-770 (1999)
- [6] Cabantous et al. *Nat Biotech* 23 (1), 102-107 (2005)

## Chemistry Division C-IIAC

|                 |  |                |
|-----------------|--|----------------|
| Name            | Beau Ballard   | LA-UR 11-02648 |
| Group:          | C-IIAC/SPO-SC  |                |
| Mentor(s):      | Eva Birnbaum, Michael Fassbender, and Kevin John   |                |
| Field of Study: | Chemistry  |                |
| Discipline:     | Isotope Production   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Bulk Production of Generator Parent $^{72}\text{Se}$ at the Los Alamos IPF using a NaBr Target |                |

### ABSTRACT

Generator radionuclides constitute a convenient tool for applications in nuclear medicine. Arsenic-72 (half life 26 h) is a medium-lived positron emitting radionuclide for PET imaging that can be produced as a daughter of  $^{72}\text{Se}$  (half life 8.5 d). A  $^{72}\text{Se}/^{72}\text{As}$  generator system would be suitable for hospital on-site utilization. No portable  $^{72}\text{Se}/^{72}\text{As}$  generator system is available on the market for convenient, repeated  $^{72}\text{As}$  elution at the point of care (“milking”). Radionuclide generator principles for  $^{72}\text{Se}/^{72}\text{As}$  have been proposed in the literature, including repeated distillation of “grown-in”  $^{72}\text{AsCl}_3$  from carrier added  $^{72}\text{Se}$  stock solutions, electroplating of  $^{72}\text{Se}$  as  $\text{Cu}_2\text{Se}$  on Cu backings, and solid phase extraction of  $^{72}\text{Se}$ . We describe a  $^{72}\text{Se}/^{72}\text{As}$  generator system analogous to a well-developed commercial  $^{82}\text{Sr}/^{82}\text{Rb}$  generator system.

Production of the parent  $^{72}\text{Se}$  via 90 MeV proton bombardment of a natural NaBr target has been successfully demonstrated at the Los Alamos National Laboratory’s Isotope Production Facility (LANL-IPF) following a thorough target safety analysis for high beam currents.

Safety analysis included a high intensity beam thermal study and product nuclide estimates utilizing Monte Carlo code MCNPX. The thermal study illustrated the high thermal stability with good thermal contact being maintained throughout the irradiation, results will be presented. The  $^{72}\text{Se}$  from proton irradiated NaBr targets was chemically recovered at the LANL Hot Cell Facility in good yield (94%). Good agreement of theoretical thick yields and experimental results were obtained. Batch recovery of  $^{72}\text{As}$  via liquid-liquid extraction was also effective at 76% yield, with minimal breakthrough of the  $^{72}\text{Se}$  parent (0.9%). Moreover, the feasibility of a solid phase generator system will be discussed.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Scott R. Daly   | LA-UR 11-03048 |
| Group:          | C-IIAC/INST-OFF   |                |
| Mentor(s):      | Stosh Kozimor and Dave Clark  |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Inorganic Chemistry   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Insights into the Selectivity of Minor Actinide Extractants: Sulfur K-edge X-ray Absorption Spectroscopy and Time Dependent-Density Functional Theory of Dithiophosphinates |                |

## ABSTRACT

Strategic goals of the U.S. Department of Energy include the implementation of an efficient closed nuclear fuel cycle encompassing proliferation-resistant separation technologies. In this context, one significant challenge is the efficient separation of trivalent actinides from lanthanide ions, a separation hampered by the similar chemical properties shared by the 5f- and 4f-elements. In certain cases, and for reasons not well understood, soft-donor ligands (e.g., dithiophosphinates) preferentially bind actinides over lanthanides, providing separation factors as high as 100,000. It is likely that this preference stems from increased covalent bonding with actinides vs. lanthanides, but despite decades of study detailed understanding of f-element participation in covalent bonding remains elusive. Until recently, experimentally determining the degree of covalency of a given bond has been difficult. This situation was altered by the pioneering work of Solomon, Hedman, and Hodgson who developed the use of ligand K-edge X-ray Absorption Spectroscopy (XAS) to directly measure covalency in bonding (Solomon, E. I. et al. *Coord. Chem. Rev.* 2005, 249, 97). In this contribution we will discuss the use of S K-edge XAS in conjunction with time dependent-density functional theory (TD-DFT) to evaluate a recently synthesized family of dithiophosphinate complexes. Specifically, we will (1) identify changes in the electronic structure of the M-S and P-S bonds as the phosphorus substituents are systematically varied and (2) investigate the relative roles of 3d, 4d, 5d, and 6d/5f-orbitals in M-S bonding. Electronic features unique to dithiophosphinates known to exhibit high separation factors will be highlighted and rationalized in terms of molecular orbital theory.

## C-PCS

|                 |   |                |
|-----------------|---|----------------|
| Name            | Christophe Galland  | LA-UR 10-08470 |
| Group:          | C-PCS   |                |
| Mentor(s):      | Victor Klimov and Han Htoon   |                |
| Field of Study: | Physics   |                |
| Discipline:     | Optical Spectroscopy - Nanomaterials  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Single Quantum Dot Spectroelectrochemistry Reveals the Role of Charging in Photoluminescence Blinking |                |

### ABSTRACT

Photoluminescence (PL) intermittency (blinking) is a universal property of molecular emitters. It has been observed for fluorescent molecules and artificial nanostructures such as nanocrystal quantum dots, carbon nanotubes, and nanowires. The occurrence of OFF periods in nanocrystal emission has been commonly attributed to the presence of an additional charge, which leads to PL quenching by nonradiative Auger recombination. However, the "charging" model was recently challenged in several reports.

Here, to clarify the role of charging in PL intermittency, we perform time-resolved PL studies of individual nanocrystals (Fig. 2) while controlling electrochemically the degree of their charging [1] (Fig. 1). We find that two distinct mechanisms can lead to PL intermittency. We identify conventional blinking (A-type) due to charging/discharging of the nanocrystal core when lower PL intensities correlate with shorter PL lifetimes (Fig. 3). Importantly, we observe a different blinking (B-type), when large changes in the PL intensity are not accompanied by significant changes in PL dynamics (Fig. 4). We attribute this blinking behavior to charge fluctuations in the electron-accepting surface sites. When unoccupied, these sites intercept hot electrons before they relax into emitting core states. Both blinking mechanisms can be controlled electrochemically and under appropriate potential blinking can be completely suppressed. These results offer an explanation to recent controversial observations on PL intermittency and should assist in the development of nanocrystals with stable, blinking-free emission for applications from quantum information to high-sensitivity detection of chemical reagents and tracking of biological molecules.

### References:

- [1] C. Galland, *et al.*, *Submitted*, (2011).

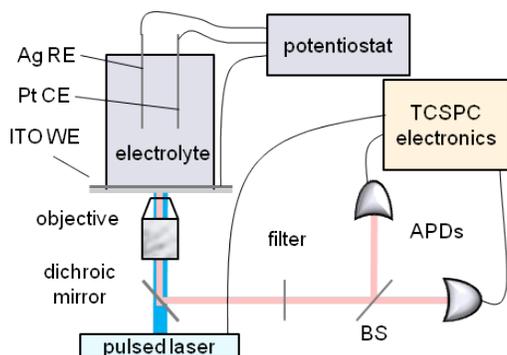


Fig. 1:  
Spectroelectrochemical setup

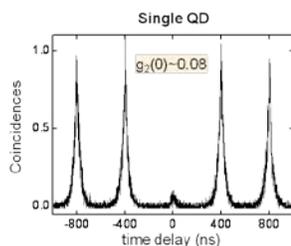


Fig. 2:  
Photon antibunching  
= single emitter

Fig. 3: A-type blinking

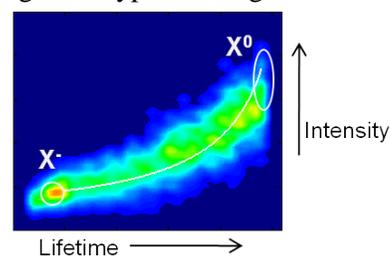
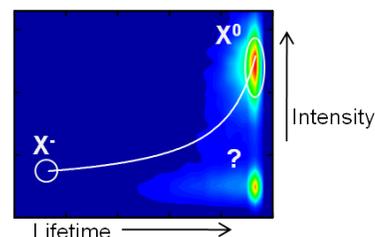


Fig. 4: B-type blinking



|                 |   |                |
|-----------------|---|----------------|
| Name:           | Sandeep Kumar   | LA-UR-11-10605 |
| Group:          | C-PCS/C-DO  |                |
| Mentor(s):      | Harshini Mukundan and Basil Swanson   |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Protein Engineering   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | High-Throughput Screening of Antibodies against Mycobacterium Tuberculosis Biomarkers |                |

## ABSTRACT

Tuberculosis (Tb) is a global health challenge with about an estimated one-third of the world population affected by it. Rapid diagnosis of Tb is important to prevent the spread of the disease as well as for global surveillance efforts. Current diagnostic methods for Tb, such as smear test, are time-consuming and often associated with high false positives and negatives. Recent focus on detection of pathogen and host biomarkers offers a robust and reliable detection strategy, but is limited by low sensitivity and specificity of the detection platform and available recognition ligands (e.g. antibodies). The Biosensor team at LANL has developed a fast and sensitive waveguide-based optical biosensor platform for the detection of *M. tuberculosis* (MTb)-associated biomarkers. However, for a successful implementation of this platform, there is a great need for sensitive and selective recognition ligands for the mycobacterial biomarkers such as Antigen 85 complex, the 6 kDa early secretory antigenic target (ESAT6), and culture filtrate protein-10 kDa (CFP-10). These antigens represent the major proteins in the culture filtrate of MTb, and critical virulence factors in disease pathology.

Most detection platforms employ monoclonal antibodies (mAbs) as capture ligands for the biomarkers. Traditionally mAbs are produced by immunization or using hybridoma-cell technology, which are relatively expensive and time-consuming. Here, we have utilized recombinant antibody libraries for the selection of specific antibodies against these biomarkers using a combination of phage display and yeast display platforms, in which phenotype and genotype are physically coupled and screened for binding to the target antigen(s). Phage display allows us to screen big libraries and identify a smaller pool of clones that can be easily subcloned in the yeast display system. The yeast-based platform allows us to screen thousands of clones in a high-throughput manner by flow cytometry, selecting those with both high specificity and high expression levels. Our results show that the antibodies selected against Ag85 Complex have very high affinity towards the target antigen, ranging from 50-200 nM binding affinity, and display very low non-specific binding in complex matrices such as serum. We have also selected mAbs against ESAT6 and CFP10 biomarker proteins. Further evaluations of their binding affinities towards the target antigens are currently underway. Our future goals include selection of antibodies that are specific to MTb and not cross-reactive with proteins from other mycobacterial species, as is required for enhanced assay specificity.

Name: Aditya Mohite LA-UR 11-02971  
Group: C-PCS/MPA-CINT  
Mentor: Han Htoon and Tom Picraux  
Field of Study: Physics  
Discipline: Electrical Engineering  
Appointment: Postdoctoral Research Associate  
Poster Title: Observation of Exceptionally Long Minority Carrier Diffusion Lengths in VLS-grown In-Situ Doped Axial Si Nanowire p-n Junctions

## ABSTRACT

VLS-grown semiconductor nanowires have emerged as for a viable prospect for future solar-based energy applications. Despite tremendous efforts invested in all areas of nanowire research, the fundamental processes critical to the functioning of a nanowire photovoltaic device such as charge dissociation, collection and recombination processes of photo-generated carriers in nanowires is still poorly understood. A direct measurement of the minority carrier diffusion lengths, and quantitative assessment of the impact of doping and diameter, is of critical importance in understanding and designing efficient 1D photovoltaic devices. To date, there have been a few published studies which report minority carrier diffusion lengths and carrier lifetimes in semiconductor nanowires, however to our knowledge no measurement has been reported for an in-situ doped, Au catalyzed VLS grown axial p-n junction nanowires. Here, we report a scanning photocurrent spectroscopy study of VLS-grown p-n junction silicon nanowires to measure the minority carrier diffusion length of the photo-generated carriers.

Photocurrent measurement studies were performed on in-situ doped Si nanowire p-n junctions and devices with Ni ohmic contacts probed separately to the p- and n-segments of the devices for p-n junction assessment as well as the field-effect properties of either segments of the junction. The measured photoresponse shows an exponential increase in the photocurrent by an order of magnitude as the laser spot ( $\lambda=532$  nm) is scanned across the p-n junction with a peak photocurrent at the center of the junction and an exponential decrease on either side as the laser spot departs from the junction. We measure minority carrier diffusion lengths ( $L_e \sim 1$  micron and  $L_h \sim 0.6$  microns), which are an order of magnitude higher than reported previously suggesting that the nanowire surface is well passivated. We also measured an external quantum efficiency (EQE) of 50%, which suggests that the nanowires have good intrinsic properties.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Young-Shin Park   | LA-UR 11-03125 |
| Group:          | C-PCS   |                |
| Mentor(s):      | Han Htoon   |                |
| Field of Study: | Physics   |                |
| Discipline:     | Optical Spectroscopy  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Controlling Radiative and Nonradiative Recombination Pathways of Multi-Excitonic States in Colloidal Nanocrystal Quantum Dots |                |

## ABSTRACT

Semiconductor nanocrystal quantum dots (NQDs) with near-perfect photoluminescence (PL) quantum yields (QYs) can be routinely synthesized using modern methods of colloidal chemistry. However, these high QYs can only be obtained for single exciton states. QYs of multiexcitons ( $Q_mX$ , with  $m > 1$ ) are, in contrast, very low ( $<10\%$ ) due to fast nonradiative Auger recombination. High values of  $Q_mX$  are, however, essential for practical realization of NQD-based applications such as lasing and generation of entangled photon pairs for quantum communication. Here, by utilizing two independent single quantum dot spectroscopic techniques, we have demonstrated that a near-unity quantum yield from biexciton emission ( $Q_2X$ ) can be achieved in a new type of core/shell NQD, in which a 3-4nm diameter CdSe core is overcoated by an ultra-thick 19-monolayer CdS shell[1]. Furthermore, we also demonstrate that the biexciton quantum yield can be further enhanced to exceed single exciton quantum yield by coupling thick shell NQDs with local plasmonic fields induced by rough silver surfaces. This strong enhancement leads to dramatic changes on photon statistics of single-NQD emission from photon anti-bunching to strong bunching, signifying a significant increase on the probability of having photon-pair emission from the cascade relaxation of a biexciton[2]. Our experimental results demonstrate that this class of thick-shell NQDs could be the foundation toward the development of photon pair sources based on metal-semiconductor hybrid nanostructure.

[1] Y.-S. Park et al., Phys. Rev. Lett. 106, 187401 (2011).

[2] Y.-S. Park et al., (in preparation).

|                 |   |                |
|-----------------|---|----------------|
| Name            | Rama Murthy Sakamuri  | LA-UR 11-10603 |
| Group:          | C-PCS/C-DO  |                |
| Mentor(s):      | Harshini Mukundan and Basil Swanson   |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Biosensors  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Binding of Lipoarabinomannan to Serum High-Density Lipoproteins Decreases its Bioavailability in the Serum of Tuberculosis Patients |                |

## ABSTRACT

Sakamuri, R.M., Price, D.P., Anderson, A.S., Grace, W.K., Mukundan, H and Swanson, B.I.  
Physical Chemistry and Applied Spectroscopy, Los Alamos National Laboratory, Los Alamos, New Mexico, USA 87545

Mannose capped Lipoarabinomannan (LAM) is a lipoglycan, which is unique to pathogenic mycobacteria. Several studies have indicated the presence LAM in the infected patients urine and serum samples, however poor sensitivity of these assays compromised the reliability. Our approach involves evaluation of *Mycobacterium tuberculosis* biomarker detection on a waveguide based optical biosensor platform. We utilized two different detection strategies, namely sandwich immunoassay and a single-ligand assay based on membrane mimetic surfaces (membrane insertion). Initial results indicated that LAM could be detected in the urine of all tuberculosis patients, whereas uninfected controls were negative by sandwich assay. Detectable concentrations of LAM in serum samples were much lower than in urine and LAM was not detected in all infected patient sera. We found that when LAM was spiked in serum and incubated over a period of time, signals for LAM were declining in a time dependent manner in membrane insertion assay. We were also able to detect LAM bound to high-density lipoprotein with a sandwich assay using biotinylated anti Apolipoprotein antibody as a capture and polyclonal LAM antibody as a reporter. This is the first report to show that LAM binds to high-density lipoprotein of serum thereby affecting the LAM concentration in the serum samples of tuberculosis patients.

## Computer, Computational, and Statistical Sciences Division CCS-2

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Guillaume Simon  | LA-UR 11-03125 |
| Group:          | CCS-2/T-3  |                |
| Mentor:         | Balu Nadiga and Phil Jones   |                |
| Field of Study: | Earth and Space Science  |                |
| Discipline:     | Stratified Rotation Turbulence   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Interactions between Balanced and Unbalanced Turbulent Cascades; or How Ocean Circulation Equilibrates |                |

### ABSTRACT

Submesoscale processes are distinguished by order-one Rossby and Richardson numbers with typical size of  $O(1-10\text{km})$  in the ocean. The dynamics of submesoscale processes are distinct from those of the largely quasi-geostrophic mesoscale (typical size of  $O(10-100\text{km})$ ) and fully three-dimensional small processes (size less than  $100\text{m}$ ).

While it's known that submesoscale turbulence arises from frontogenesis due to mesoscale strain and submesoscale instabilities, an understanding of their influence on large-scale circulation is only nascent. We focus on a) their role in mediating energy exchanges between the larger scale, balanced, circulations and smaller scale, fully-unbalanced three dimensional processes, and b) the vertical penetration of such ageostrophic circulations and how they affect the air-sea interactions that drive global ocean circulation.

A computational challenge in this project is the simultaneous and proper simulation of a range of scales ranging from the balanced mesoscales down to the unbalanced scales, still well removed from the regime of full three dimensional turbulence. We use a full dynamical model across the range of scales in a configuration that is compatible with complex forecasting code. An idealized configuration generating submesoscale turbulence in ocean will be presented.

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Tie Wei  | LA-UR 11-02630 |
| Group:          | CCS-2  |                |
| Mentor:         | Daniel Livescu and Malcolm Andrews   |                |
| Field of Study: | Engineering  |                |
| Discipline:     | Mechanical Engineering   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Effects of Initial Conditions on Single and Two-Mode Rayleigh-Taylor Instability |                |

## ABSTRACT

The dependence on initial conditions of single and two-mode Rayleigh-Taylor instability (RTI) is investigated using Direct Numerical Simulations (DNS). The numerical results of single-mode RTI simulation compare well with the linear stability analysis, the analytical prediction of Goncharov and the experimental results of Waddell et al. To ensure that the solution is fully converged, extensive resolution studies were also performed. A new stage, chaotic development stage, was found after the re-acceleration stage in single-mode RTI. During the chaotic stage, the instability experiences seemingly random acceleration and deceleration phases as a result of complex vortical motions. The vortices are generated at the interface and the subsequent interactions are very sensitive to details of the initial perturbation shape, such as diffusion thickness and perturbation amplitude. Although the initial perturbation shape influences the early and late time behavior, it has a minimal role during the potential flow regime and Goncharov's "constant" velocity prediction remains robust.

We have also studied the effect of initial conditions on two-mode RTI, and found that the mixing layer growth is strongly affected by the combination of mode numbers and amplitude as well as phase shift between modes. At late time, the motions become quite complicated, however, some new phenomena, such as 'leaning', 'ejection', and 'mode resonance,' can be identified as significantly influencing the mixing layer growth rate.

## DECISION APPLICATIONS DIVISION D-5

|                 |   |                |
|-----------------|---|----------------|
| Name            | Wenzhong Zhou   | LA-UR 11-02971 |
| Group:          | D-5   |                |
| Mentor(s):      | Jinsuo Zhang and Holly Trelue                                       |                |
| Field of Study: | Engineering   |                |
| Discipline:     | Nuclear Engineering   |                |
| Appointment:    | Postdoctoral Research Associate                                     |                |
| Poster Title:   | Model and Simulation Code Development for Actinide-Containing Fuels |                |

### ABSTRACT

Actinide recycle into a fast-spectrum reactor has been found to be an effective way to manage the disposition of transuranic isotopes, such as Americium and Neptunium, which have long half-lives and dominate the calculated long-term dose associated with releases from repositories. However, the properties of actinide-containing-fuel materials are not well established. The key properties, such as thermal conductivity, enthalpy, and melting temperature, and the key performance, such as gas release, cracking, swelling and fuel relocation, of the fuel must be determined and verified.

The research is conducted in developing constitutive models and simulation codes to predict actinide-containing-fuel materials' properties and performances under irradiation in fast reactor applications. Specifically, the proposed research will use MOOSE/BISON framework and develop a BISON-OXIDE and BISON-METAL fuel performance codes to predict the fuel behavior under steady state and transient conditions for fast reactor applications. That includes the implementation of existing fast reactor constitutive models into BISON fuel performance code. The existing legacy fuel properties and models will be taken from LIFE IV, LIFE IV Metal and FEAST codes for oxide, and metal fuels. These models will be assessed to predict the existing EBR and FFTF databases for validation purposes. Then the proposed research will use a high performance simulation framework called MOOSE (written in C++) to develop a new model for actinide-containing fuels.

Using the new model developed, the properties of actinide containing fuels will be analyzed and semi-empirical models and implementation algorithms will be developed for this data. These new models will be implemented into BISON-OXIDE and BISON-METAL fuel codes and irradiation behavior of these fuels will be assessed using these new codes.

## Earth and Environmental Sciences Division

### EES-14

|                 |   |                |
|-----------------|---|----------------|
| Name:           | Allison C. Aiken  | LA-UR 11-10521 |
| Group:          | EES-14/ISR-2  |                |
| Mentor:         | Manvendra Dubey and Petr Chylek   |                |
| Field of Study: | Earth and Space Science   |                |
| Discipline:     | Atmospheric Aerosols  |                |
| Appointment:    | Director's Postdoctoral Fellow  |                |
| Poster Title:   | Laboratory Studies of the Optical Properties of Warming Aerosols with the SP2 and Photoacoustic Spectrometer: Soot and Hematite |                |

### ABSTRACT

Most aerosols cool the atmosphere by scattering radiation. Absorbing aerosols, such as black carbon (BC) from combustion and hematite in dust, absorb radiation, resulting in a warming of the atmosphere. It is currently thought that BC is the second most important factor in global warming behind carbon dioxide, while dust is one of the major components of ambient aerosols globally. Direct on-line measurements of BC and hematite, an absorbing dust aerosol, can be made with the Single Particle Soot Photometer (SP2), which measures the size and mass of the particles by incandescence and scattering on an individual particle basis. Measurements from the SP2 are combined with absorption measurements from the three-wavelength photoacoustic soot spectrometer (PASS-3) at 405, 532, and 781 nm and the ultraviolet photoacoustic soot spectrometer (PASS-UV) at 375 nm in order to determine wavelength-dependent mass absorption cross sections (MACs). Aerosols are generated by atomizing particles from aqueous solution, dried with a diffusion drier, and can be size-selected with a diffusion mobility analyzer (DMA) before being sent simultaneously to the SP2, PASS-3, PASS-UV, and a laser aerosol spectrometer (LAS) for measuring size distributions. Aerosol samples include flame-generated soot, fullerene soot, Aquadag, glassy carbon, and hematite. MACs from the absorbing aerosols measured in the laboratory are compared with those from ambient aerosols. Size-resolved information with bulk spectroscopic data are used to predict optical properties and are compared with our ambient observations for closure.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Rebeka Derseh  | LA-UR-11-10532 |
| Group:          | EES-14   |                |
| Mentor:         | Thom Rahn  |                |
| Field of Study: | Earth and Space Science  |                |
| Discipline:     | Atmospheric science  |                |
| Appointment:    | Postdoctoral Research Associate                                |                |
| Poster Title:   | Isotopic Tracer for Climate Relevant Secondary Organic Aerosol |                |

## ABSTRACT

At a global level, 1,350 Tg of volatile organic compounds (VOC) are emitted annually into the atmosphere. Many of these VOCs become secondary organic aerosols through reactions with atmospheric oxidants, like hydroxyl radicals or ozone. Secondary organic aerosols (SOA) have a profound influence on Earth's radiation budget, cloud and precipitation distribution and climate. Overall, these influences are poorly quantified. Recent research has demonstrated that SOA inflict worse damage on the respiratory system than VOCs. Hence, heavy exposure to SOA can result in adverse health effects. In order to illuminate SOA formation mechanisms, we traced changes in stable isotope composition through various stages of terpene/ozone SOA formation. To further characterize SOA, we analyzed SOA by ultrahigh resolution mass spectrometry at the National High Magnetic Field Laboratory (NHMFL). This provided detailed knowledge of the chemical composition of SOA produced from ozonolysis reactions. Such approaches greatly enhance our knowledge of SOA and can be incorporated in global and regional climate models to improve current global climate change predictions.

The SOA studied was generated in a 1.5m<sup>3</sup> Teflon chamber by reacting ozone with a variety of biogenic VOCs ( $\alpha$ -pinene,  $\beta$ -pinene, limonene, D-carene Caryophellene and isoprene). Terpenes were volatilized into the chamber, followed by ozone, and allowed the two to react over a period of time. SOA was formed immediately after introducing ozone into the chamber. The SOA produced was collected on a quartz fiber filter. We used a stable isotope ratio mass spectrometer (IRMS) to measure the bulk carbon isotope composition of that SOA. Separately, filter samples were extracted for injection into the ultrahigh resolution mass spectrometer at the NHMFL. From this data, empirical formulas could be unambiguously assigned to hundreds of individual compounds. Currently, we are exploring the potential of <sup>17</sup>O anomaly as a tracer for ozone-derived atmospheric SOA. Because there is no previously published technique to measure <sup>17</sup>O in organic compounds, we are developing a method to measure <sup>17</sup>O/<sup>16</sup>O ratio in oxygen containing organic matter.

This research will add depth and breadth to the current knowledge of SOA production and aging, thus contributing significantly to aerosol science and related climate change issues. Notably, the triple oxygen isotope technique is applied routinely by only a handful of labs worldwide and its potential application to forensics and homeland security issues cannot be understated. This especially, a highlight of the research project, demonstrates the utility of LANL's recent investments in isotopic expertise and instrumentation and may inspire further program development with relevance in many fields.

Name: Bradley Flowers LA-UR 11-03125  
Group: EES-14/ C-PCS  
Mentor: Manvendra Dubey and Bryan Henson  
Field of Study: Earth and Space Science  
Discipline: Physical Chemistry  
Appointment: Postdoctoral Research Associate  
Poster Title: Wavelength-Dependent Optical Properties, Mass Absorption Coefficients and Closure Studies for Carbonaceous Aerosols: Quantifying Absorption Enhancements of Absorptive and Non-Absorptive Coatings on Black Carbon Particles

## ABSTRACT

Soot (black carbon, BC) aerosols are emitted into the atmosphere as a result of combustion activities and make a significant positive contribution to climate forcing. As they are transported and processed in the atmosphere, particles become coated with absorbing (so-called brown carbon) and non-absorbing material, which has a dynamic and uncertain effect on their absorption and radiative properties. Integrated photoacoustic absorption/ nephelometer sensors (IPNs) operating at 781, 532, 405, and 375nm and single particle laser-induced incandescent techniques are used to measure aerosol absorption and scattering as well as BC mass in real-time using on-line measurements. Combined, these techniques are useful to quantify the wavelength-dependent mass absorption coefficient ( $MAC(\lambda)$ ) of BC aerosol as well as the coating effects on optical properties. The absorption enhancement is very sensitive to the composition of the coating material. We report measurements of  $4-\lambda$  aerosol absorption and scattering coefficients and BC mass for ambient aerosols and laboratory generated soot particles and develop a framework for directly quantifying wavelength dependent aerosol absorption properties for black, brown, and organic components of carbonaceous aerosol. We observe coating enhancements of BC absorption by ~ 20% - 30% for freshly emitted soot and much larger enhancements for aerosol having undergone significant atmospheric processing and transport. Quantitative impacts of atmospheric processing to aerosol climate forcing are derived and discussed.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Chandana Gangodagamage  | LA-UR 11-02971 |
| Group:          | EES-14/ISR-2  |                |
| Mentor:         | Cathy Wilson and Steven Brumby  |                |
| Field of Study: | Engineering   |                |
| Discipline:     | Civil Engineering   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Scaling Laws in Arctic Permafrost River Basins: Statistical Signature in Transition |                |

## ABSTRACT

The Arctic landscape has been shown to be fundamentally different from the temperate landscape in many ways. Long winters and cold temperatures have led to the development of permafrost, perennially frozen ground, that controls geomorphic processes and the structure of the Arctic landscape. Climate warming is causing changes in permafrost and the active layer (the seasonally thawed surface layer) that is driving an increase in thermal erosion including thermokarst (collapsed soil), retrogressive thaw slumps, and gullies. One of the dominant features of permafrost basins are immature surficial water tracks which often run parallel to each other down the face of hillslope rather than coalesce into dendritic networks typical of non-permafrost environments. These rudimentary flow-paths are less likely to incise into hillslopes apparently due to permafrost, which ultimately leads to relatively undissected landscapes. These geomorphic anomalies in the arctic landscapes have not been well quantified, even though some of the landscape geomorphic and hydrologic characteristics and changes are detectable by our existing sensor networks. We currently lack understanding of the fundamental fluvio-thermal-erosional processes that underpin Arctic landscape structure and form, which limits our ability to develop models to predict the landscape response to current and future climate change.

In this work, we seek a unified framework that can explain why permafrost landscapes are different from temperate landscapes. We use high resolution LIDAR data to analyze arctic geomorphic processes at a scale of less than a 1 m and demonstrate our ability to quantify the fundamental difference in the arctic landscape. We first simulate the arctic hillslopes from a stochastic space-filling network and demonstrate that the flow-path convergent properties of arctic landscape can be effectively captured from this simple model, where the simple model represents a landscape flowpath arrangement on a relatively impervious frozen soil layer. Further, we use a novel data processing algorithm to analyze landscape attributes such as slope, curvature, flow-accumulation, elevation-drops and other geomorphic properties, and show that the pattern of diffusion and advection dominated soil transport processes (diffusion/advection regime transition) in the arctic landscape is substantially different from the pattern in temperate landscapes. Our results suggest that Arctic landscapes are characterized by low soil production rates and relatively undissected, long planar hillslopes, which convey sediment to quasi-fluvial valleys through long (~ 1 km) flow-tracks. Further, we also document that broad planar hillslopes abruptly converge, forcing rapid subsurface flow accumulation at channel heads. This topographic characteristic can successfully be used to explain the position of erosion features. Finally we estimate the landscape model parameters for the arctic landscape that can be successfully used to model development and validation purposes.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Jiabin Han  | LA-UR 11-02971 |
| Group:          | EES-14  |                |
| Mentor:         | Bill Carey  |                |
| Field of Study: | Earth and Space Science   |                |
| Discipline:     | Corrosion   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Effect of Carbonated or Leached Cement on Corrosion of Mild Steel in Simulated Wellbore Systems |                |

## ABSTRACT

In wellbore systems, Portland cement can passivate and protect steel against corrosion by forming an iron oxide film. However, exposure to CO<sub>2</sub> changes the cement properties and may damage the pre-formed passive film and allow enhanced corrosion rates of steel. In order to investigate this effect, steel-cement composites with varying thicknesses of cement were exposed to CO<sub>2</sub>-brine mixtures. Electrochemical techniques were employed to probe the corrosion behavior of steel as the cement was progressively carbonated by CO<sub>2</sub>.

In high-pressure experiments (100-bar CO<sub>2</sub> pressure), the initial corrosion rates on pre-passivated steel were negligibly small (0.002-0.006 mm/year) compared with rates of unprotected bare steel (10 mm/year). The rates increased three orders of magnitude to 1.0 mm/yr as the pre-formed iron oxide passive film was damaged by infiltrating CO<sub>2</sub> brine. With time, an iron carbonate scale developed eventually resulting in final steady corrosion rates that were almost equal to those of the initial passivated steel surface. This indicates that the corrosion surface was re-healed by iron carbonate formation after the pre-formed iron oxide was damaged by CO<sub>2</sub> brine. Although the corrosion rates of the initial and final states were almost the same, the corrosion potentials were significantly different (0.3 vs. 0.6 V) reflecting the different properties of the iron-oxide passivated film compared with the iron carbonate scale. We also observed that corrosion rate was a function of the thickness of cement coating with a 1 mm coating having a corrosion rate two times higher than that with a 5 mm thick coating, indicating improved protection with greater cement thickness. In addition, we observed that the steady state corrosion rate was two orders of magnitude higher when the cement was completely leached (decarbonated and decalcified) compared with that covered by carbonated cement.

Based on the experimental observations, we proposed the guideline for wellbore integrity criteria in CO<sub>2</sub> sequestration operation: Maintain well bonded and non-leached cement sealing.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Chonggang Xu  | LA-UR 11-02971 |
| Group:          | EES-14  |                |
| Mentor:         | Cathy Wilson and Nate McDowell                        |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Environmental Sciences                                |                |
| Appointment:    | Postdoctoral Research Associate                       |                |
| Poster Title:   | Simulating the Shrub Abundance Increase in the Arctic |                |

## ABSTRACT

The future of carbon balance in the Arctic depends on the responses of both plant growth and soil carbon release to surface warming. One key limitation of plant growth in the arctic is the low inorganic nitrogen availability; however, the arctic warming can enhance nitrogen availability and thus substantially stimulate vegetation growth (especially for shrub species). This will lead to the transition from tundra to shrubland, which can have important feedbacks to global climate by modifying the arctic carbon and energy balances. To predict the transition of tundra to shrubland, we developed an integrated ecosystem dynamic model by coupling an ecosystem demography model (ED) with an arctic hydrology model (ARCHY). The coupled ARCHY-ED model has been parameterized to validate against a 20-year fertilization experiment at Toolik Lake, Alaska. Our results show that the key drivers for the dominance of deciduous shrub is its relatively high ability to take nitrogen and to compete for light. Our coupled model is the first ecosystem dynamics model for the arctic that integrates plant species competition, microbial community dynamics and permafrost.

## EES-16

|                 |  |                |
|-----------------|--|----------------|
| Name            | Min Chen   | LA-UR 11-02971 |
| Group:          | EES-16   |                |
| Mentor:         | Richard Middleton and Cathy Wilson   |                |
| Field of Study: | Earth and Space Science  |                |
| Discipline:     | Hydrology  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Understanding Seasonal and Inter-Annual Lake Area Change Dynamics in Yukon Flats, Alaska |                |

### ABSTRACT

Lake area changes due to global warming can substantially affect arctic hydrology. These changes can have important feedbacks to future global climates by modifying the energy fluxes and carbon balances. In recent studies, lake area change has been used to detect the temporal rate and spatial extent of permafrost degradation in the arctic. Because of the limited availability of long-term clouds-free remote sensing images, lake area from different months (May through September) of different years were commonly compared to quantify the long-term lake area change. However, natural seasonal and inter-annual variability of lake area change can significantly interfere with the signal of long-term lake area change used to indicate the permafrost degradation. In this study, Landsat 7 images of seven time periods from 1999 and 2000 were used to quantify the seasonal and inter-annual lake area changes for the study area within Yukon Flats, Alaska. A total of 7,877 lakes were identified. Total lake areas varied greatly between seasons, ranging from 19,586 ha in the dry season (August 22, 1999) to 35,871 ha in flood season (June 6, 2000). Both intra-annual and inter-annual lake area variability in August and September was smaller than that in June and July, suggesting that images from later summer season are more appropriate for long-term lake area change detection. The surface connection to the rivers played an important role in lake area variability. The area variability of no closure lakes (i.e., with channel connection to rivers) during the two years was twice that of closed basin lakes (i.e., without channel connection to rivers) as measured by coefficient of variation. Seasonal area changes of closed basin lakes can be well explained by the seasonal water balance, defined as cumulative precipitation minus potential evapotranspiration between two corresponding seasons; this is especially true for closed basin lakes. In contrast, area change of no closure lakes was controlled by both seasonal water balance and the changing stage of rivers. For a given time period, total lake area was more strongly correlated with the cumulative water balance since the preceding October when snow became the dominant form of precipitation, rather than with the cumulative water balance in the preceding 12 months as reported in previous studies. We conclude that regardless of the lake area extent of previous fall, the cumulative precipitation (mainly snow fall) during the previous winter was the single critical factor that determined the peak lake area extent in June. In addition, we find that both precipitation (rainfall) and evapotranspiration are important factors driving seasonal lake area change. Spatial heterogeneity in seasonal area change of individual lakes was observed across the study region, a result of different local topographical and geological characteristics around and beneath the lakes, such as elevation and presence of permafrost. The quantification of seasonal and inter-annual lake area variability, along with identification of key factors influencing lake area and area change, are key components for the quantification of long-term lake area change in response to global warming.

Name: Hailin Deng LA-UR-11-10385  
Group: EES-16  
Mentor: Phil Stauffer and Zhenxue Dai  
Field of Study: Earth and Space Science  
Discipline: Hydrogeology and Geochemistry  
Appointment: Postdoctoral Research Associate  
Poster Title: Assessment of Storage Capacity, Injectivity, and Leakage Using Multiscale Reservoir Simulation of CO<sub>2</sub> Sequestration at Rock Springs Uplift, Wyoming

## ABSTRACT

CO<sub>2</sub> geological sequestration in subsurface saline water reservoirs is a practical way to reduce release of anthropogenic CO<sub>2</sub> into the atmosphere and mitigate global warming. Many geological, geochemical, geomechanical and hydrogeological factors control CO<sub>2</sub> storage. Among them, heterogeneity in rock properties in the saline water reservoir can seriously influence design of injection wells, CO<sub>2</sub> injection rate, CO<sub>2</sub> plume migration, storage capacity, and potential leakage and risk assessment. To quantify spatial heterogeneities in porosity and permeability in a target reservoir and overlying cap-rocks, a methodology has been developed to apply index geostatistics and a Markov chain model at the Rock Springs Uplift, Wyoming. We first generate facies-based heterogeneous fields for porosity and permeability in the target saline water reservoir (Pennsylvanian Weber sandstone) and surrounding cap-rocks (including Phosphoria, and Madison and cap-rock Chugwater). A multiphase flow simulator FEHM is then employed to model injection of CO<sub>2</sub> into the saline water reservoir. Monte Carlo simulations are performed with different combination of random fields of porosity and permeability within the saline water reservoir and cap-rocks. The CO<sub>2</sub> storage capacity at the Rock Springs Uplift is estimated to be 6.6 - 0.3 Gt at 95% confidence interval. Uncertainty in storage capacity and well injectivity are quantified based results from these simulations. Finally, we present uncertainty analysis of CO<sub>2</sub> leakage into overlying formations due to heterogeneity in both the target saline reservoir and surrounding formations. The amount of CO<sub>2</sub> leaked into the Chugwater formation is below 0.6% of total injected CO<sub>2</sub> for 50 years of injection. The uncertainties in injectivity, storage capacity, and leakage derived from this method are much more robust than previous estimates and are being used to inform the next generation of risk assessment models.

|                 |   |                |
|-----------------|---|----------------|
| Name:           | Dylan Harp  | LA-UR 11-10322 |
| Group:          | EES-16  |                |
| Mentor:         | Velimir Vesselinov and Kay Birdsell   |                |
| Field of Study: | Engineering   |                |
| Discipline:     | Civil Engineering   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | An Agent-Based Approach to Global Uncertainty and Sensitivity Analysis (ABAGUS) |                |

## ABSTRACT

A novel sampling approach for global uncertainty and sensitivity analyses of modeling results utilizing concepts from agent-based modeling is presented (Agent-Based Analysis of Global Uncertainty and Sensitivity (ABAGUS)). A plausible model parameter space is discretized and sampled by a particle swarm where the particle locations represent unique model parameter sets. Particle locations are optimized based on a model performance metric using a standard particle swarm optimization (PSO) algorithm. Locations producing a performance metric below a specified threshold are collected. In subsequent visits to the location, a modified value of the performance metric, proportionally increased above the acceptable threshold (i.e. convexities in the response surface become concavities), is provided to the PSO algorithm. As a result, the methodology promotes a global exploration of a plausible parameter space, and discourages, but does not prevent, reinvestigation of previously explored regions. This effectively alters the strategy of the PSO algorithm from optimization to a sampling approach providing global uncertainty and sensitivity analyses. The viability of the approach is demonstrated on 2D Griewank and Rosenbrock functions. This also demonstrates the set-based approach of ABAGUS as opposed to distribution-based approaches. The practical application of the approach is demonstrated on a 3D synthetic contaminant transport case study. The evaluation of global parametric uncertainty using ABAGUS is demonstrated on model parameters defining the source location and transverse/longitudinal dispersivities. The evaluation of predictive uncertainties using ABAGUS is demonstrated for contaminant concentrations at proposed monitoring wells.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Kayla Lewis  | LA-UR 11-02971 |
| Group:          | EES-16   |                |
| Mentor:         | George Zyvolski  |                |
| Field of Study: | Earth and Space Science  |                |
| Discipline:     | Physics  |                |
| Appointment:    | Postdoctoral Research Associate                                      |                |
| Poster Title:   | Soil Subsidence Associated with Permafrost Degradation in the Arctic |                |

## ABSTRACT

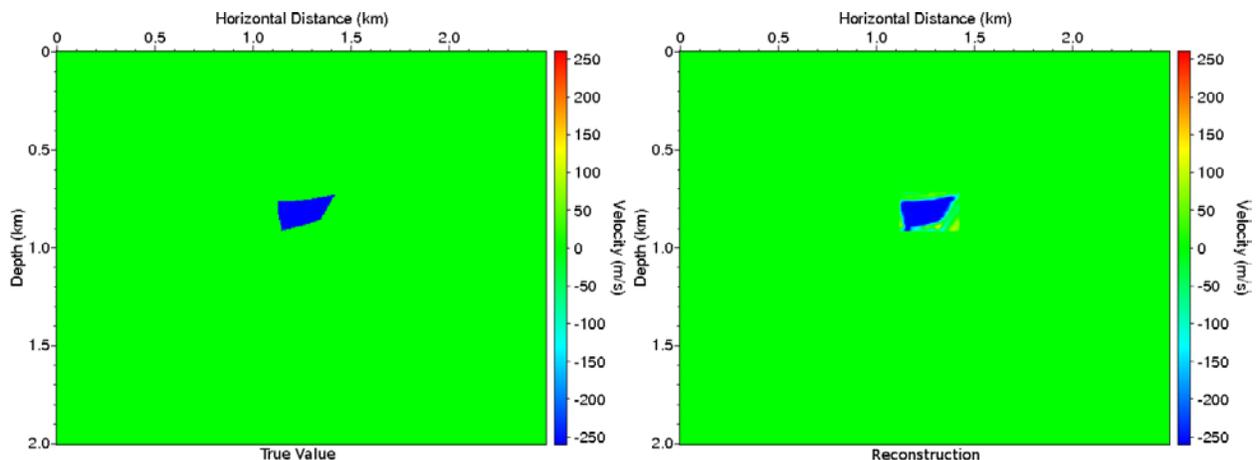
Arctic sources of greenhouse gas associated with permafrost degradation constitute a large uncertainty in existing climate models. Greenhouse gas release from the arctic subsurface is mediated by numerous interconnected biogeochemical processes; one facet of these is the interplay between surface deformation and melting of subsurface ice. I study this interplay via numerical modeling of an initially frozen, fluid saturated, porous, 2D matrix with a subsequent thaw zone advancing from the surface downward. I include an ice-rich region by setting the porosity in a 10 x 20 m rectangular shaped region near the surface to twice that of the surrounding medium (0.6 vs 0.3). With the surface temperature fixed at 5C, a thaw front propagates to ~10 m depth within 20 years and, due primarily to drainage of fluid from the pore space, a zone of soil depressed by ~4.5 meters forms above the initially ice-rich zone. Soil underlying this depressed zone has its permeability reduced by between one and two orders of magnitude. In addition to these numerical results, an analytic model provides the porosity and permeability as functions of time in a 1D column, as well as a group of model parameters that determines a characteristic time scale for soil subsidence.

## EES-17

|                 |  |                |
|-----------------|--|----------------|
| Name            | Youzuo Lin   | LA-UR-11-10597 |
| Group:          | EES-17   |                |
| Mentor:         | Lianjie Huang  |                |
| Field of Study: | Earth and Space Science  |                |
| Discipline:     | Geophysics   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Double-Difference Waveform Inversion with Spatially-Variant Regularization for Quantitative Reservoir Monitoring |                |

### ABSTRACT

It is a challenging problem to monitor subsurface changes using seismic data acquired on the surface. Double-difference waveform inversion is a promising tool for quantitative estimation of reservoir changes due to injection/production of fluids, such as geologic carbon sequestration and enhanced geothermal systems. The method uses seismic data acquired at different times to jointly invert for changes in geophysical properties within reservoirs. Due to limited data, waveform inversion is an ill-posed problem and regularization techniques can be utilized to alleviate the problem. To improve the fidelity of quantitative monitoring, we develop a spatially-variant regularization scheme for double-difference waveform inversion. The method employs different regularization parameters within and outside target monitoring regions to optimize estimations of physical parameters in each region. We use numerical examples to demonstrate the significant improvement of the new approach in estimating reservoir changes compared to the conventional scheme that uses a constant regularization parameter.



|                 |   |                |
|-----------------|---|----------------|
| Name:           | Jonathan MacCarthy  | LA-UR 11-03125 |
| Group:          | EES-17  |                |
| Mentor:         | Charlotte Rowe and Monica Maceira   |                |
| Field of Study: | Earth and Space Science   |                |
| Discipline:     | Geophysics  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Imaging Lithospheric Structure of Intercontinental Mountains through Simultaneous Inversion of Disparate Geophysical Data Types |                |

## ABSTRACT

We explore the tectonic processes of intracontinental mountain building by comparing the Southern Rocky Mountains (SRM) and the Tien Shan (TS) of western China. Both over 1000 km from the nearest plate margin, they have similar tectonic environments, yet different origins. It is thought that shallow oceanic subduction during the Laramide orogeny transmitted stresses into the continental interior to uplift the SRM, but there is no subducted oceanic lithosphere beneath the TS. Instead, stresses have been transmitted across the undeformed Tarim Basin (TB) into the TS. Both mountain belts lie adjacent to broad orogenic plateaus between two tectonically stable blocks, but orogeny has ceased in the SRM, and the western US lithosphere is overprinted by extension and thinning. Mountain building is ongoing in the TS, hence it is a contemporary natural laboratory of intracontinental mountain building. We will leverage new seismic data sets in western China and satellite gravity observations to model seismic and thermal structure of the lithosphere in western China, and compare to the SRM.

Simultaneous inversion of multiple geophysical data sets leverages the sensitivities of each data type to produce comprehensive earth models. We present a nonlinear simultaneous inversion of teleseismic travel time delays and crust-corrected Bouguer gravity for models of P wave velocity, applied to the uppermost mantle of the SRM. Challenges in the method include 1) finding an appropriate mapping between data types to produce a unified geophysical model, 2) ensuring appropriate use of data sensitivities, and 3) finding optimal relative weighting of the data sets. We present our solutions to these difficulties and ongoing efforts to finalize our approach for use with the upcoming Chinese modeling effort.

## High Performance Computing Division HPC-5

|                 |  |                |
|-----------------|--|----------------|
| Name            | Adam Manzanares  | LA-UR 11-10426 |
| Group:          | HPC- 5   |                |
| Mentor:         | John Bent and Meghan Wingate                               |                |
| Field of Study: | Mathematics and Computer Science                           |                |
| Discipline:     | Computer Science   |                |
| Appointment:    | Metropolis Postdoctoral Fellow                             |                |
| Poster Title:   | Reducing Concurrency Bottlenecks in Parallel I/O Workloads |                |

### ABSTRACT

The Parallel Log Structured File System was developed to improve shared file write performance by decoupling a shared file into component pieces. This allowed a shared nothing approach, and improved write performance significantly at the cost of read performance. In this work we develop three collective I/O strategies capable of improving the read performance of PLFS. We also investigate the read performance of PLFS across a set of parallel I/O kernels and identify read patterns where PLFS can improve the read performance of a parallel file system.

In this work we also demonstrate how the transformative properties of PLFS can be leveraged to federate a set of metadata servers leading to increased metadata performance. PLFS is leveraged to reduce bottlenecks in parallel I/O workloads leading to increased performance from the underlying parallel file system. This leads us to believe that PLFS will be a part of our Exascale I/O stack.

## LANL Institutes Office INST-OFF

|                 |  |                |
|-----------------|--|----------------|
| Name            | David Mascarenas   | LA-UR 11-02025 |
| Group:          | INST- OFF  |                |
| Mentor:         | Chuck Farrar   |                |
| Field of Study: | Engineering  |                |
| Discipline:     | Wireless Sensor Networks   |                |
| Appointment:    | Director's Postdoctoral Fellow   |                |
| Poster Title:   | The Development of Active Self-Preservation Policies for Ensuring the Cyber-Physical Security of Unattended, Car-Like, Mobile Sensor Nodes |                |

### ABSTRACT

In recent years there has been a significant interest in the development of car-like mobile sensor nodes. The Google Street View service and the CarTel Project are two prime examples. Contemporary car-like mobile sensor nodes require that a human operator oversee their operation. The next evolution is to enable the deployment of mobile sensor node fleets that operate unattended for long periods of time with a minimum of supervision. In order to make this vision a reality, the cyber-physical security challenges surrounding unattended, car-like mobile sensor nodes must be addressed. Mobile sensor nodes are inherently cyber-physical systems in the sense that they possess tight interplay between their mechanical, electrical, computational, and information systems. As such, the security issues surrounding mobile sensor nodes will typically display a tight coupling between physical security and cyber security concerns. A mobile sensor node could be compromised in a variety of ways that would impact both cyber and physical security. In some situations, a mobile sensor node may be targeted for theft, and as a result, appropriate physical security measures should be taken to avoid this possibility. In the event that the mobile sensor node is physically stolen, cyber-security security challenges arise in the sense that data onboard the node or its network may be compromised, altered, or destroyed. Alternatively, breaches in cyber-security can lead to the breach of a mobile sensor node's physical security. For example, an attack mounted against the wireless communications between a mobile sensor node and its base-station can open a window of opportunity to physically steal or tamper with the node, with a reduced chance of detection.

The focus of this work is to develop control policies to ensure the self-preservation of car-like mobile sensor nodes subject to precision immobilization technique (PIT maneuver) attacks. The PIT maneuver is a technique originally developed by law enforcement to bring high speed vehicular pursuits to an end in a quasi-safe manner. Fig 1. illustrates the execution of a PIT maneuver. It is easy to imagine that the PIT maneuver could be used by thieves to immobilize a car-like mobile sensor node for the purpose of stealing it and compromising its data. Previous work in this area has focused on developing strategies for mobile sensor nodes to both execute and resist the PIT maneuver using mobile sensor nodes. These strategies have been demonstrated in simulation, and are currently being field tested on board small-scale models. The next stage of this effort is to begin developing control policies to recover from, and counter the PIT maneuver. J-turn active recovery will be explored to help mobile sensor nodes recover from PIT maneuvers with a minimum disturbance to their escape route. The "reverse-PIT" maneuver will also be developed to enable a mobile sensor node to apply the PIT maneuver to hostile agents when no other means of escape is practical. This research will be explored using simulation as well as small-scale, car-like mobile sensor node models. The control policies developed in this and previous work will later be integrated into an intelligent framework dedicated to ensuring the cyber-physical security of car-like mobile sensor nodes.

Name David Mascarenas (continued)  
Group: INST- OFF  
Mentor: Chuck Farrar  
Field of Study: Engineering  
Discipline: Wireless Sensor Networks  
Appointment: Director's Postdoctoral Fellow  
Poster Title: The Development of Active Self-Preservation Policies for Ensuring the Cyber-Physical Security of Unattended, Car-Like, Mobile Sensor Nodes



Figure 1: The manual execution of the PIT maneuver on a car-like mobile sensor node.

Name: Christopher Stull  
Group: INST-OFF  
Mentor: Chuck Farrar  
Field of Study: Engineering  
Discipline: Structural Engineering  
Appointment: Postdoctoral Research Associate  
Poster Title: Toward Quantifying the Predictive Maturity of Computer Codes

LA-UR 11-02404

## ABSTRACT

As our understanding of the physical world increases, the experimental methods developed to measure ever-increasingly complex phenomena often become both less reliable and more expensive. It is thus not surprising that many fields of science and engineering are relying more and more heavily on numerical models to simulate real-world phenomena. Commensurate with this increased reliance on computer codes, is the motivation to define a standard framework to measure the “predictive maturity” of these codes. In this context, predictive maturity relates to the confidence an analyst has with regard to the ability of his computer code to make predictions in the absence of experimental data.

The development of such a framework is of particular importance to Los Alamos National Laboratory’s national security mission of stockpile stewardship, for which the Comprehensive Nuclear Test Ban Treaty prohibits experimental testing of our nuclear weapons. This presents a situation where certification of the U.S. nuclear stockpile relies to a great extent on results from numerical simulations. As such, research efforts at Los Alamos National Laboratory have focused on the development of a predictive maturity framework, centered on a quantitative metric, which we call the Predictive Maturity Index or PMI.

The PMI incorporates the following concepts that we assert as important indicators of the predictive maturity of computer codes.

- Coverage - the extent to which experimental data “covers” the design space over which a computer code will be executed.
- Discrepancy – the level of agreement between experimental measurements and model predictions resulting from a computer code.
- Complexity – the level of complexity associated with one or more aspects of a computer code.
- Robustness - the admissible level of ignorance about the calibration variables composing a computer code.

This poster summarizes recent research efforts aimed at further developing this framework, with an eye toward future enhancements for FY12 and beyond.

## International, Space, and Response Division ISR-1

|                 |  |                |
|-----------------|--|----------------|
| Name            | Jeremie Lasue  | LA-UR 11-03125 |
| Group:          | ISR-1/EES-14/C-PCS   |                |
| Mentor:         | Roger Wiens, Dave Vaniman, and Sam Clegg                       |                |
| Field of Study: | Earth and Space Science  |                |
| Discipline:     | Space Research   |                |
| Appointment:    | Postdoctoral Research Associate                                |                |
| Poster Title:   | Mars Science Laboratory ChemCam Fast Motion Field Test Results |                |

### ABSTRACT

Chemcam is a Laser-Induced Breakdown Spectroscopy (LIBS) instrument that will arrive on Mars in 2012, on-board the Mars Science Laboratory (MSL) Rover. LIBS is an active analytical technique that makes use of a pulsed laser to ablate material of interest at a distance. The atoms constituting the high temperature plasma emit at specific wavelengths and the light can be analyzed by spectrometers (from the UV to the NIR) to determine the composition of the target. The technique has been validated for planetary exploration purposes under low pressure and can ablate dust covering rocks. During the MSL mission, ChemCam analyses will be crucial to accurately identify samples and quantify elemental abundances at up to 7 m from the rover.

During the first week of June, NASA organized a "Fast Motion" Field Test (FMFT) of all the MSL instruments including ChemCam. The scope of the field work is to assess the communication efficiency of the teams during the exploratory mission by sending teams equipped with instruments with the same capabilities as MSL's to an unknown geological field site. The data taken in the field are then analyzed by the MSL teams (~200 scientists) at their home institutes without direct communication with the field team to simulate the rover operations. To simulate ChemCam operations, a portable backpack LIBS system from LANL will be taken to the field to analyze geological samples.

While the backpack unit specifications are not as good as the ChemCam flight model, it will allow us to classify the targets and give us a first elemental quantitative analysis. 79 standards (including igneous rocks, sulfates and sediments) were used as a calibration set in the laboratory. O, Si, Al are predicted with relative accuracies better than respectively 10, 20, 30%. Other major elements (Fe, Ca, Mn, Mg, Na, Ti, K) are predicted with a relative accuracy of about 40%. The following elements are not predicted with good accuracy, except if they are highly abundant: H, Li, C, P, S, Cl, Cr, Ni, Cu, Zn, Rb, and Ba.

We will report on the results of the FMFT with respect to the efficiency of the ChemCam team in collecting data and analyzing them to interpret the geology of an unknown site with the MSL instrument suite.

## ISR-6

|                 |                                     |                |
|-----------------|-------------------------------------|----------------|
| Name:           | Vitaly Pavlenko                     | LA-UR 11-02971 |
| Group:          | ISR-6/T-4                           |                |
| Mentor:         | Nathan Moody and Lev Boulaevskii    |                |
| Field of Study: | Physics                             |                |
| Discipline:     | Solid State Physics                 |                |
| Appointment:    | Postdoctoral Research Associate     |                |
| Poster Title:   | Superconducting Tunable THz Sources |                |

### ABSTRACT

Low terahertz range (approximately 0.5 to 2 THz) is of great interest for medical diagnosis, nondestructive materials imaging and spectroscopy. However, currently it lacks efficient oscillators and detectors as it lies between the high frequency limit of semiconductor devices and the low frequency limit of lasers (the so-called “THz gap”).

Sources utilizing the ac Josephson effect allow direct conversion of dc bias voltage across the Josephson junction into electromagnetic wave and can be considered promising candidates for filling in this frequency gap. However, there are two major problems associated with the conventional (mostly Nb-based) Josephson junctions: (a) relatively small value of the superconducting gap limits the frequency by ~600 GHz, and (b) to obtain a practical output power of the source one has to arrange a large number of identical junctions within the space of much less than the wavelength of the emitted electromagnetic radiation (~100 microns).

An alternative approach pursued by the authors is a device based on high temperature superconductor, BSCCO. The specific crystalline structure of this compound accounts for the fact that it exhibits pronounced intrinsic Josephson effect, i.e. the Josephson effect observed between elementary superconducting cuprate layers separated by the insulating Bi- and Sr-oxide layers. Tens of thousands of such elementary junctions (forming a stack) are contained within the THz band wavelength. Presently, non-tunable BSCCO THz source has been demonstrated by several groups with the relatively low (< 1000) number of emitting elementary Josephson junctions. The fixed operational frequency of such type of THz source is set by the size of BSCCO crystal itself in the direction of the electromagnetic wave propagation. The crystal acts as a cavity thus this size has to be about 50-100 microns for the low THz frequency band.

We propose a different design also based on the intrinsic Josephson effect that enables a tunable, rather than a fixed-frequency THz operation. The crystal in this design has to be very thin (~10 microns) in the direction of the electromagnetic wave propagation. There are several other constraints to the device geometry that make the realization of this type of device rather complicated but numerical calculations show that the dc-to-rf efficiency of such source can be as high as 30% with ~1 mW emitted power. We discuss the possibility of using different techniques for fabrication of the tunable superconducting THz source. We show that the desired geometry of the device can be realized through subsequent processing of BSCCO single crystals by precision wire saw and masked broad ion beam milling. As considerable amount of power will still lead to self-heating of the device several approaches to the cooling design are also discussed.

## Los Alamos Neutron Science Center

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Peng Wang  | LA-UR 11-02683 |
| Group:          | LANSCE-LC/EES-DO   |                |
| Mentor:         | Jaroslav Majewski and Don Hickmott   |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Surface Science  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | High Pressure and High Temperature Neutron Reflectometer Cell for Solid-Fluid Interface Research |                |

### ABSTRACT

To understand the interfacial behaviors of materials under high pressure (P) and temperature (T) are of great importance and interest since lots of natural phenomena and practical applications involve those conditions. For instance, mineral surface/fluid interactions control success or failure of many attempts to engineer Earth's subsurface for energy and/or environmental applications. The corrosion of metals and alloys in high subcritical aqueous systems, and especially in supercritical environments is an important safety issue in nuclear power plants.

However, due to the fact that most interface characterization techniques are difficult to implement at elevated P-T, little experimental attention has focused on solid/fluid interfaces at high P-T. Neutron reflectometry (NR) is increasingly being used as a characterization tool to study the surface/interface of planar substrates. SPEAR at Lujan center is a Time-of-Flight (ToF) NR facility, which is specifically designed to study solid-liquid interface and is able to in-situ monitor the surface/interface behavior with a space resolution of a few angstroms. The obtained real space model from reflectivity curve fitting can provide a lot of physical and chemical information about the interface. One key gap to study the interfacial behaviors of materials under high P-T conditions is the lack of well-designed pressure cell capable of handling P-T conditions close to or above supercritical conditions. To build up the capability of studying high P-T surface/interface, Lujan Center developed a special designed pressure cell which allows us to reach 200 MPa and 250 °C (in the future such cell will be equipped with in-situ spectroscopic Raman and IR capabilities). Neutron is highly penetrating, which is able to "see through" high P-T aluminum cell walls and examining the surface/interface properties. Besides the pressure cell itself, the high P-T cell system includes three other subsystems: temperature, pressure and sample chamber environment control systems.

## Materials Physics and Applications Division

### MPA-11

|                 |  |                |
|-----------------|--|----------------|
| Name            | John Brady   | LA-UR 11-03048 |
| Group:          | MPA-11   |                |
| Mentor:         | Dipen Sinha and Cristian Pantea                            |                |
| Field of Study: | Physics  |                |
| Discipline:     | Physical Acoustics   |                |
| Appointment:    | Postdoctoral Research Associate                            |                |
| Poster Title:   | Acoustic Imaging System for Oil Well Downhole Applications |                |

#### ABSTRACT

Objects sometimes fall into and become lodged within oil well boreholes during maintenance or production. The industry currently has no good way to determine the shape of the object or its location within the well, leaving removal largely to trial and error. This often results in very costly production delays.

In principle, an acoustic imaging device could be developed for such applications; however, significant challenges need to be overcome. First, the fluids encountered in oil wells (drilling mud, crude oil) are highly viscous and attenuate sound rapidly—especially at the frequencies used by conventional acoustic imaging systems (MHz range). As a result, lower frequencies (below 500 kHz) must be used. This forces a second challenge: the system must maintain high directionality while operating at these lower frequencies or spatial resolution will be poor. Third, the system must generate enough acoustic intensity in the fluid or the required depth-of-field (at least one foot) will not be achievable. Fourth, the system must operate within a narrow cylinder (eight-inch inner diameter) under high pressures and temperatures.

Directional arrays, phase-steered arrays, and parametric arrays could all be used; however, their practical applicability is limited by electrical complexity, spatial resolution, or inefficiency. A relatively new type of multi-beam array—the frequency-steered array—may overcome these issues. In addition, a novel concept for a real-time, three-dimensional acoustic imaging system will be presented.

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Blake Sturtevant   | LA-UR 11-03125 |
| Group:          | MPA-11   |                |
| Mentor:         | Cristian Pantea and Dipen Sinah  |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Applied Physics  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Coupling Layer Corrections in Pulse-Echo Time-of-Flight Measurements in Solids Revisited |                |

## ABSTRACT

Accurate quantification of the elastic and piezoelectric properties of solids is essential for technological applications such as acoustic based sensors and frequency control devices as well as for basic research into the thermodynamic properties of materials. Ultrasonic time-of-flight measurements have been used to extract the elastic and piezoelectric tensors since these properties can be determined from the acoustic wave phase velocities in a material.

It is well known that to extract highly accurate phase velocities from ultrasonic time-of-flight measurements, one must properly account for the influence of the medium used to acoustically couple the transducer (or buffer rod) to the sample being measured. This correction is typically on the order of 0.1% and is usually achieved by fitting experimental data to a scalar transmission line model in which echoes undergo phase shifts upon transmission through or reflection from the various boundaries. Fitting data to such a model involves varying two free parameters, the thickness of the coupling bond layer and the speed of an acoustic wave in the sample. When performing the fit, one must choose between multiple solutions corresponding to different bond lengths and sample sound speeds. This work quantifies the importance of the couplant correction in selected cases and discusses the error introduced to the extracted velocities by selecting a “wrong” fit to the data. For the first time, criteria and methods for choosing the “correct fit” without making independent measurements of the bond length will be discussed.

## MPA-CINT

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Jeong-Hyun Cho   | LA-UR 11-02971 |
| Group:          | MPA-CINT   |                |
| Mentor:         | Tom Picraux  |                |
| Field of Study: | Engineering  |                |
| Discipline:     | Electrical, Mechanical, and Materials Engineering                                      |                |
| Appointment:    | Director's Postdoctoral Fellow   |                |
| Poster Title:   | Silicon NW Growth on Metal Substrates for a High Performance Lithium-Ion Battery Anode |                |

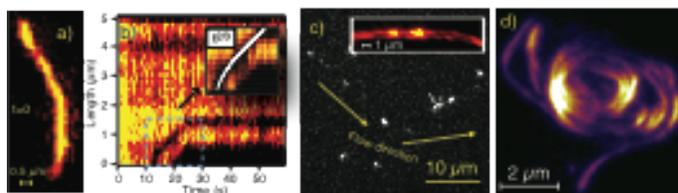
### ABSTRACT

Lithium-ion batteries are widely used in portable electronic systems and electric vehicles because of their relatively high energy density, lack of a memory effect, and low self-discharge. However, the pace at which the energy capacity of batteries is improving is not fast enough to mitigate the energy consumption of new electronic systems. It is known that the energy capacity can be up to an order of magnitude larger than today's commercially available products by using silicon (Si) as an anode material. However, the mechanical stress due to silicon's volume change (approx. 400%) during the addition of Li ions quickly destroys the electrode and leads to loss of electrical contact between the anode material (Si) and a current collector. Recently, it is found that one-dimensional (1D) structures, heterogeneous nanomaterials (silicon nanowires), allow lateral relaxation and can be used to reduce pulverization of a silicon-based anode material. However, the growth of high-density arrays of silicon nanowires (SiNWs) on metal current collectors is challenging due to wetting of the nanowire growth catalyst, which leads to formation of micro-scale Si clumps as well as to competing metal silicide formation during the Si nanowire growth process. The Si clump and silicide formation reduces overall capacity and leads to capacity fade during cycling. Here, we demonstrate high-density, electrically contacted Si nanowire growth on stainless steel substrates (metal current collectors) with minimal unwanted substrate-silicide and Si clump formation for high Li ion battery performance. Specific energy capacity and Li ion cycling results with SiNW half-cell batteries will be presented to illustrate the beneficial effects of our new approach.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Jared Crochet   | LA-UR 11-10326 |
| Group:          | MPA-CINT/C-PCS  |                |
| Mentor:         | Steve Doorn and Han Htoon   |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Nanoscale Materials   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Advanced Microscopic Imaging of Single-Wall Carbon Nanotubes: From One-Dimensional Surface Science to Nano-Scale Rheology |                |

## ABSTRACT

The highly stable, but environmentally sensitive one-dimensional, excitonic near infrared luminescence of single SWNTs can be exploited for applications in single molecule detection in both chemical and biological media. However, the full potential of SWNTs as imaging agents has not been realized because of a lack of homogeneity in the optical properties at the ensemble level. Our laboratory has recently developed methods to produce high quality SWNT colloids with extraordinary tube lengths and photoluminescence quantum yields nearly an order of magnitude larger than previously reported. We demonstrate how high quality SWNTs enable for the first time direct imaging of adatom motion confined to a one-dimensional surface. Also, the unique electronic structure of SWNTs can be used to determine the nature of impurity levels associated with adatoms. A direct application of having high quality colloidal suspension of SWNTs has arisen in the field of low dimensional particle imaging velocimetry for fluid flow visualization. Examples of imaging fluid flow through a nano-porous gel as well as direct image of the dynamics of a reaction-diffusion system involving SWNT aggregation is presented.



**Figure:** a) Photoluminescence (PL) image of an  $\sim 6 \mu\text{m}$  SWNT. b) The same SWNT as in a) spatio-temporally resolved after chemical attack by a single  $\text{AuCl}_4^-$ . The inset shows the non-Brownian motion of the adatoms. c) PL image of colloidal SWNTs flowing through a TMOS gel. The inset is a stacked image showing a vein of flow that was confined to less than  $1 \mu\text{m}$ . d) PL Image of a spiral aggregate of SWNTs formed by a localized chemical wave on a  $\text{MgCl}_2$  treated substrate.

|                 |   |                |
|-----------------|---|----------------|
| Name:           | Shadi Dayeh   | LA-UR 11-02971 |
| Group:          | MPA-CINT  |                |
| Mentor:         | Tom Picraux   |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Electronic Materials  |                |
| Appointment:    | Oppenheimer Distinguished Postdoctoral Fellow   |                |
| Poster Title:   | An Atomic Scale Understanding of Defect Nucleation and Propagation in Heterostructure Nanowires |                |

## ABSTRACT

By the virtue of the nature of the vapor-liquid-solid (VLS) growth of semiconductor nanowires (NWs) - for which ledge nucleation occurs at the triple line interface -, nucleation of defects during the VLS growth can be dramatically different from that in planar thin films. Ge-Si NW heterostructures serve as an excellent test bench system for studying defect nucleation at interfaces in semiconductor NWs.

We present detailed microscopy analysis of ledge and defect nucleation in axial Ge/Si NW heterostructures coupled with molecular dynamics (MD) simulations of defect site preference and stability. We intentionally control the supersaturation in our liquid growth seed to control the creation or elimination of such defects in our NWs. Faults can only occur at three of the inclined (111) facets with respect to the growth orientation that pin the VLS ledge nucleation which in turn progressively shift with layer-by-layer growth at an angle of  $19.5^\circ$  with respect to the NW axis, therefore preventing access to the initial low energy (111) facets and nucleation of any other defect. Two stacking faults form a stable  $\langle 211 \rangle / \langle 111 \rangle$  twin that cannot be terminated (grows parallel to the NW axis). Nucleation and propagation of such defects provide a unique tool for new understanding of the VLS growth in semiconductor NWs on an atomic scale not attainable by in-situ microscopy, nor available in earlier literature. We demonstrate experimentally several orders of magnitude improved performance of transistors made of these heterostructures when compared to their homogenous counterparts.

In addition, the epitaxial growth of different concentric core/shell materials allows engineering the local strain, quantum size, and electronic band offsets that in turn can be tailored to control the spatial distribution of charge carriers and achieve novel opto-electronic devices. It is therefore particularly important, experimentally and theoretically, to assess the coherent limits for the growth of such epitaxial shells and to identify the mechanisms by which the strains are relaxed. Here, we observe two types of relaxed shell structures using HRTEM, provide the first experimental quantification of critical thicknesses in heterostructure core/shell nanowires that matches very well with analytic predictions and explain their strain relaxation mechanisms both axially and radially as well as validate these observations by molecular dynamics simulations. Further, we experimentally probe for the first time ballistic hole transport in such heterostructures over a length scale of  $\sim 220$  nm at room temperature, which is better than any expected ballistic length in conventional semiconductors and is comparable to what is achieved with carbon nanotubes and graphene, yet with better ability to tailor the transport properties and enable bandgap engineering when compared to these graphitic materials.

|                 |   |                |
|-----------------|---|----------------|
| Name:           | Yagnaseni Ghosh   | LA-UR 11-03048 |
| Group:          | MPA-CINT  |                |
| Mentor:         | Jenn Hollingsworth  |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Inorganic Chemistry   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Understanding “Giant” Nanocrystal Quantum Dots by Synthetic Manipulations and Spectroscopic Methods |                |

## ABSTRACT

Semiconductor nanocrystal quantum dots (NQDs) are increasingly being considered as nearly ideal candidates for light-emission applications due to high quantum efficiencies and narrow-band and particle-size-tunable photoluminescence. However, they suffer from certain disadvantages, including chemical-environment-dependent photo-instability at the ensemble level and intermittency in fluorescence intensity, or “blinking”, at the single NQD level. Prior work in our research team showed for the first time that the growth of ultra-thick shells (number of shell monolayers,  $n$ , = 10-20) of the higher bandgap material, CdS, over CdSe NQD cores leads to remarkable photostability and significant suppression of blinking behavior,<sup>1,2</sup> which is likely related to the concurrently observed suppression of nonradiative Auger recombination.<sup>3,4</sup> The new photophysical behavior afforded by this structurally new class of NQD, the so-called “giant” NQD (g-NQD), promises significant advantages for their application in novel light emitting devices (LEDs).

We now emphasize further improvements and tunability by manipulating the relative core-shell volume (by changing the overall core and shell diameter) and also the interfacial composition (by means of fine tuning the percent composition of shelling material). These variations lead to control over optical properties, viz., emission wavelength, single and multi-excitonic decay lifetimes, and fluorescence intermittency (blinking) at single NQD levels. We report syntheses of these novel CdSe/nCdS core-shell NQDs, and also demonstrate their unique optical properties by ensemble and single quantum dot spectroscopy. Additionally we utilize relatively unexplored field of electrochemistry, viz., cyclic voltammetry (CV) and differential pulse voltammetry (DPV) to accurately and directly determine the energy levels of the Highest Occupied Molecular Orbitals (HOMO) and Lowest Unoccupied Molecular Orbitals (LUMO) and conclusively comment on the electronic structures in solution dispersed semiconductor NQDs. This important understanding of conduction and valence-band energy-level alignments allows us to design g-NQD based devices.

*In collaboration with: Benjamin D. Mangum, Han Htoon, Joanna L. Casson, and Jennifer A. Hollingsworth*

1. Chen, Y. *et al.*, *J. Am. Chem. Soc.*, **2008**, 130, 5026.
2. Vela, J. *et al.*, *J. Biophotonics*, **2010**, 3, 706.
3. García-Santamaría, F. *et al.*, *Nano Lett.*, **2009**, 9, 3482.
4. Htoon, H. *et al.*, *Nano Lett.*, **2010**, 10, 2401.

Name: Steve Gilbertson  
 Group: MPA-CINT  
 Mentor: George Rodriguez  
 Field of Study: Physics  
 Discipline: Optical Physics  
 Appointment: Director's Postdoctoral Fellow  
 Poster Title: Quasiparticle Lifetime Near the Dirac Point in Graphene

LA-UR 11-02971

## ABSTRACT

We report measurements on the rise and decay times of electrons pumped above the Dirac point in graphene using 1.5 eV and 3 eV, femtosecond laser pulses as pumps and extreme ultraviolet photons as probe. The experiment is conducted looking at photoemission from graphene samples. The results indicate a fast rise time independent of pump photon energy. The decay times do however depend on the pump photon energy and the kinetic energy of the emitted photoelectron implying that relaxation back to the ground state is heavily influenced by electron-electron and electron-phonon coupling effects after pumping. Figures 1(a) and (b) show the results for 1.5 eV pump and 3 eV pump pulses, respectively. The peak located near delay zero and above the Fermi edge represents electrons pumped to states above the Dirac point while a “dip” in the plots below the Fermi energy represents the formation of holes. These results also indicate the lifetimes of quasiparticle state formation near the Dirac point with the states closest to the Dirac point decaying slowest due to the small volume of the phase space available for scattering processes to take place. Additionally, the change in lifetime at energies moving away from the Dirac point represents the increasing interband scattering processes and lattice coupling, hence shorter lifetimes at higher energies. A qualitative analysis of the results also indicates the electrons and holes have two distinct temperature and chemical potential dependences for at least several hundred femtoseconds after pumping. Figures 2 (a) and (b) show normalized energy spectra of graphene for different delays for 1.5 eV and 3 eV pump pulses, respectively. The plots show the holes below the Dirac point and the electrons promoted to states above the Dirac point. Also seen is the shifting of the peak electron counts to lower energy with increasing delay which can be partially explained by the temperature and chemical potential dependence. This may help settle the debate over whether graphene acts more like a semi-conductor or a metal in the linear dispersion region. The results suggest a limit on electron relaxation times, which along with a fundamental understanding of the ultrafast non-equilibrium dynamics in graphene, is of importance when designing graphene devices.

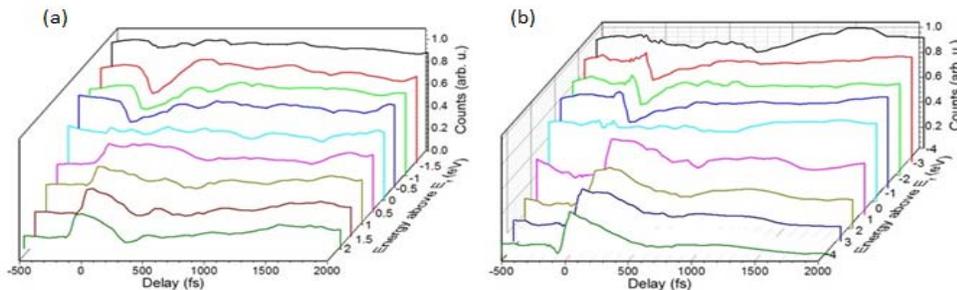


Figure 1: Population versus delay for various energies above and below the Fermi energy,  $E_F$  for (a) 1.5 eV and (b) 3 eV pump photon energy. The data is modified so that counts above  $E_F$  are weighted more heavily than counts below  $E_F$ . This is done to accentuate the features from the raw data.

|                 |   |
|-----------------|---|
| Name            | Steve Gilbertson (continued)                            |
| Group:          | MPA-CINT  |
| Mentor:         | George Rodriguez  |
| Field of Study: | Physics   |
| Discipline:     | Optical Physics   |
| Appointment:    | Director's Postdoctoral Fellow                          |
| Poster Title:   | Quasiparticle Lifetime Near the Dirac Point in Graphene |

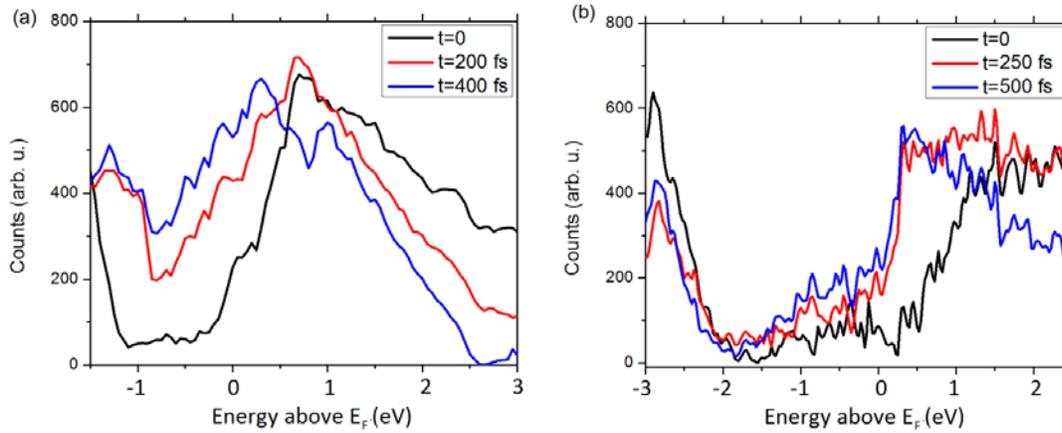


Figure 2: Population versus energy for three different delays for (a) 1.5 eV and (b) 3 eV pump photon energy. The counts above  $E_F$  are weighted more heavily than those below  $E_F$  to accentuate the features.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Jaemyeong Jung   | LA-UR 11-02882 |
| Group:          | MPA-CINT/B-9   |                |
| Mentor:         | Peter Goodwin, Jim Werner, and Andrew Bradbury   |                |
| Field of Study: | Physics  |                |
| Discipline:     | Biophysics   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Molecular Level Understanding of Cellulase-Catalyzed Hydrolysis of Cellulose: A Single-Molecule Approach |                |

## ABSTRACT

Developing bioenergy is germane to both national energy security and the environment. Lignocellulosic biomass, the woody inedible material from plant cell walls is the most abundant biological material on earth. The efficient conversion of biomass to biofuels such as ethanol would meet a large portion of transportation energy requirements in the near future. A crucial step in this process is the enzyme-catalyzed hydrolysis of cellulose to glucose that is then converted into fuel by fermentation. However, this step is a roadblock to the economical, large-scale conversion of the biomass to fuel and therefore, prevents its widespread use as an economically viable alternative to fossil fuel. The enzyme-catalyzed hydrolysis of cellulose is complex – it entails the cooperative (synergistic) action of multiple enzymes known collectively as cellulases: endoglucanase, exoglucanase and beta-glucosidase on both insoluble and soluble substrates. In contrast to homogeneous solution-phase catalysis, the overall efficiency of this heterogeneous catalysis process depends on factors in addition to the catalytic rates of the cellulases, including: cellulase absorption, desorption and diffusion rates on the insoluble cellulose substrate, endoglucanase-catalyzed conversion of cellulose from its crystalline to amorphous forms, and the processivity of exoglucanase-catalyzed hydrolysis of individual cellulose strands. To date, due in large part to limitations of the bulk analysis methods used for its study, this heterogeneous reaction is poorly understood. Here we use single-molecule imaging to directly elucidate molecular-level details of cellulase activity that cannot be readily inferred from ensemble averages reported by conventional, bulk analyses. In our research, the motion of these enzymes on cellulose microfibrils is investigated at the single-molecule level. Total internal reflection fluorescence microscopy (TIRFM) is used to monitor the activity of individual fluorescently-labeled exoglucanases interacting with insoluble cellulose substrates during hydrolysis. Using wide field imaging, we are able to simultaneously record the motion of multiple, individual cellulases with nanometer spatial resolution over intervals up to ~20 minutes. By following the motion of individual cellulases during catalysis, our analysis will provide insight on: (i) Binding and diffusion of the enzyme to ‘active’ sites on cellulose; (ii) Lifetime of enzyme activity for the hydrolysis; (iii) The processivity of the enzyme and the distribution of catalytic turnover numbers during the hydrolysis by a single enzyme; (iv) The nature of the synergy between cellulase enzymes. Data obtained from these measurements will inform coarse-grain molecular dynamics simulations of cellulase activity currently being developed at Los Alamos. Our goal, a molecular-level understanding of cellulase activity, will guide the rational design of superior cellulases and their cocktails, and contribute towards a carbon-neutral fuel economy based on the efficient conversion of abundant lignocellulosic biomass to biofuels.

|                 |   |                |
|-----------------|---|----------------|
| Name:           | Rawiwan Laocharoensuk   | LA-UR 11-03125 |
| Group:          | MPA-CINT  |                |
| Mentor:         | Jenn Hollingsworth  |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Inorganic Chemistry   |                |
| Appointment:    | Director's Postdoctoral Fellow  |                |
| Poster Title:   | Flow Solution-Liquid-Solid Growth: Novel Solution-Phase Technique for Fabrication of Axially Heterostructured Semiconductor Nanowires |                |

## ABSTRACT

Semiconductor nanowires (SC-NWs) constitute “next-generation” nanoscale building blocks for a range of applications from nanoelectronics and photonics to energy harvesting. SC-NWs can be fabricated using either vapor- or solution-phase methods, where solution-phase approaches offer advantages in simplified processing and scaleup, ultra-small diameters for enhanced quantum-confinement effects, and an almost unlimited choice of materials systems from Group III-V to Groups IV, II-VI, IV-VI, and III-VI<sub>2</sub> semiconductors (e.g., InP, InAs, GaP, GaAs, ZnTe, CdSe, PbSe, and CuInSe<sub>2</sub>). Despite these advantages in terms of composition and size control, there is currently no clear way to use the solution-phase methods to grow complex axial heterostructures. A prominent solution-based approach to SC-NW synthesis is known as Solution-Liquid-Solid (SLS) growth, which provides exceptionally high quality single-crystalline NWs. Unfortunately, this “single-pot” approach, where all chemical precursors, stabilizing agents and metal catalyst nanoparticles are injected into a reaction vessel at high temperature to facilitate immediate and rapid NW growth, is not conducive to fabrication of axial heterostructures. In contrast, the vapor-phase analog, Vapor-Liquid-Solid (VLS) growth, permits controlled heterostructuring along the length of growing NWs by employing sequential addition of different chemical precursors to a solid-state array of catalyst particles. To enable a similar approach for SLS, we transformed “conventional-SLS” into a flow-based method called “flow-SLS” (FSLs). With this new approach that allows for facile sequential feeding of solution-phase precursors to arrays of catalyst particles, we have demonstrated for the first time synthesis of axially heterostructured NWs comprising >4 segments of ZnSe and CdSe.

-----

In collaboration with Kumaranand Palaniappan (*MPA-CINT*), Nikolaus A. Smith (*MST-7*), Joanna Casson (*C-PCS*), Jon K. Baldwin (*MPA-CINT*), Jennifer A. Hollingsworth (*MPA-CINT*)

|                 |  |                |
|-----------------|--|----------------|
| Name            | Daniel Perea   | LA-UR 11-03125 |
| Group:          | MPA-CINT   |                |
| Mentor:         | Tom Picraux  |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Semiconductor Nanostructure Engineering  |                |
| Appointment:    | Director's Postdoctoral Fellow   |                |
| Poster Title:   | Synthesis of Abrupt Interfaces without Kinking in VLS-Grown Si-Ge Axial Nanowire Heterostructures by Novel In Situ Catalyst Alloying |                |

## ABSTRACT

Vapor-liquid-solid (VLS) grown axial semiconductor heterostructures have garnered much attention due to their potential for novel or enhanced optical, electronic, and thermoelectric properties compared to conventional planar technology. Of particular interest are Si-SiGe and Si-Ge axial superlattice heterostructures, which are being explored for thermoelectric and tunnel field-effect transistor applications. However, it is commonly found that due to the VLS growth process, the interfaces are significantly broadened and a high percentage of Si-Ge heterostructured nanowires form undesired structural kinks by changing growth direction shortly after the change in composition. Using electron beam based analysis, we report recent results in which the interfaces are much more abrupt and kinking is significantly reduced. The new process involves in situ alloying of the liquid Au catalyst with Ga by the introduction of trimethylgallium. This resulting novel liquid alloy catalyst significantly reduces the solubility of Si and Ge in the liquid, which sharpens the interface, while at the same time reduces the growth rate at the higher precursor partial pressures favorable to nanowire growth, thus promoting a significant reduction in kinking. For example, considering a ~65nm diameter nanowire, for the transition from Ge to Si, the solubility of Ge is significantly decreased and the interface sharpness increases from a width of 45 nm to 11 nm for growth at 380 C using a Au<sub>0.67</sub>Ga<sub>0.33</sub> alloy, as compared to growth from pure Au. At the same time, the growth rate decreases from 2.8 nm/s for kinked Si segments grown from a pure Au catalyst, to 0.2 nm/s with a 10X increase in unkinked Ge/Si heterostructure growth from approximately 95% kinking to <10%. While the underlying mechanisms for kinking which drive a nanowire to change growth direction is not well understood, it is known that this effect is sensitive to the kinetics of growth and becomes a significant issue when changing the growth precursors or temperature. In this presentation we will present detailed results for this new approach to achieving high quality nanowire heterostructure interfaces, discuss the underlying mechanisms.

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Minah Seo  | LA-UR 11-03125 |
| Group:          | MPA-CINT/EES-16  |                |
| Mentor:         | Rohit Prasankumar and Houtong Chen   |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Materials Science  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Polarization Anisotropy of Transient Carrier Dynamics in Single Silicon Nanowire |                |

## ABSTRACT

We have measured polarization-dependent ultrafast carrier dynamics on single- and ensemble-silicon nanowires (SiNWs) using non-degenerate pump-probe spectroscopy to excite and probe carriers above the indirect band gap ( $E_g = 1.12$  eV). In particular, the first measured polarization dependence of transient carrier dynamics in single Si NWs can give deep insight into the influence of light polarization on light-matter interactions in Si NWs. The Si NWs used for this measurement were grown through vapor-liquid-solid (VLS) synthesis using chemical vapor deposition and were dry transferred onto a sapphire substrate with diameters from  $d = 240$  nm to  $d = 50$  nm. A nanomanipulator was then used to transfer an isolated Si NW onto a patterned sapphire substrate. To measure the polarization-dependent transient carrier dynamics, femtosecond Ti:sapphire laser oscillator is used with 420 nm pump and 840 nm probe pulses. The magnitude of the photoinduced changes in probe transmission were  $\sim \Delta T/T \sim 10^{-5}$ . Polarization-sensitive pump-probe experiments on Si NW ensembles reveal that the magnitude of the  $\Delta T/T$  signal is maximum for both beams polarized parallel to the NW axis and minimum for both beams polarized perpendicular to the NW axis, as expected since light absorption is maximum for light polarized parallel to the NW axis; however, there was no significant anisotropy in the measured relaxation times. The photoinduced change in transmission was then measured on the single NW sample (and compared to measurements on the NW ensemble and bulk Si) to explore polarization-dependent carrier dynamics without the complications resulting from the broad NW size and alignment distribution in the NW ensemble. The faster decay process in the NW ensemble as compared to bulk silicon can be explained by the increased influence of surface traps and recombination centers as the degree of spatial confinement increases. Carrier relaxation is even faster in the single Si NW measured here, although this will depend on the specific parameters (diameter, length, alignment) of a given NW. Further polarization-dependent experiments on the single NW sample show the strong influence of the laser polarization on carrier relaxation. The transient transmission is maximum for both polarizations parallel to the NW axis, as in the NW ensemble. However, in stark contrast to our measurements on the NW ensemble, there is a clear anisotropy in the ultrafast dynamics measured for light polarized parallel and perpendicular to the long axis of the NW, with an overall faster decay for parallel polarizations. Density-dependent effects such as Auger recombination, which typically cause carrier lifetimes to decrease with increasing carrier density, may thus lead to the observed polarization dependence of the carrier dynamics. The observed anisotropy in single NWs could enable advanced applications, such as optical switching and polarization-sensitive photodetection, on the nanoscale, where directional control and high spatial resolution are much desired.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Jinkyoun Yoo  | LA-UR 11-02971 |
| Group:          | MPA-CINT  |                |
| Mentor:         | Tom Picraux   |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Materials Science: Semiconductors                                 |                |
| Appointment:    | Postdoctoral Research Associate                                   |                |
| Poster Title:   | Si Nanopillar-Based Radial <i>p-n</i> Junction Photovoltaic Cells |                |

## ABSTRACT

One of the most important directions of photovoltaics (PVs) research is enhancement of photovoltaic efficiency. Semiconductor nanostructures and their heterostructures have opened up novel opportunities of enhancing PV efficiency due to their exotic properties such as no severe limitation of epitaxial relation for obtaining high-quality materials, enhanced light absorption, low carrier loss, and so on. Enhancing the efficiency of PV devices based on these new nanoscale materials requires in-depth study of the structure of materials, electronic band structure, and carrier transport. In vertically-aligned radial NW *p-n* junctions, the direction of light absorption and that of carrier transport can be separated orthogonally. The inherent problem in thin film and bulk structures, a trade-off between efficiency of light absorption and that of carrier collection, can be solved by using radial NW *p-n* junctions.

The growth of vertically-aligned Si radial nanopillar *p-n* junctions with specific geometrical architectures was achieved by a combination of lithographic technique and chemical vapor deposition method. The feature sizes of nanopillar radial *p-n* junction arrays at a sub-wavelength scale can generate interesting behavior of light absorption with different geometric effects determined by sizes and spacings of nanopillars.

In this research, demonstration of nanopillar radial *p-n* junction-based PV devices and fundamental understanding on the transport properties in Si nanopillar radial *p-n* junctions were tried. Especially the comprehensive understanding on carrier transport and optical absorption in Si nanopillar radial *p-n* junction arrays will be discussed.

## MPA-CMMS

|                 |   |                |
|-----------------|---|----------------|
| Name            | Miles Beaux   | LA-UR 11-02662 |
| Group:          | MPA- CMMS   |                |
| Mentor:         | John Joyce  |                |
| Field of Study: | Physics   |                |
| Discipline:     | Photoemission   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Hard X-Ray Photoelectron Spectroscopy and Electronic Structure of Single Crystal UPd3, UGe2, and USb2 |                |

### ABSTRACT

Hard X-ray Photoelectron Spectroscopy (HAXPES) with 7.6 keV photons has been performed on single crystals of UPd3, UGe2, and USb2 at the European Synchrotron Radiation Facility (ESRF). The greatly reduced surface sensitivity of HAXPES enabled observation of the bulk core levels in spite of surface oxidation. Two distinct features separated by 800 meV were observed for the Sb 3d core level. These two features are attributed to manifestations of two distinct Sb sites within the USb2 single crystal as supported by consideration of interatomic distances and enthalpy-of-formation. Photoelectron mean-free-path vs oxide layer thickness considerations were used to model the effectiveness of HAXPES for probing bulk features of in-air cleaved samples.

## MPA-MC

|                 |   |                |
|-----------------|---|----------------|
| Name            | Jonathan Cape   | LA-UR 11-03048 |
| Group:          | MPA-MC  |                |
| Mentor:         | Jim Boncella  |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Biosensors and Biomaterials                               |                |
| Appointment:    | Director's Postdoctoral Fellow                            |                |
| Poster Title:   | DNA Aptamer Based Detection of O,O-Dialkyl Halophosphates |                |

### ABSTRACT

Nucleic acid aptamers are single stranded DNA molecules containing specific sequences that tightly bind target molecular species with antibody-like strength and specificity. These macromolecules have been widely evaluated for clinical diagnostic and chemical/biological detection applications. The long term goal of this project is to develop new methodologies for DNA-aptamer based chemical sensing and to develop practical solid-state material platforms for these systems. Our current work has focused on the detection of organo-phosphates by aptamer-bound dyes in a cationic surfactant matrix. This assay relies on covalent modification of the aptamer-bound dye with a reactive target organophosphate. Specific interactions between the dye and the aptamer binding site result in fluorescence enhancement being observed when the system is exposed to certain O, O'-dialkyl halophosphates. This work investigates the structure and thermodynamics of dye and surfactant complexation with the DNA aptamer, the spectral properties of the bound dye and its phosphorylated derivatives, and the relative specificity of this assay for O, O'-dialkyl halophosphates. The results of these studies demonstrate fairly specific and sensitive responses to these targets, and suggest that this system may potentially offer a practical and inexpensive field test for O, O'-dialkyl halophosphates.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Robert Jilek  | LA-UR 11-02971 |
| Group:          | MPA-MC  |                |
| Mentor:         | Jim Boncella  |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Organometallic Chemistry  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | New Frontiers in Actinide Imido Chemistry: Preparation and Reactivity of Uranium (IV) Imido Dihalides |                |

## ABSTRACT

The study of multiple bonding in the actinide series has been of considerable interest in recent years. Such research is critical to understanding f-orbital participation in actinide-element bonding and sheds light on reactivity differences between the actinides and transition metals. Initially, we discovered that the comproportionation reaction between a uranium (V) bis(imido) dimer,  $[\text{U}(\text{NtBu})_2\text{I}(\text{tBu}_2\text{bpy})]_2$ , and  $\text{UI}_3(\text{THF})_4$  resulted in the formation of a uranium(IV) imido dihalide complex,  $\text{U}(\text{NtBu})\text{I}_2(\text{tBu}_2\text{bpy})(\text{THF})_2$ . Soon thereafter, we found that reactions of  $\text{UCl}_4$  or  $\text{UI}_4(\text{OEt}_2)_2$  with two equivalents of  $\text{LiNHR}$ ,  $\text{R} = 2,6$ -diisopropylphenyl (dipp), 2-tert-butylphenyl, also produced imido dihalides,  $[\text{U}(\mu\text{-NR})\text{Cl}_2(\text{THF})_2]_2$  or  $\text{U}(\text{Ndipp})\text{I}_2(\text{THF})_4$ . Analogous reactions of  $\text{UCl}_4$  in the presence of triphenylphosphine oxide (tppo) result in the formation of  $\text{U}(\text{Ndipp})\text{Cl}_2(\text{tppo})_3$  or  $[\text{U}(\mu\text{Nmes})\text{Cl}_2(\text{tppo})_2]_2$ , mes = 2,4,6-trimethylphenyl, suggesting that imido, halide, and Lewis base all play an important role in determining the nuclearity of these compounds. The synthesis, characterization, and reactivity of these intriguing complexes will be discussed in detail.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Katherine Lovejoy  | LA-UR 11-10503 |
| Group:          | MPA-MC/B-8   |                |
| Mentor:         | Rico Del Sesto and Andy Koppisch                           |                |
| Field of Study: | Chemistry  |                |
| Discipline:     | Materials Chemistry  |                |
| Appointment:    | Reines Distinguished Postdoctoral Fellow                   |                |
| Poster Title:   | Materials Designed for Identification of Forensic Analytes |                |

## ABSTRACT

We have developed a single-platform forensic method to denature wool keratin, reliably extract dyes from wool fibers and identify the extracted dyes and dye mixtures. Wool is composed of the fibrous protein keratin, which is extremely durable and difficult to solubilize. To solve this problem, we have applied our expertise in designing, synthesizing, and manipulating room temperature ionic liquids, which are molten organic salts that act as unique solvents. Ionic liquids can have strong electrostatic interactions with solute molecules and are known to solubilize highly insoluble, fibrous materials, such as lignin and cellulose. We have also used ionic liquids to solubilize inks, dyes, pigments, and inorganic solids in similar applications. For this project, ionic liquids with tetraalkylphosphonium cations were used in a single-platform method to 1) dissolve wool keratin, 2) efficiently extract wool dyes from aqueous solution, and 3) identify the dyes using MALDI mass spectrometry. These ionic liquids were found to be appropriate matrices for MALDI mass spectrometry, which allows for direct measurement of dye-ionic liquid preparations and streamlines the method. Our goal is to facilitate forensic comparison of wool fibers obtained from IED sites and other relevant sources.

Name: Nicholas Travia LA-UR 11-03125  
Group: MPA-MC  
Mentor: Jackie Kiplinger  
Field of Study: Chemistry  
Discipline: Inorganic Chemistry  
Appointment: Postdoctoral Research Associate  
Poster Title: Snapshots of Thorium-Mediated THF Ring-Opening Reactions Using bis(pentamethylcyclopentadienyl)

## ABSTRACT

The thorium tetraiodide  $\text{ThI}_4(\text{THF})_4$  is not a well-behaved starting material for synthesis of the metallocene diiodide complex  $(\text{C}_5\text{Me}_5)_2\text{ThI}_2$ . This appears to be a consequence of the donor ability of the  $\text{C}_5\text{Me}_5$  ligand, which proves insufficient toward preventing metal-mediated ring-opening of coordinated THF and subsequent decomposition. In contrast, parallel reaction chemistry using the isoelectronic bidentate ferrocene diamide ligand  $[(1,1'\text{-fc}(\text{NSitBuMe}_2)_2)]\text{-2}$ , (fcNN), cleanly yields the diiodide complex  $(\text{fcNN})\text{ThI}_2(\text{THF})$ . This observation suggests that compared to the  $(\text{C}_5\text{Me}_5)_2$  framework, the electronically-flexible fcNN framework is better able to stabilize the Th(IV) metal center. This presentation will provide insight into thorium-mediated THF ring-opening reactions as well as general synthetic implications for thorium iodide complexes.

## Materials Science and Technology Division

### MST-7

|                 |  |                |
|-----------------|--|----------------|
| Name            | Lakshminarayana Gandham  | LA-UR 11-02131 |
| Group:          | MST-7  |                |
| Mentor:         | Markus Hehlen  |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Glasses and Glass Ceramics   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Structural, Thermal, and Optical Characterization of Transparent Glass Ceramics Containing LaF <sub>3</sub> : Ce <sup>3+</sup> Nanocrystals for Scintillation Applications |                |

#### ABSTRACT

A series of optically transparent oxy-fluoride glass ceramics containing LaF<sub>3</sub>: Ce<sup>3+</sup> nanocrystals were fabricated by the sol-gel and melt-quench techniques. These glasses and respective glass ceramics were studied with respect to their structural, thermal, and optical properties. From the X-ray diffraction measurement, the glass structure was established. The respective internally nucleated LaF<sub>3</sub>: Ce<sup>3+</sup> nanocrystals containing glass ceramics were obtained by proper heat treatment of the precursor glasses. The nanocrystallisation of LaF<sub>3</sub> was achieved by controlling both time and temperature parameters. It was found that the mean crystal size and the crystal fraction increase with the heat treatment temperature. The Fourier transform infrared spectroscopy and <sup>29</sup>Si, <sup>27</sup>Al, and <sup>23</sup>Na nuclear magnetic resonance measurements have shown good chemical stability and complexation between selected glass former SiO<sub>2</sub>, chief intermediate Al<sub>2</sub>O<sub>3</sub> and network modifier Na<sub>2</sub>O in the glass matrices, respectively. The thermogravimetric analysis, differential thermal analysis, and differential scanning calorimetry measurements confirmed that the glasses were thermally stable. The effect of added fluoride content on the microstructure of the glass ceramics was studied by transmission electron microscopy micrographs. No phase separation at the surfaces and a homogeneous distribution of all elements was observed, indicating that these glass ceramics with LaF<sub>3</sub> nanocrystalline phase are homogeneous at nanoscale. An average crystallite size of around ~10 nm is achieved with a narrow size distribution. Optical absorption, emission and excitation spectra and luminescence decay kinetics of all the prepared glasses and respective glass ceramics have been studied with respect to temperature (77-300 K) and glass composition. Compared with Ce<sup>3+</sup>-doped glasses, their respective glass ceramics have shown stronger emissions due to the presence of the LaF<sub>3</sub> crystalline phase in the glass matrix. Here, in the prepared transparent oxyfluoride glass-ceramics, the optically active (Ce<sup>3+</sup>) ion tends to be located in the crystalline fluoride phase (the latter possesses a significantly lower phonon energy than the vitreous oxide matrix) thereby increasing the intensity of the characteristic emission of Ce<sup>3+</sup>. These preliminary results indicate that the glass ceramics synthesized in this work are promising materials for scintillation applications and future gamma ray detectors.

## MST-8

|                 |  |                |
|-----------------|--|----------------|
| Name            | Levente Balogh   | LA-UR 11-03048 |
| Group:          | MST-8  |                |
| Mentor:         | Donald Brown and Carlos Tome   |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Materials Physics  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | The Nature of Dislocations in Irradiated Zirconium Determined by Diffraction Line Profile Analysis |                |

### ABSTRACT

Diffraction line profile analysis (DLPA) is a powerful method for characterization of the microstructure of crystalline materials [1-3]. Until now, the DLPA method has been used mostly with X-ray diffraction patterns. There is interest in using Time-of-Flight (TOF) neutron diffraction data for DLPA due to the high penetration of neutrons and because TOF diffraction records many peaks simultaneously with collinear diffraction vectors [4].

Zircaloy samples removed from a nuclear power reactor were investigated using the Neutron Powder Diffractometer instrument, to determine the microstructural changes induced by heavy neutron irradiation. Several years spent inside a nuclear reactor causes a dramatic change in dislocation density, arrangement and Burgers vector ratio. It is shown that DLPA combined with TOF neutron diffraction is a valuable tool for the characterization of irradiated materials. These investigations are of great technological interest as Zr alloys are used as structural material in nuclear reactors.

1. T. Ungar, J. Gubicza, G. Ribarik & A. Borbely, *J. Appl. Cryst.* 34 (2001), 298.
2. G. Ribarik & T. Ungar, *Mat. Sci. Eng. A* 528 (2010) 112.
3. G. Ribarik, J. Gubicza & T. Ungar, *Mat. Sci. Eng. A* 387-389 (2004) 343.
4. D.W. Brown, T.A. Sisneros, B. Clausen, S. Abeln, M.A.M. Bourke, B.G. Smith, M.L. Steinzig, C.N. Tomé & S.C. Vogel, *Acta Mat.* 57 (2009) 972.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Juan Escobedo  | LA-UR 11-00924 |
| Group:          | MST-8/WX-9   |                |
| Mentor:         | Ellen Cerreta and Darcie Dennis-Koller   |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Dynamic Deformation  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Effects of Grain Size and Boundary Structure on the Dynamic Tensile Response of Copper |                |

## ABSTRACT

Plate impact experiments have been carried out to examine the influence of grain boundary characteristics on the dynamic tensile response of Cu samples with grain sizes of 30, 60, 100 and 200  $\mu\text{m}$ . The peak compressive stress is  $\sim 1.50\text{GPa}$  for all experiments, low enough to cause an early stage of incipient spall damage that is correlated to the surrounding microstructure in metallographic analysis. The experimental configuration used in this work permits real-time measurements of the sample free surface velocity histories, soft-recovery, and post-impact examination of the damaged microstructure. The resulting tensile damage in the recovered samples is examined using optical and electron microscopy along with micro x-ray tomography. The free surface velocity measurements are used to calculate spall strength values and show no significant effect of the grain size. However, differences are observed in the free surface velocity behavior after the pull-back minima, when re-acceleration occurs. The magnitude of the spall peak and its acceleration rate are dependent upon the grain size. The quantitative, post-impact, metallographic analyses of recovered samples show that for the materials with grain sizes larger than 30  $\mu\text{m}$ , the void volume fraction and the average void size increase with increasing grain size. In the 30 and 200  $\mu\text{m}$  samples, void coalescence is observed to dominate the void growth behavior, whereas in 60 and 100  $\mu\text{m}$  samples, void growth is dominated by the growth of isolated voids. Electron backscatter diffraction (EBSD) observations show that voids preferentially nucleate and grow at grain boundaries with high angle misorientation. However, special boundaries corresponding to 1 (low angle,  $<5^\circ$ ) and 3 ( $\sim 60^\circ$   $\langle 111 \rangle$  misorientation) types are more resistant to void formation. Based on these findings, mechanisms for the void growth and coalescence are proposed.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Saryu Fensin  | LA-UR 11-02062 |
| Group:          | MST-8   |                |
| Mentor:         | Rusty Gray, Ellen Cerreta, and Steve Valone   |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Materials Engineering   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Structure and Shock Response of a Sigma 11 Asymmetric Tilt Grain Boundary in Copper at Finite Temperature |                |

## ABSTRACT

Grain boundaries play an important role in governing the microstructure and deformation evolution in a material. Hence, it is important to understand the structure of grain boundaries that are subjected to high homologous temperatures. Boundaries that are susceptible to extreme structural disorder as the temperature is increased might drastically change the dynamic damage in a material under shock loading conditions. In this talk we will present the results of molecular dynamics simulations studying the shock response of an asymmetric tilt grain boundary in copper as a function of temperature. At high homologous temperatures a grain boundary can either form a disordered structure or can completely premelt. The change in grain boundary structure can be drastic enough to alter its response to an applied external force.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Tongsik Lee   | LA-UR 11-02444 |
| Group:          | MST-8/MST-6   |                |
| Mentor:         | Steve Valone and Chris Taylor   |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Materials Modeling  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Atomistic Modeling of the Thermodynamic Equilibrium and Phase Transitions in Solids |                |

## ABSTRACT

An accurate description of structural transitions and resulting changes of physical properties is one of the central themes in computational materials modeling. A proper scheme to describe phase behavior must be built on the basis of a detailed microscopic approach in terms of both a reasonable model of the energetics and a method of statistical mechanics. The Monte Carlo (MC) method can be an efficient yet robust technique to determine the thermodynamic equilibrium of a given system at the atomic scale. When the method is combined with a reliable interatomic potential model, it acquires powerful predictive ability. Recall that the free parameters in an interatomic potential model are normally fitted only to some zero temperature material properties (e.g. the second-order elastic moduli) at a certain bulk reference structure of the system of interest. In many cases, large-scale molecular dynamics simulations using such a potential are thereupon conducted to draw conclusions regarding the thermal or temporal aspects of the system. However, the performance at finite temperature or transferability to other structures of the model potential is not necessarily guaranteed. It is vital that one ensure at least the reproduction of the bulk equilibrium properties prior to the application of the model potential to studies of the dynamics or defects of the system.

In the present study, we address the thermodynamic equilibrium and phase stability of numerous metals and metallic alloys. The modified embedded atom method is adopted as an interatomic potential model. A general MC methodology for simulation of crystalline solids with the isobaric or isotension ensemble has been developed, being enhanced with the parallel tempering method in order to overcome the sampling inefficiency in the standard Metropolis scheme. We conduct systematic computation of various thermodynamic response functions with respect to temperature and pressure. Examples of these properties are the heat capacity, thermal expansion, and elasticity, that as a whole constitute the full equation of state of solids. Further, calculations of the Gibbs free energies utilizing thermodynamic integration are performed to discuss the relative phase stability among multiple phases. Reliability and transferability of a model potential are ensured by testing against broader regions of the phase diagram. Only with our fully equipped MC simulations are we able to gain a comprehensive perspective of the structure/property relations of solids at a quantitative level.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Enrique Martinez Saez  | LA-UR 11-02971 |
| Group:          | MST-8/MPA-CINT   |                |
| Mentor:         | Jose Caro and Mike Nastasi   |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Computational Materials Science  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Synchronous Parallel Kinetic Monte Carlo: Diffusion in Heterogeneous Systems |                |

## ABSTRACT

A new hybrid Molecular Dynamics-kinetic Monte Carlo algorithm has been developed in order to study the basic mechanisms taking place in diffusion in concentrated alloys under the action of chemical and stress fields. Parallel implementation of the kMC part based on a recently developed synchronous algorithm [J. Comp. Phys. 227 (2008) 3804-3823] resorting on the introduction of a set of null events aiming at synchronizing the time for the different subdomains. added to the parallel efficiency of MD, provides the computer power required to evaluate jump rates 'on the fly', incorporating in this way the actual driving force emerging from chemical potential gradients and the actual environment-dependent jump rates.

We have applied the model to study the fluxes of vacancies around edge dislocations. Calculations of the accumulation of these vacancies in the dislocations as well as the segregation of alloying elements towards them have been carried out. The importance of the results is two-fold. One, the determination of fluxes is of paramount significance in higher level calculations like continuum mechanics and rate theory models, and second, the evolution of the microstructure in complex structures is captured directly from the simulation results.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Alejandro Perez-Bergquist  | LA-UR 11-02066 |
| Group:          | MST-8  |                |
| Mentor:         | Ellen Cerreta and Rusty Gray   |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Dynamic Properties   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Grain Boundary Response in Shocked Copper Multicrystals: TEM Characterization and Atomistic Modeling |                |

## ABSTRACT

To understand the role of interface structure during shock loading, and specifically the role of interfaces in damage evolution due to shock, four copper bi-crystal boundaries were studied both experimentally and through atomistic modeling simulations under shock loading and incipient spall conditions. These boundaries, two 001/111 boundaries and two 001/001 boundaries, were characterized prior to deformation using both electron back scattered diffraction (EBSD) and transmission electron microscopy (TEM) to determine axis/angle pair relationships, interface planes, and grain boundary structure. Samples containing these boundaries were then subjected to incipient spall at 2.5 GPa and shock loading at 10 GPa, respectively. Samples were soft recovered and characterized post-mortem via EBSD and TEM. Molecular dynamics (MD) simulations were also performed where grain boundaries representative of those present in the experimental samples were subjected to shock loading conditions. Given similar strain rates between experiments and computer simulations, the MD simulations provide perspective into the in situ damage mechanisms within the shocked crystals and also allow for improved atomic-scale grain boundary structure analysis in conjunction with TEM. Preliminary results indicate that typical grain boundaries readily form damage during shock loading but that special boundaries, such as twin boundaries, are resistant to failure. Both experimental evidence and computer simulations indicate that differences in slip and defect transmissibility across these types of boundaries likely play a role in this response.

## Nuclear Nonproliferation Division

### N-4

|                 |   |                |
|-----------------|---|----------------|
| Name            | Sara Kutchesfahani  | LA-UR 11-02034 |
| Group:          | N-4   |                |
| Mentor:         | Brian Boyer and Jim Doyle   |                |
| Field of Study: | Political Sciences  |                |
| Discipline:     | International Relations/Security  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | How to Strengthen International Safeguards: Moving Forward with the Additional Protocol |                |

### ABSTRACT

This poster will illustrate that one way to strengthen international safeguards would be to ensure the signature of the Additional Protocol (AP) by all IAEA member states. Events in the early 1990s, including the dissolution of the Soviet Union, events in Iraq, South Africa and the DPRK prompted the International Atomic Energy Agency (IAEA) to request recommendations on strengthened and more efficient safeguards in order to extend the classical safeguards system. As a result, the model protocol – the IAEA Additional Protocol (INFCIRC 540) – was agreed by the IAEA Board of Governors in 1997. The AP provides better tools to carry out inspections on a more routine basis and in a less confrontational manner since it provides access rights to suspect locations at short notice, additional information and verification on nuclear and nuclear-related activities, and the use of environmental sampling and remote monitoring techniques to detect illicit activities.

Currently, 139 countries have signed the AP. However, there are a number of countries, including Argentina, Brazil, Iran, Egypt, Syria, Venezuela, and Burma that have not yet signed the AP. This poster will outline possible reasons for why these countries have yet to sign the AP and will offer recommendations to ensure the signatures of the AP by all IAEA member states, thereby moving forward the IAEA's desire to strengthen international safeguards.

## Physics Division

### P-21

|                 |  |                |
|-----------------|--|----------------|
| Name            | Evgeny Burmistrov  | LA-UR-11-10491 |
| Group:          | P-21   |                |
| Mentor:         | Michelle Espy and Andrei Matlashov                         |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Methods and Instruments for Bioscience                     |                |
| Appointment:    | Postdoctoral Research Associate                            |                |
| Poster Title:   | Helmet Shaped SQUIDS Array for Ultra-Low Field MRI and MEG |                |

#### ABSTRACT

Investigating dynamics in the human brain requires studies with both excellent temporal and spatial resolution. Resolving synchronous oscillations in the visual cortex, for example, requires  $\sim 2.5$  ms temporal resolution and  $\sim 5$  mm spatial resolution. Recently, it has become practical to perform magnetic resonance imaging (MRI) at much lower fields (from  $\mu\text{T}$  to mT), the so-called ultra-low field (ULF) regime [1, 2]. The reduced signal-to-noise can be compensated by using pre-polarizing fields and SQUID (Superconducting QUantum Interference Device) sensor technology. Due to the very low operating fields, ULF MRI is compatible with simultaneous MEG. In this work we propose a new system for simultaneous ULF MRI and magnetoencephalography (MEG) measurements, which will achieve the required spatial and temporal resolution while eliminating co-registration errors.

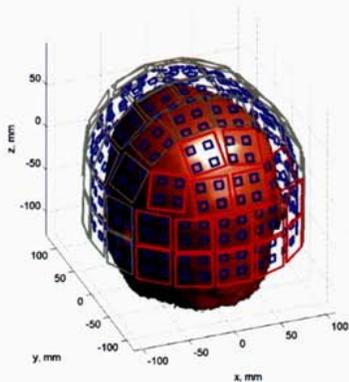
Magnetic detectors, using low temperature superconductivity (LTS) SQUID technology, will be placed on the internal surface of a helmet surrounding the subject's head. Figure 1 shows the locations of SQUID magnetometers for MEG channels (blue colored squares) and input coils for SQUIDS that will be used for ULF MRI (red colored squares). In this system we will build an imaging system for the occipital region of the head using 16 MRI and 64 MEG channels. SQUIDS with 8 mm square input coils will be used for detection of MEG; for ULF MRI detection we will use SQUIDS with 40 mm square input coils. The helmet will be placed on the bottom of the cryostat insert as shown in Figure 2. The sensor array will reside in a liquid helium cryostat made by Neuromag.

The MRI coils are shown in Figure 3. Helmholtz coils will generate the measurement field,  $B_m$ , which will range from  $100 \mu\text{T}$  to  $500 \mu\text{T}$  (precession frequency 4 kHz to 22 kHz). The other three sets of coils will generate gradients  $B_{zz}$ ,  $B_{zx}$ ,  $B_{zy}$  for 3-D imaging, with magnitudes up to  $350 \mu\text{T/m}$ . To create the pre-polarizing field,  $B_p$ , in the range of 100 – 200 mT, we will use a pair of liquid nitrogen cooled coils.

[1] Michelle A. Espy et al. "SQUID-Based Simultaneous Detection of NMR and Biomagnetic Signals at Ultra-Low Magnetic Fields", IEEE Trans. on Appl. Supercond., Vol. 15, No 2, June 2005

[2] Andrei N. Matlashov et al. "Instrumentation for Simultaneous Detection of Low Field NMR and Biomagnetic Signals", IEEE Trans. on Appl. Supercond., Vol. 15, No 2, June 2005

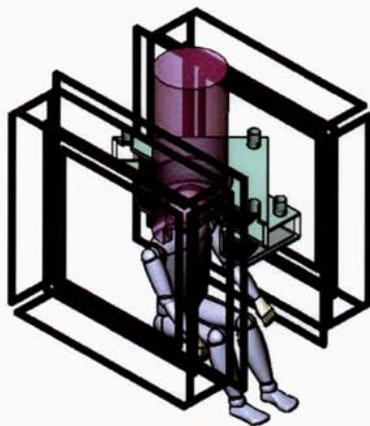
Name: Evgeny Burmistrov (continued)  
 Group: P-21  
 Mentor: Andrei Matlashov  
 Field of Study: Bioscience  
 Discipline: Methods and Instruments for Bioscience  
 Appointment: Postdoctoral Research Associate  
 Poster Title: Helmet Shaped SQUIDs Array for Ultra-Low Field MRI and MEG



**Figure 1.** Helmet shaped SQUID measurement system.



**Figure 2.** Inside of the liquid helium cryostat. The measurement helmet is shown in green at the bottom.



**Figure 3.** MRI Coils, cryostat, and cutaway of pre-polarization coils positioned around subject.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Chaitanya Chandrana   | LA-UR-11-10596 |
| Group:          | P-21  |                |
| Mentor:         | Pulak Nath and Michelle Espy  |                |
| Field of Study: | Engineering   |                |
| Discipline:     | Electrical Engineering  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | 'Shim-a-Ring' Magnets: Coaxial Shimming of Ring Magnets for Nuclear Magnetic Resonance (NMR) and Magnetic Separations |                |

## ABSTRACT

Magnetic field is a critical component in many important applications including Magnetic Resonance Imaging (MRI), Nuclear Magnetic Resonance (NMR) Spectroscopy, and High Gradient Magnetic Separation (HGMS) etc. Generally, there are two ways to generate a magnetic field: (1) Electromagnetic Circuits, and (2) Permanent Magnets. Our focus is on the use of permanent magnets. Permanent magnets have several advantages over electromagnets. A permanent magnet does not require a power source to generate the magnetic field. Magnetic fields generated by a permanent magnet do not dissipate heat under normal conditions and therefore, unlike electromagnets, permanent magnets can be operated continuously with no cooling requirements.

Patterns of the magnetic fields are critical to the type of applications. For example, a gradient magnetic field is required for magnetic separation, where as a highly uniform field is required for magnetic detection using NMR. Typically magnetic fields for magnetic separation and detection are obtained using an array of precisely oriented permanent magnets. (e.g. Quadrupole magnet, Halbach array etc). Precise alignments of multiple magnets make the fabrication of such magnetic circuits difficult, time consuming and expensive. In this work, we will present a ring magnet with a ferromagnetic co-axial shim (hence the name, 'shim-a-ring' magnet), for separation and detection applications. The design was developed and optimized using commercial software FEMLAB 3.1 (COMSOL, Inc, Burlington, MA). The novel design proposed in this work utilizes a single ring magnet with co-axial shimming, and therefore eliminates the need for precise alignment reducing the overall fabrication cost and time. Our model shows well-defined magnetic fields (uniform or gradient field distributions) comparable to the traditional designs. Once fully developed and implemented, these 'shim-a-ring' magnets could replace the existing state-of-the art magnets and open up doors for next generation magnetic separation and detection platforms.

Name: Amy Guthormsen

LA-UR 11-03048

Group: P-21

Mentor: John George

Field of Study: Psychology

Discipline: Cognitive

Appointment: Postdoctoral Research Associate

Poster Title: Using ERPs to Track the Timecourse of Visual Object Recognition

## ABSTRACT

People are able to discriminate natural scenes containing animals from those with no animals very quickly. Event related potentials (ERPs) are a tool by which investigators can study the time course of rapid perception. However, the extent to which target/non-target differences in ERPs reflect object recognition is a matter of controversy. Here, we present preliminary data from an ERP study in which participants were presented briefly with an image and asked whether it represents a member of a target category. The target category was either dog or cat. Stimulus images were dogs, cats or natural scenes without animals. This design allows us to examine both the effect of stimulus similarity and target status on ERP waveforms. Among images that were not targets, we observed early (<150 ms) differences between the most physically dissimilar image sets (no animal scenes vs. dogs or cats). More physically similar image sets (dogs vs. cats) produced differences that were weaker, later, and more variable between participants. We compare these patterns to data from a speed of sight task in which participants had to identify the same targets in a two alternative forced choice task. When the two choices are highly similar (dog, cat) the visual system requires a longer exposure to perform the task accurately than when the stimuli are less similar (dog, no animal). We then extend this paradigm to explore an alternative set of images in which we compare physically similar images (male and female faces) to a less similar set (non-face images). Overall, our data support the conclusion that, while the visual system may be able to discriminate some classes of images from each other in a very short time, true object recognition takes longer. One should therefore look carefully at the task and image sets used in any study that uses the fast speed of object recognition to support purely feed-forward models of vision.

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Todor Karaulanov   | LA-UR-11-10696 |
| Group:          | P-21   |                |
| Mentor:         | Igor Savukov and Michelle Espy   |                |
| Field of Study: | Physics  |                |
| Discipline:     | NMR/MRI  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Demonstration of Anatomical Imaging with a Portable Non-Cryogenic Ultra-Low Field MRI System |                |

## **ABSTRACT**

Ultra-low field (ULF) MRI has many potential advantages such as low cost, portability, convenience, enhanced contrast, open design, absence of susceptibility artifacts, and some others. However, previous anatomical imaging was demonstrated only with SQUIDs and in a shielded room, which would limit many applications. At Los Alamos, to make ULF MRI applications commercially viable, we have worked on developing alternative non-cryogenic detection methods. By changing the frequency from 3 kHz to 60-80 kHz (still keeping most of the advantages of the ULF regime) and by increasing the prepolarization field strength from 400 G to 1 kG, we were able to improve sensitivity by more than an order of magnitude. As a result, we obtained MRIs with a resolution of 2-3 mm in 5-20 minutes of acquisition time, with longer times required for better visibility of anatomical features. The hand image is the first step showing feasibility of the non-cryogenic ULF method of anatomical imaging. Work on the development of a ULF MRI non-cryogenic scanner for the human brain is in progress. The results of this work and further detail on the system design and image properties will be reported at the poster session.

Name: Warren Lybarger  
Group: P-21  
Mentor: Malcolm Boshier  
Field of Study: Physics  
Discipline: AMO Physics; Quantum Technologies; & Precision Measurement  
Appointment: Postdoctoral Research Associate  
Poster Title: Single-Ion Heisenberg-Limited Quantum Phase Sensors

LA-UR 10-07993

## ABSTRACT

We report on our efforts to construct a single-ion-qubit sensor capable of Heisenberg limited detection of external fields that can be efficiently coupled to the ion qubit. Based on a single-qubit iterative phase estimation algorithm (IPEA) [1, 2], a quadratic enhancement in quantum phase estimation precision is achieved when compared to standard shot-noise limited measurement protocols without using any entanglement. This approach also has the advantage that it does not require an understanding of the quantum Fourier transform, and it is readily related to more conventional approaches for measuring phases. The bit-by-bit estimation of an unknown phase only requires standard quantum information processing (QIP) protocols in addition to the use of single-qubit rotations that are each of a relative phase that is conditioned on all previous classical outcomes in the measurement sequence. Successful implementation of the IPEA will demonstrate a working quantum circuit with relatively immediate and useful applications in basic science, remote sensing, and clock synchronization [3]. We also describe the potential application of novel ion trap architectures previously put forth [4, 5, 6] to the problem of miniaturizing the IPEA experiment as well as other single- and multi-qubit quantum enhanced metrology experiments. While these architectures were initially conceived in the context of large-scale QIP and quantum simulation, we face similar technical challenges in developing deployable ion trap based quantum sensors. This provides further impetus for developing relevant enabling technologies with both long- and short-term applications.

[1] Knill et al., Phys. Rev. A 75, 012328 (2007)

[2] Higgins et al., Nature 450, 393-396 (2007)

[3] de Burgh and Bartlett, Phys. Rev. A 72, 042301 (2005)

[4] J. Chiaverini and W. E. Lybarger, Jr., Phys. Rev. A, 77, 022324 (2008)

[5] J. Chiaverini, "Dynamically Configurable Trapped-Ion Arrays for Streamlined Quantum Processing," presented at the Workshop on Integrated Atomic Systems II, Seattle, Washington USA, February 2009.

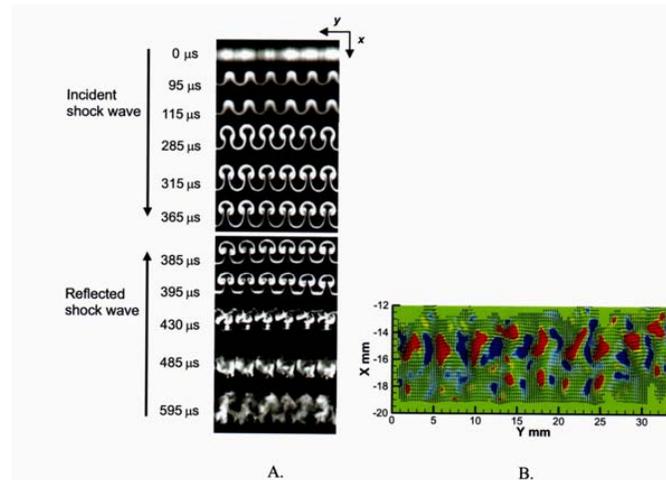
[6] W. E. Lybarger, Jr., Ph.D. thesis, University of California, Los Angeles (2010)

|                 |  |                |
|-----------------|--|----------------|
| Name            | Sridhar Balasubramanian  | LA-UR 11-02703 |
| Group:          | P-23   |                |
| Mentor:         | Kathy Prestridge   |                |
| Field of Study: | Engineering  |                |
| Discipline:     | Mechanical Engineering   |                |
| Appointment:    | Postdoctoral Research Associate                                      |                |
| Poster Title:   | Initial Condition Effects on Richtmyer-Meshkov Mixing and Turbulence |                |

## ABSTRACT

Recent computational studies have shown that carefully imposed initial conditions can be used to control late time mixing and turbulence in buoyancy-driven Rayleigh Taylor (RT) and shockdriven Richtmyer Meshkov (RM) flows. Such dependence has not been confirmed in experiments, which is important for Verification and Validation (V&V) purposes. A systematic experimental study is carried out to study the dependence of initial condition parameters, namely the amplitude and wavelength of perturbations, on turbulence and mixing in RM flows. A stable, single mode, membrane-free varicose heavy gas curtain (air-SF<sub>6</sub>-air) at a shock Mach number  $M = 1.2$  and Atwood number,  $A=0.60$  was used in our experiments. The density (concentration) and velocity fields for various initial configurations were characterized using Planar Laser Induced Fluorescence (PLIF) and Particle Image Velocimetry (PIV) respectively. The evolution of RM instability after the incident shock and subsequent reshock obtained using simultaneous PLIF and PIV is shown in Figure 1. A non-dimensional length scale is proposed to parametrically link the initial condition dependence to R-M mixing. It was observed experimentally that high wave number (short wavelength) modes are necessary to enhance the mixing and transition to turbulence. Statistics such as non dimensional growth widths, density self correlation, turbulent kinetic energy, Reynolds stresses and variances of velocity fluctuations were measured to quantify the amount of mixing for different initial condition configuration. The results indicate a strong correlation between initial condition parameters and mixing at late times. These results present an opportunity to predict and “design” late-time turbulence, with transformative impact on our understanding and prediction of Inertial Confinement Fusion (ICF) and general fluid mixing processes. The experimental results obtained are being compared with data from ongoing 3-D ILES numerical simulations.

This work is supported by Los Alamos Laboratory Directed Research & Development Program.



**Figure 1.** (A) - An image of the concentration field using PLIF showing time evolution of RM instability after single shocking the varicose curtain and re-shocking the structure at 385  $\mu$ s. White line is the demarcation showing the re-shocked morphologies. (B) - An image of the vorticity field of the shocked curtain with overlaid velocity vectors.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Megan Leftwich   | LA-UR 11-02045 |
| Group:          | P-23   |                |
| Mentor:         | Kathy Prestridge   |                |
| Field of Study: | Engineering  |                |
| Discipline:     | Mechanical Engineering   |                |
| Appointment:    | Agnew National Security Postdoctoral Fellow                    |                |
| Poster Title:   | Motivation, Design, and Fabrication of the Vertical Shock Tube |                |

## ABSTRACT

Shock-driven mixing occurs in supernovae, inertial confinement fusion capsules, and weapons. To study shock driven turbulence and contribute to turbulence models and simulation validations, we need an unsteady driver (a shock wave) that can be repeatedly generated on a laboratory scale so that large ensembles of data can be collected. Shock tubes provide this capability as well as flexibility in experimental parameters. Our shock tube facilities allow us to use high-resolution diagnostics on repeatable experiments, and important flow parameters are easily varied (Mach number, Atwood number, etc.). However, the current shock tube can only produce small variations in initial conditions, and they are 2D. However, priority research requires an interface that is: 3D, multi-mode, multi-directional, statistically stationary, minimally diffuse, single interface and membraneless. The a new vertical shock tube (the VST) will have this capability. A custom designed co-flow initial condition generation system will be able to produce a multi-mode three-dimensional interface between a light gas (air) and a heavy one (sulfur hexafluoride). The decision to make the shock tube vertical was to accommodate the need for a single interface. By aligning the tube with gravity, this can be done without a membrane. When designing the VST, we considered not only the current research needs, but also anticipated the needs and capabilities of the future. All of the components of the test section and diagnostics are modular and can be changed to meet different data acquiring objectives. While current diagnostic techniques are suitable to Mach 3, the VST can achieve higher Mach numbers so as to remain useful when new methods are developed. Several sub-systems of this lab-scale facility have been fabricated—the pneumatic driver, initial condition generation system, and support structure—and the VST has been designed and is currently being made. We will take the first shots this summer.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Suhas Pol   | LA-UR 11-02451 |
| Group:          | P-23  |                |
| Mentor:         | B. J. Balakumuar  |                |
| Field of Study: | Engineering   |                |
| Discipline:     | Mechanical Engineering (Fluid Dynamics)                             |                |
| Appointment:    | Postdoctoral Research Associate                                     |                |
| Poster Title:   | Understanding Wind Turbine Fatigue Using advanced Fluid Diagnostics |                |

## ABSTRACT

The design criterion of today's commercial on-shore and off-shore wind turbines expects turbines to operate for a span of twenty years. Nonetheless, the turbines fail far more often due to extreme fatigue conditions under which they operate, resulting in a steep increase in the cost of wind energy. The precise mechanism of early wind turbine failure has not been identified. However, it is likely that fatigue loading on turbines is augmented due to the complex nature of the varying inflow winds and turbulent wakes generated at the upstream turbines. This leads to the amplification of unsteady aerodynamic loads impacting the whole turbine assembly. Diagnostics to measure the large scale flows around wind turbines are limited to LIDARs, SODARs, sonic and thermal anemometry. Each of these diagnostics either suffer from limitations in accuracy or data yield, resulting in an incomplete understanding of flow features around wind turbines such as wake structures and boundary layer flows around the blades.

Two new diagnostic implementations of Particle Image Velocimetry (PIV) are being developed at LANL to facilitate understanding of wind turbine aerodynamics in unprecedented detail. We have developed a Large-Field PIV (LF-PIV) diagnostic at LANL to measure large scale flow fields (of up to 100cm x 75cm per camera) in the wake of wind turbines operating under field conditions. This diagnostic, which represents a significant leap in the field of view of existing PIV systems, allows the measurement of velocity fields at multiple points with high accuracy. As a validation exercise, a comparison study of large field PIV measurements with typical PIV measurements (field size of ~10cm x 7.5cm) was conducted under laboratory conditions. The mean velocity statistics obtained from both measurement methods are within 1% agreement of each other for a flow turbulence intensity levels as high as about 50%.

In addition, one of the hindrances in accurately predicting wind turbine performance is the lack of understanding of flow separation around the blades as they rotate in an unsteady inflow environment. In order to understand this problem, we have developed an in-situ rotating PIV system (patent application in progress) that is capable of measuring blade boundary layers on a rotating turbine. The system is currently being prepared for deployment at LANL's wind turbine field station at TA-49.

## Theoretical Division

### T-1

|                 |   |                |
|-----------------|---|----------------|
| Name            | Valery Borovikov  | LA-UR 11-03048 |
| Group:          | T-1/T-5   |                |
| Mentor:         | Art Voter and Xianzhu Tang  |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Computational Condensed Matter Physics  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Influence Of Interstitials or Vacancies Introduced into Grain Boundary on Sliding Process in bcc Tungsten |                |

### ABSTRACT

Atomistic computer simulations were performed to study the influence of radiation-induced damage on grain boundary (GB) sliding process in bcc tungsten (W). For a number of GBs, we found the surprising result that introducing interstitials or vacancies into GB can reduce the average sliding-friction force under shear by more than an order of magnitude. Moreover, because these GBs typically shear in a well-known “coupled” way, we speculate that this may provide W with a built-in “self-healing” capability under irradiation conditions, as follows. A collision cascade produces vacancies and highly mobile interstitials; the diffusing interstitials find, and are trapped at, a nearby GB. The interstitial-loaded GB is now so easy to shear that internal stresses in the crystal may start it moving, and the coupled motion causes it to sweep past the cascade center, sweeping up the vacancies as it goes. We have also observed that as the number of interstitials in the GB is varied, the direction of the coupled motion sometimes reverses, causing the GB to sweep in the opposite direction under the same applied shear stress.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Ivana Matanovic  | LA-UR 11-02695 |
| Group:          | T-1/MPA-11   |                |
| Mentor:         | Neil Henson and Fernando Garzon  |                |
| Field of Study: | Materials Science  |                |
| Discipline:     | Theoretical Electrochemistry   |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | Theoretical Study of Electrochemical Processes on Novel Platinum Group Metal Catalysts |                |

## ABSTRACT

Future energy security concerns demand a transition from fossil-fuels to a more environmental benign energy sources. The use of fuel cells to directly convert chemical energy of fuels to electricity is a promising route for achieving this. Efficient fuel cell performance however requires the engineering of platinum group metal catalysts with higher mass activity and more stability. For designing catalysts with such performances better theoretical understanding of elementary electrochemical processes on the solid surfaces are crucial. We have, therefore, undertaken a comprehensive and systematic computational study of the structure, reactivity and stability of different materials based on platinum group metals such as Pt-Ni alloys and Pt nanotubes using the plane wave, pseudopotential implementation of DFT. The change in the catalytic activity of the platinum surface induced by the structural or compositional changes are studied by calculating equilibrium adsorption potentials for oxygen reduction reaction (ORR) intermediates and by constructing free energy diagrams in the ORR dissociative mechanism network. In addition, the stability of these materials in aqueous environments is investigated in the terms of relative electrochemical dissolution shifts and by determining the most stable state of the surface as a function of pH and potential as represented in Pourbaix diagrams.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Aaron Pierpont  | LA-UR 11-03125 |
| Group:          | T-1   |                |
| Mentor:         | Enrique Batista and Richard Martin  |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Theoretical Chemistry   |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | DFT Study of Cp <sub>2</sub> Th and Cp <sub>2</sub> U Catalysts for Hydrodenitrogenation (HDN) and Hydrodesulfurization (HDS) |                |

## ABSTRACT

As of 2009, fossil fuels comprised over 80% of US energy consumption, despite global dwindling of fossil fuel reserves. In order to prevent an economic catastrophe, a transition period has been proposed, where abundant, low quality (“dirty”) petroleum feedstocks would bridge the gap between fossil fuels and alternative energy sources. These dirty feedstocks, typically tar sands and oil shales, are contaminated with N- and S-containing organic impurities that pose environmental hazards after combustion. Once the impurities are removed, the upgraded feedstock may be safely used for fuel.

N/S-heterocycles such as pyridine and thiophene are some of the most persistent contaminants in dirty petroleum and are conventionally removed via hydrotreating, in which the heterocycle is reacted with hydrogen over a suitable heterogeneous catalyst to remove the nitrogen as ammonia [hydrodenitrogenation (HDN)] or sulfur as hydrogen sulfide [hydrodesulfurization (HDS)]. However, due to the drawbacks of current hydrotreating processes (high pressures and temperatures required, poorly-understood reaction mechanisms, etc.), there has been renewed interest in homogeneous catalysts, albeit with mixed results; even though potent transition metal catalysts have been discovered, they are only active towards a narrow range of substrates and tend to be stoichiometric as opposed to catalytic.

Fortunately, early actinide catalysts of the type Cp<sub>2</sub>An(R)<sub>2</sub> (Cp\* = pentamethylcyclopentadienyl; An = Th, U; R = Me, Ph) have been more potent towards the strong C-N and C-H bonds of substrates such as pyridine-N-oxide and 2-picoline (2-methylpyridine). Here, DFT calculations are performed on model Cp\*<sub>2</sub>U(Ph)<sub>2</sub> and Cp\*<sub>2</sub>Th(Ph)<sub>2</sub> catalysts to predict how well this chemistry extends to pyridine as well as thiophene (C-H/C-S activation).

|                 |   |                |
|-----------------|---|----------------|
| Name            | Xiaodong Wen  | LA-UR 11-03125 |
| Group:          | T-1   |                |
| Mentor:         | Richard Martin and Sven Rudin                                   |                |
| Field of Study: | Materials Science   |                |
| Discipline:     | Electronic Properties   |                |
| Appointment:    | Postdoctoral Research Associate                                 |                |
| Poster Title:   | The High Temperature UC <sub>2</sub> Phase - A Rotational Solid |                |

## ABSTRACT

The structural, optical and electronic property of the high temperature UC<sub>2</sub> phase (cubic phase) is examined utilizing hybrid DFT method (HSE0<sub>6</sub>). The high temperature UC<sub>2</sub> phase contains C<sub>2</sub> units with the computed C-C distance in 1.45 Å, which is in the range of CC double bond. From the molecular orbital point of view, there should be 12 valence electrons per C<sub>2</sub> unit to make a double C-C bond (the antibonding orbital, 1π\* is half occupied). Therefore, we proposed that the C<sub>2</sub> units would formally be C<sub>24-</sub>, indicating that there are 2 electrons in f states of the U atoms (as confirmed by the calculated magnetic moment and the density of states). The calculated high-temperature UC<sub>2</sub> AFM, FM and NM structures are converged to paramagnetic one, as expected. The calculated density of states shows that the cubic UC<sub>2</sub> structure is semiconductor, which is confirmed by experimental observation at LANL. Interestingly, the C<sub>2</sub> units can be rotated freely or partially freely, indicating the high temperature UC<sub>2</sub> phase is a kind of rotational solid. In addition, The high pressure properties of the low (tetragonal phase) and high temperature UC<sub>2</sub> phase are investigated; no phase transition occurs up to 100 GPa. Molecular dynamics simulations are performed to consider the effect of temperature; the result shows that the C<sub>2</sub> units in the low temperature phase start to rotate above 1500°C, which is in agreement with experiment.

## T-4

|                 |  |                |
|-----------------|--|----------------|
| Name            | Jason Haraldsen  | LA-UR 11-02101 |
| Group:          | T-4  |                |
| Mentor:         | Alexander Balatsky   |                |
| Field of Study: | Physics  |                |
| Discipline:     | Condensed Matter   |                |
| Appointment:    | Postdoctoral Research Associate                                |                |
| Poster Title:   | Emergent States in Paraelectric and Superconducting Interfaces |                |

### **ABSTRACT**

We examine the modified electronic states at the interface between superconducting and ferroelectric/paraelectric films. We find that the coupling of a classical fluctuating paraelectric and superconducting order parameters can significantly modify these orders at the interface. Using an effective action and a Ginzburg-Landau formalism, we show that terms linear in the electric polarization produce a modulation of the polarization and superconducting order parameters while in the ordered states. We also show that the paraelectric state creates an interface-induced ferroelectric polarization. These effects are limited to the interfacial region and we will discuss implications of this work for the experiments on the epitaxial oxide films.

## T-5

|                 |   |                |
|-----------------|---|----------------|
| Name            | Tsvi Achler   | LA-UR 11-03125 |
| Group:          | T-5   |                |
| Mentor:         | Luis Bettencourt  |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Computational Neuroscience                              |                |
| Appointment:    | Postdoctoral Research Associate                         |                |
| Poster Title:   | Processing Mixtures of Patterns Using Generative Models |                |

### ABSTRACT

The brain has capabilities to process pattern mixtures that remains unmatched by computer algorithms. We hypothesize that recognition centers of the brain construct an internal copy of inputs using knowledge the brain has previously accumulated, in accordance with a class models called "generative models". Subsequently, it minimizes the error between the internal copy and the input from the environment. We study how this strategy may overcome known combinatorial problems associated with pattern mixtures and display cognitive phenomena.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Alexander Gutfraind  | LA-UR 11-02971 |
| Group:          | T-5/T-CNLS/D-6   |                |
| Mentor:         | Aric Hagberg and Feng Pan  |                |
| Field of Study: | Mathematics and Computer Science                                       |                |
| Discipline:     | Network Science  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | The Sendai Network Problem: Optimizing Network Deployment and Recovery |                |

### ABSTRACT

While network design problems attempt to optimize the network topology, we consider the problem of installing a specified network. Assume that the cost of installing a node depends on which other nodes have already been installed. This leads to a NP-hard optimization problem over  $n!$  permutations. Fortunately, there exist efficient approximations, and dynamic programming can find optimal solutions to small instances. Using those techniques, it becomes possible to optimize the recovery schedule of infrastructure networks, helping prepare for an attack or a large-scale natural disaster.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Zhengping Ji  | LA-UR 11-03048 |
| Group:          | T-5/ISR-2   |                |
| Mentor:         | Luis Bettencourt and Steven Brumby  |                |
| Field of Study: | Mathematics and Computer Science  |                |
| Discipline:     | Neural Computation  |                |
| Appointment:    | Postdoctoral Research Associate   |                |
| Poster Title:   | Deep Generative Networks as Systems Level Models of Primate Visual Cortex |                |

## ABSTRACT

Building cortex-like visual representations is a long-standing goal of computational vision. Many existing models of visual cortex (e.g., HMAX [1]) use learned hierarchical (sparse) representations to describe visual scenes, and present state-of-the-art accuracy on image recognition. However, some fundamental mysteries still remain in this area, such as why the over-completeness of primary visual cortex (vs. its LGN inputs) is necessary and what the functional role of extensive lateral and feedback connections is.

Here, we describe a deep generative network model, following the architecture of visual cortex but emphasizing feedback processes as generators of semantically informed, locally self-consistent image predictions. Our approach is a generalization of generative models with sparse constraint, from primary visual cortex (V1) to a hierarchy of (deep hidden) cortical layers, corresponding to visual areas V2, V4, and IT in the primate ventral pathway. The Bayesian framework is utilized to address visual inference in the hierarchical structure, where each cortical area is an expert for inferring certain aspects of the visual scene, constrained by the bottom-up data from the feedforward connections, lateral data with temporal contexts, and the top-down data from feedback connections. An optimized continuation method is adopted to iteratively search a converged solution with high efficiency.

This generative network is applied to natural images, and develops internal presentation that matches the neuroscience findings in primate visual cortex. The primary visual cortex, V1, presents an over-complete set of Gabor-like filters, while higher layers in the ventral pathway contains more complex features than V1. A degree of visual invariance regarding objects is emergent via local pooling of the hierarchical presentations. Using the benchmark object identification data sets like Caltech 101 [2], our new systems-level computational model is able to generate hierarchical internal representation better than the well-known SIFT-based approach [3] and convolutional networks [4], etc.

## Reference:

- [1] T. Serre, A. Oliva and T. Poggio. A feedforward architecture accounts for rapid categorization. In PNAS, 2007.
- [2] L. Fei-Fei, R. Fergus, and P. Perona. Learning generative visual models from few training examples: an incremental Bayesian approach tested on 101 object categories. In CVPR, 2004.
- [3] K. Jarrett, K. Kavukcuoglu, M. Ranzato, and Y. LeCun. What is the best multi-stage architecture for object recognition? In ICCV, 2009.
- [4] S. Lazebnik, C. Schmid, and J. Ponce. Beyond bags of features: Spatial pyramid matching for recognizing natural scene categories. In CVPR, 2006.

## T-6

|                 |  |                |
|-----------------|--|----------------|
| Name            | Ghanim Ullah   | LA-UR 11-03125 |
| Group:          | T-6/P-21   |                |
| Mentor:         | John Pearson and Garrett Kenyon  |                |
| Field of Study: | Bioscience   |                |
| Discipline:     | Theoretical Chemistry  |                |
| Appointment:    | Postdoctoral Research Associate  |                |
| Poster Title:   | A Data-Driven Model of a Modal Gated Ion Channel: The IP3 Receptor in Insect Sf9 Cells |                |

### ABSTRACT

The inositol 1,4,5-trisphosphate (IP3) receptor (IP3R) calcium release channel plays a central role in the generation and modulation of intracellular calcium signals in animal cells. To gain insight into the complex mechanisms regulating the gating kinetics of this ubiquitous channel, we developed a quantitative model to account for all the experimentally observed gating behaviors of single native IP3R channels from insect Sf9 cells. The model can closely reproduce the equilibrium open probability, as well as the channel open probability, mean durations and relative prevalence for all three gating modes of the channel, observed over a broad range of ligand concentrations. It also reproduces the distribution of channel response latencies following different kinds of ligand concentration changes. Furthermore, the model predicts gating behaviors as yet unexplored. Our approach demonstrates a simple and transparent technique to construct the simplest kinetic state network that accounts for complex observed behaviors of a system, which can be adapted to Markov chain models in general.

|                 |   |                |
|-----------------|---|----------------|
| Name            | Jingshan Zhang  | LA-UR 11-02971 |
| Group:          | T-6   |                |
| Mentor:         | Alan Perelson and Ruy Ribeiro                                       |                |
| Field of Study: | Bioscience  |                |
| Discipline:     | Biophysics  |                |
| Appointment:    | Director's Postdoctoral Fellow                                      |                |
| Poster Title:   | Quantifying the Role of FDC as a Long Term Reservoir of HIV-1 Virus |                |

### ABSTRACT

HIV-1 infections cannot be completely eradicated by drug therapy because the virus can persist in some reservoirs for a long time. It has been established that follicular dendritic cells (FDC) act as such a reservoir for HIV-1, although the long-term ability for FDC to retain HIV-1 is yet to be quantified. With the help of data on long-term plasma viremia and the FDC virus pool, we study the property of FDC as an HIV-1 reservoir, and find evidence that FDC could be the main source of low-level viremia between a few months to ~2 years after therapy initiation. We then evaluate the effects of potential drug therapies to drive HIV-1 out of the FDC reservoir, a possible next step toward eliminating the infection.

## Weapons Experiments Division

### WX-7

|                 |   |                |
|-----------------|---|----------------|
| Name            | Amanda Duque  | LA-UR 11-02735 |
| Group:          | WX- 7   |                |
| Mentor:         | Lee Perry   |                |
| Field of Study: | Chemistry   |                |
| Discipline:     | Chemical Kinetics   |                |
| Appointment:    | Director's Postdoctoral Fellow  |                |
| Poster Title:   | Temperature Measurements of High Explosives Under Microwave Irradiation for Kinetic Analysis of Thermally Induced Transitions |                |

### ABSTRACT

Microwave (MW) irradiation offers the unique ability to uniformly heat material at extremely high rates while maintaining a uniform temperature distribution. Compared to the large number of modeling studies that exist on predicting the temperature of a sample under MW exposure, there are few experimental temperature measurements. One primary difficulty is that conventional methods for measuring temperature adversely affect the MW distribution within the system, and are themselves affected by the presence of the microwaves. Metal thermocouples may be introduced after the MW irradiation has ceased, but this does not give accurate real-time measurements. For this reason, fiber-optic thermometers are being explored to make single-point measurements of samples while undergoing MW irradiation. We utilize this technique for the temperature acquisition of high explosives heated by MWs for kinetic analysis of thermally induced transitions.

Our goal is to acquire temperature measurements in real time for the study of decomposition kinetics of high explosives, specifically HMX. Understanding how the material will interact with MWs is an important component of this study, and involves measuring the material's dielectric properties. Beginning at 160 °C, HMX undergoes a  $\beta$ - to  $\delta$ - conformational phase transformation; the  $\delta$ -form of HMX produces a second-harmonic generation (SHG) at 532 nm when irradiated with 1064 nm laser light. Detection of the SHG intensity, and thus mole fraction of  $\delta$ -HMX present, as a function of temperature will be a useful probe for describing the HMX decomposition kinetics in a fast kinetic regime ( $< 0.1$  s) that has never been explored. Previous work performed at LANL studied similar HMX behavior and though very successful, used external heating methods that are inherently transport limited and cause a low heating rate and large temperature gradients. The incorporation of MWs will aid in building a more complete model of HMX decomposition and understanding the role that the crystalline phases play in a kinetic regime that has been sparsely investigated.

To date, we have shown that fiber-optic temperature measurement techniques can be effectively interfaced with our current microwave setup. We have shown reproducible surface temperature measurements of a non-HMX microwave sensitized explosive upon exposure to a 200 ms pulse of 2.5 kW MW energy (2.45 GHz) that closely follows modeling results. A key step to obtaining accurate temperatures is careful calibration that mimics the actual experimental setup as closely as possible. The next-generation fixture design that minimizes sample temperature gradients has been developed and is currently being machined for use in future experiments. Additionally, dielectric property measurements are currently underway for microwave-sensitized HMX composites.

Name: Amanda Duque (continued)

LA-UR 11-02735

Group: WX- 7

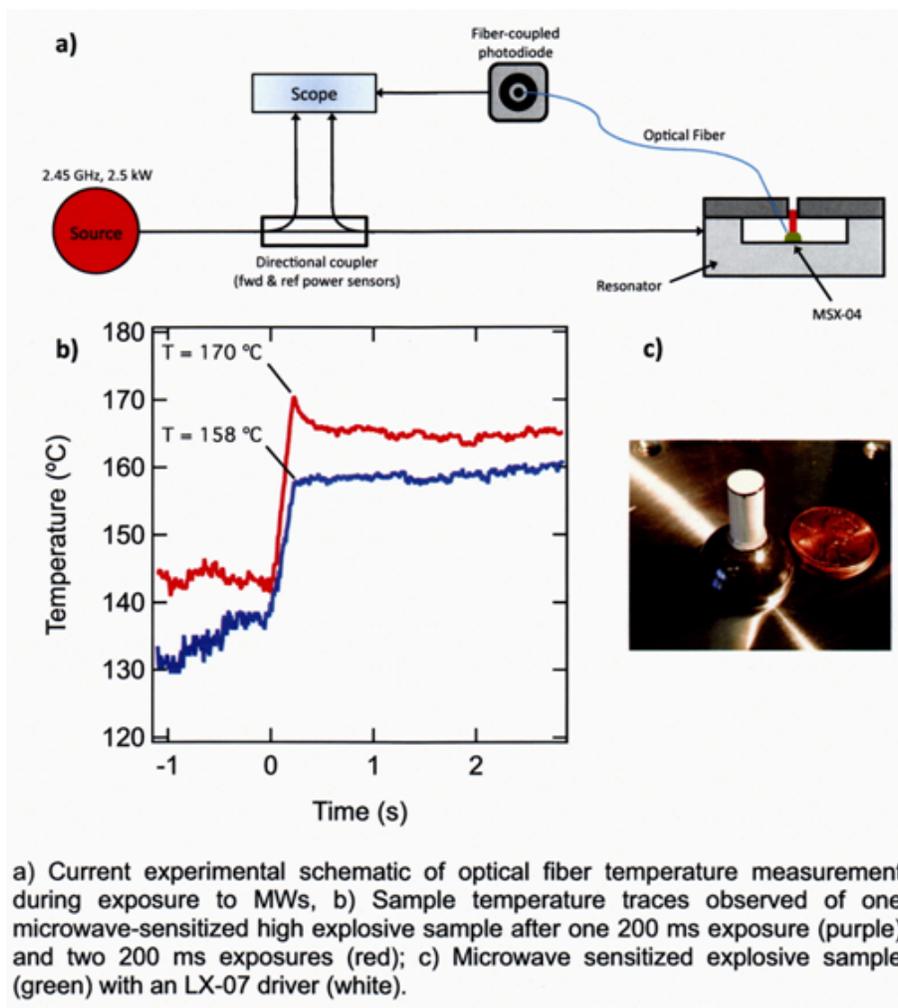
Mentor: Lee Perry

Field of Study: Chemistry

Discipline: Chemical Kinetics

Appointment: Director's Postdoctoral Fellow

Poster Title: Temperature Measurements of High Explosives under Microwave Irradiation for Kinetic Analysis of Thermally Induced Transitions



## WX-9

|                 |  |                |
|-----------------|--|----------------|
| Name            | Nhan Dang  | LA-UR 11-03048 |
| Group:          | WX-9   |                |
| Mentor:         | Shawn McGrane and David Moore                          |                |
| Field of Study: | Physics  |                |
| Discipline:     | Spectroscopy   |                |
| Appointment:    | Postdoctoral Research Associate                        |                |
| Poster Title:   | Picosecond Temperature Measurement in Condensed Phases |                |

### ABSTRACT

In a manner analogous to the measurements of molecular vibrational temperature using the spontaneous Raman anti-Stokes to Stokes ratio, we demonstrate the capability of femtosecond stimulated Raman scattering (FSRS) data to measure the temperature of condensed matter with sub-picosecond temporal resolution. We present experimental results of the temperature dependence of FSRS in a Calcite single crystal from cryogenic to room temperature. Measured temperature using Raman loss to Raman gain ratios for low frequency modes ( $< 300 \text{ cm}^{-1}$ ) are compared to thermocouple temperature and shown to be in agreement with theoretical predictions. We also present temperature jump measurements following a femtosecond ultraviolet pump pulse, demonstrating that FSRS can measure the nonequilibrium time evolution of mode specific vibrational temperatures on picosecond time scales. Improvements for accuracy and sensitivity of picoseconds temperature determinations using FSRS method are discussed.

|                 |  |                |
|-----------------|--|----------------|
| Name            | Carl Johnson   | LA-UR 11-03048 |
| Group:          | WX-9   |                |
| Mentor:         | Von Whitley  |                |
| Field of Study: | Physics  |                |
| Discipline:     | Shock and Detonation Physics                                   |                |
| Appointment:    | Postdoctoral Research Associate                                |                |
| Poster Title:   | Revisiting the Munroe Effect, New Experiments and Applications |                |

## ABSTRACT

In 1888, Charles Munroe reported surprising witness plate results when testing explosive charges that had holes drilled in their faces. He discovered that a charge that had a hole drilled in its face would produce significantly larger dents below the hole than in the areas where the charge was solid. In other words, removal of some of the explosive mass caused more damage. We believe the damage below the removed explosive is caused by decomposition products from the detonating explosive being driven into the witness plate at velocities approaching 10 km/s. The interaction mechanisms between the high-velocity decomposition gases and the solid witness plate material are still poorly understood, owing principally to the extreme violence of this interaction environment and the difficulties in making measurements there.

To further our understanding of the damage mechanism, now known as the Munroe effect, we have designed high explosive (HE) shaped charges amenable to high-speed camera measurements. Measurements of gas jet propagation velocity and morphology have been made using both framing camera and streak camera equipped detonations. Witness plate materials were varied, with properties carefully selected to span the range of strength, density, and heat capacity. Witness plates were sectioned and analyzed microscopically in the damaged area to understand damage mechanisms and the extent of damage for each material. In addition to this experimental effort, we have completed hydrocode calculations using both CTH (an Eulerian hydrocode from Sandia National Laboratory) and ALE3D (an arbitrary Lagrange-Eulerian hydrocode from Lawrence Livermore National Laboratory). The results of experiments and calculations are compared and the limitations of the current hydrocodes are discussed.

This hollow charge HE technology has practical applications in mining/drilling for minerals, the defeat of improvised explosive devices (IEDs), and other military applications such as wall breaching. Currently, metal lined shape charges are used to perforate down-hole well bores. Material displaced by the shaped charge jet becomes densely packed, making subsequent oil production more difficult. Hollow charges alleviate this affect since no solid projectile is formed. Hollow charges also prove useful in the defeat of IEDs, as a gas jet can perforate a bomb casing and deflagrate the target HE fill without initiating a detonation.

## X-Computational Physics Division

### XCP-4

|                 |   |                |
|-----------------|---|----------------|
| Name:           | Amy Lee   | LA-UR 11-02531 |
| Group:          | XCP-4   |                |
| Mentor:         | Randy Bos and Thomas Dey                          |                |
| Field of Study: | Physics   |                |
| Discipline:     | Computational Physics                             |                |
| Appointment:    | Postdoctoral Research Associate                   |                |
| Poster Title:   | Modeling the Response of Glazing to Blast Loading |                |

### ABSTRACT

Glass fragmentation due to an explosive force in an urban setting will cause of the majority of injuries. The development of an accurate and detailed model to simulate the response of window glazing to a blast load is the focus of this research. Historically the potential hazard to building occupants has been determined from explosive testing of window systems. Current available models and prediction software packages rely on simple empirical expressions developed from the data collected from experimental testing. Post-breakup and fly-out of the shards of glass is a complex phenomenon that has not been widely modeled. Recent models have resulted in overly conservative estimates of damage and injuries. The work for this research will use the advantage of hydrocodes to capture the complex behavior of the blast wave. Fragment size, shape and velocity distribution are anticipated to be a function of the incident angle of the blast wave. Combined finite-discrete element code will be used to describe the fracture and fly-out behavior of the glazing. Blast load calculations will be coupled with the glazing response analysis so the deflection of the glazing can be computed simultaneously with increasing blast pressures.

## XCP-5

|                 |  |                |
|-----------------|--|----------------|
| Name:           | Charles Starrett                                     | LA-UR 11-02080 |
| Group:          | XCP-5  |                |
| Mentor:         | Didier Saumon and Jonathan Boettger                  |                |
| Field of Study: | Physics  |                |
| Discipline:     | Plasma Physics                                       |                |
| Appointment:    | Postdoctoral Research Associate                      |                |
| Poster Title:   | Many Body Correlations in a Variational Average Atom |                |

### ABSTRACT

Modeling hot dense plasma is crucial to understanding numerous physical phenomena in inertial confinement fusion plasmas, stellar interiors, planetary science and geophysics. It is also extremely difficult for two main reasons. First, the densities and temperatures encountered are precisely those where electrons can no longer be clearly distinguished as being either bound or free, as they can be in liquids, solids or fully ionized plasmas. And second, the ion structure is somewhere between being long range ordered, as in a solid, and being completely disordered, as in fully ionized plasmas. These hot dense plasmas lie at the intersection of two well-understood regimes, and to model them accurately is a challenge.

Building on existing work, we have derived from a variational standpoint an average atom style model, which is applicable from liquid to fully ionized plasma conditions. The model is generic in that it can be applied to any element in the periodic table, with nuclei treated as classical particles and electrons treated with quantum mechanics through density functional theory. Many body interactions are taken into account with the local density approximation (electron-electron), the hypernetted chain (nucleus-nucleus), and the quantum hypernetted chain (electron-nucleus) approximations.

In this poster we present the theoretical background and early results of numerical simulations, focusing mainly on the equation of state and average ionization, and comparing to other established models and experimental results.

## XCP-6

|                 |   |                |
|-----------------|---|----------------|
| Name            | Chengkun Huang  | LA-UR 11-03048 |
| Group:          | XCP-6   |                |
| Mentor:         | Brian Albright and Tom Kwan   |                |
| Field of Study: | Physics   |                |
| Discipline:     | Plasma Physics  |                |
| Appointment:    | Director's Postdoctoral Fellow  |                |
| Poster Title:   | A Double-Foil Target for Improving Beam Quality In Laser Ion Acceleration with Thin Foils |                |

### ABSTRACT

Mid-Z ion driven fast ignition inertial fusion requires ion beams of 100s of MeV energy and  $< 10\%$  energy spread. An overdense nm-scale foil target driven by a high intensity laser pulse can produce an ion beam that has attractive properties for this application. The Break Out Afterburner (BOA) is one laser-ion acceleration mechanism proposed to generate such beams, however the late stages of the BOA tend to produce too large of an energy spread. The spectral and spatial qualities of the beam quickly evolve as the ion beam and co-moving electrons continue to interact with the laser. Here we show how use of a second target foil placed behind a nm-scale foil can substantially reduce the temperature of the co-moving electrons and improve the ion beam energy spread. Particle-In-Cell simulations reveal the dynamics of the ion beam under control. Optimal conditions for improving the spectral and spatial spread of the ion beam is explored for current laser and target parameters, leading to generation of ion beams of energy 100s of MeV and 6% energy spread, a vital step for realizing ion-driven fast ignition.