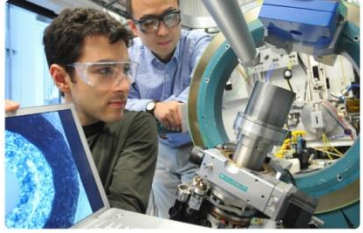

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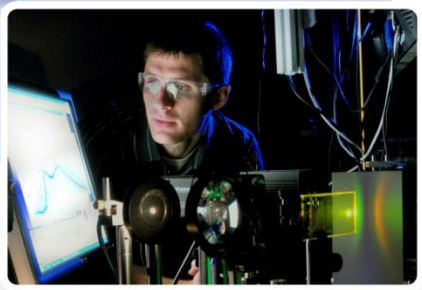

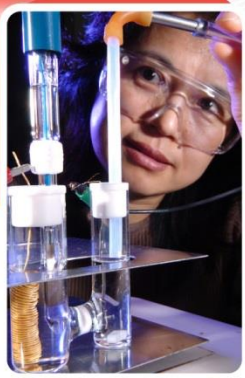

2014 Postdoctoral Research and Career Symposium

Argonne National Laboratory Postdoctoral Research and Career Symposium

October 23, 2014

Co-sponsored by:

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2014 Postdoctoral Research and Career Symposium

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2014 Postdoctoral Research and Career Symposium Agenda

Morning Session: TCS Conference Center

8:00–8:30 AM	**Continental Breakfast and Registration**
8:30–8:35 AM	**Welcome Remarks from Postdoctoral Society of Argonne**
8:35–9:05 AM	**Keynote Address by Seth Darling**
9:05–9:30 AM	**Career Skills Plenary by Meridith Bruozas**
9:30–11:30 AM	**Company Exhibit Booths: TCS Room 1416** **9:30–10:00 AM:** Designated booth set up time
9:40–10:30 AM	**Academic Panel Discussion: TCS Room 1406–1407** Daniel Shoemaker — University of Illinois Sunshine Silver — Concordia University Brittany B. Nelson-Cheeseman — University of St. Thomas
10:40–11:30 AM	**Industry Panel Discussion: TCS Room 1406–1407** Erin Broderick — UOP-Honeywell Steven Kraft — Cabot Microelectronics Elina Vitol — Ecolab

Lunch Provided to Symposium Participants: Building 213 Cafeteria

11:45 AM–1:15 PM	Postdoctoral Research Poster Presentations

Afternoon Session: TCS Conference Center

1:30–1:45 PM	**Research Plenary by Al Sattelberger: TCS Room 1416**
1:45–2:45 PM	**Associate Laboratory Director Nominated Postdoctoral Speakers:** Sebastien Boisvert — Computing, Environment and Life Sciences Doga Gursoy — Photon Sciences Brandon R. Long — Physical Sciences and Engineering Canan Uckun — Energy Engineering and System Analysis
2:50–4:20 PM	**Parallel Company Presentations and Booth Time** Booths: TCS Room 1416 Presentations: Breakout rooms 1404–05 and 1406–07
4:30–6:00 PM	**Networking Reception with Closing Remarks by Director Littlewood and Poster Award Presentations**

NOTE—Due to time constraints and space availability, a tour of the Leadership Computing Facility will be available for external registrants only at 5:00 PM.

Special thanks to our 2014 Sponsors!

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2014 Postdoctoral Research and Career Symposium

Company Presentations

Time	TCS Conference Rooms 1404	TCS Conference Rooms 1405	TCS Conference Rooms 1406–1407
3:00 PM	Oak Ridge National Laboratory	Allstate Insurance	Clean Energy Trust
3:15 PM	Institute for Defense Analysis	AbbVie	Chicago Innovation Exchange
3:30 PM	International Atomic Energy Agency	Coskata, Inc.	Ware Connections
3:45 PM	General Motors	Donaldson Company, Inc.	H-CORE, LLC
4:00 PM	Rubicon Technology	LanzaTech	

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2014 Keynote Address

A Random Walk through Science… and Drawing on Those Experiences

Seth Darling, PhD, Nanoscience and Technology Division
Argonne National Laboratory

Seth B. Darling is a Scientist at Argonne National Laboratory and a Fellow at the Institute for Molecular Engineering at the University of Chicago. After receiving his PhD from the University of Chicago in physical chemistry, he joined Argonne as the Glenn Seaborg Distinguished Postdoctoral Fellow in the Materials Science Division where he studied directed self-assembly of polymers and polymer/nanoparticle hybrid systems. Following his postdoc, Darling joined the Center for Nanoscale Materials at Argonne as a staff scientist. His group's research centers around polymer molecular engineering with a particular emphasis on solar cells, water treatment, and advanced lithography. He also serves as the solar energy strategy leader for Argonne, through which he interfaces with a spectrum of internal scientists, engineers, and managers as well as external domestic and international stakeholders in industry, government, museums and foundations, national laboratories, market analysis firms, academia, and the media.

Welcome Remarks

Jeremy Love, PhD, Postdoctoral Researcher, High Energy Physics Division (HEP), Argonne National Laboratory, Vice President, Postdoctoral Society of Argonne

Jeremy Love is a Postdoctoral Researcher in the HEP Division working on the ATLAS experiment on the Large Hadron Collider (LHC) at CERN, developing and performing novel searches for new experimental evidence of fundamental symmetries of nature. Additionally, he works on integration and commissioning of custom electronics used in the ATLAS data acquisition system designed at Argonne. Love received his PhD from Boston University in 2011 working on the ATLAS Experiment, he was awarded the Alvaro Roccaro Giamporcaro Memorial Award for achievements over a graduate career. He attended Carnegie Mellon University receiving a BS in Physics in 2004 graduating with research honors for contributions to the CLEO collaboration.

Closing Remarks

Dr. Peter Littlewood, Director, Argonne National Laboratory

Peter B. Littlewood is the Director of Argonne National Laboratory, one of the nation's largest science and engineering research centers, and a Professor of Physics in the James Franck Institute at the University of Chicago. Littlewood came to Argonne in 2011 after being appointed Associate Laboratory Director of Argonne's Physical Sciences and Engineering directorate, which focuses on discovery science across a broad range of disciplines, and on creating and understanding new materials and chemistries that address the grand challenges in energy and the environment.

Before that, he spent 14 years at the University of Cambridge in the United Kingdom, where he last served as the head of the Cavendish Laboratory and the Department of Physics. Littlewood started his career at Bell Laboratories, beginning in 1980 as a postdoctoral member of the technical staff; by 1992, he had worked his way up to head of Theoretical Physics Research. Littlewood is an internationally respected scientist who holds six patents, has published more than 200 articles in scientific journals and has given more than 200 invited talks at international conferences, universities and laboratories. He is a fellow of the Royal Society of London, the Institute of Physics and the American Physical Society, and is an associate member of The World Academy of Sciences. Littlewood holds a bachelor's degree in Natural Sciences (Physics) and a PhD in Physics, both from the University of Cambridge.

Career Skills Plenary
Networking at a Social Event: The Keys to Working a Room

Meridith Bruozas, MS, Manager of Educational Programs
Argonne National Laboratory

Meridith Bruozas is the Manager of Educational Programs and Outreach with a focus on developing high quality educational programs that are aligned to mission science and support the development of the next generation of scientists and engineers. She oversees on- and off-site programming that ranges from inspiring and connecting middle school youth to STEM experiences to providing undergraduate and graduate students a once in a life time internship experience. She also focuses on developing key partnerships with local and regional organizations and school systems around STEM education. Bruozas is an educator by training and has spent the past 15 years in a combination of district, not-for-profit and academic service positions researching and promoting STEM education. She earned her MS in Learning Sciences from Northwestern University and a BS in Secondary Education and Biology from Ball State University. Her publications include several national curriculum resources for the K-12 classroom and numerous professional presentations and research articles. She is a member of the National Science Teacher Association, International Society of Technology in Education, Women in Science and Technology and Chicago Council of Science and Technology.

Academic Career Panel Speakers

Brittany Nelson-Cheeseman, PhD Assistant Professor, School of Engineering, University of St. Thomas

Brittany Nelson-Cheeseman is beginning her third year in the unique environment of the School of Engineering at the University of St. Thomas, a liberal arts college of 10,000 students in St. Paul, MN. She holds degrees in Materials Science and Engineering from the UC–Berkeley (PhD, MS) and the UW–Madison (BS). Before becoming a professor, she was a postdoctoral researcher at Argonne for three years, working with the Materials Science Division and the Center for Nanoscale Materials (CNM). She continues to be a CNM user, bringing her undergraduate research students to Argonne National Laboratory to participate in nanoscale growth and characterization. She also utilizes growth and characterization facilities at the University of Minnesota. Her research group investigates novel nanoscale oxide materials for energy applications by constructing new materials one atomic layer at a time. She is also expanding into constructing novel layered composite materials via 3D-printing, as well as research on new techniques to facilitate materials

engineering education. As an engineering professor at a liberal arts college, she has had the opportunity to become involved with diverse initiatives, including innovative teaching methods (e.g., flipped classroom), women in engineering, STEM outreach, writing across the curriculum, and mindfulness & meditation in the classroom.

Daniel Shoemaker, PhD Assistant Professor,
University of Illinois, Urbana-Champaign

Daniel Shoemaker received his BS with Honors in Materials Science and Engineering from the University of Illinois in 2006 and his PhD in Materials from the University of California, Santa Barbara in 2010. His doctoral work focused on using neutron scattering and real-space modeling to understand the structure-property relationships of disordered magnetic and electronic oxides. In 2011 he began a postdoctoral appointment in the Materials Science Division of Argonne National Laboratory where he investigated the synthesis of superconductors and semiconductors with a focus on *in situ* spectroscopy and x-ray diffraction. Shoemaker joined the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign as an Assistant Professor in August 2013.

Sunshine Silver, PhD, Assistant Professor of Chemistry,
Concordia University Chicago

Sunshine Silver received her BS in chemistry from St. Cloud State University, MN, where enzymatic biochemistry caught her attention. During her doctoral studies at Montana State University, Bozeman, she developed an interest in teaching at the undergraduate level. Following a postdoctoral appointment at Argonne in the Solar Energy Conversion group, she accepted an academic appointment at Concordia University Chicago as an Assistant Professor of Chemistry. She currently teaches a wide variety of chemistry and science courses for undergraduate students, although her passion still lies in the area of biochemistry. Silver's research interests include elucidating enzyme mechanisms, understanding protein-protein interactions and finding renewable and sustainable energy sources.

Industry Career Panel Speakers

Steven Kraft, PhD, Scientist,
Cabot Microelectronics

Steven Kraft received his PhD in Inorganic Chemistry from Purdue University in 2012 as a Robert R. Squires Fellow synthesizing and studying uranium organometallic compounds, and his BS in Chemistry from St. Norbert College in 2008. In early 2014, Kraft completed a postdoctoral research position at Argonne National Laboratory studying heterogeneous and homogeneous transition metal catalysts in the catalysis group in the CSE division. Currently he is a formulation scientist at Cabot Microelectronics developing products to polish materials for the semiconductor industry.

Elina Vitol, PhD, Scientist, Automation Department R&D, NALCO—an Ecolab Company

Dr. Elina Vitol has multidisciplinary expertise in optical engineering, materials science and biomedical engineering, with work experience in environments ranging from academia and a start-up company to a Fortune 500 corporation. Vitol is currently a Scientist and a Project Leader at Nalco–an Ecolab company, where she is leading a diverse team of scientists and engineers, developing optical sensors for industrial applications. In addition to technical leadership and project management at the R&D level, she is overseeing the process of technology transfer from prototyping to production stage. She also serves as a subject matter expert in evaluating external technologies. Prior to joining Ecolab, Vitol completed her postdoctoral training at the Materials Science Division, Argonne National Laboratory. During her PhD studies, she developed a nanoparticle-based sensor for *in situ* surface-enhanced Raman spectroscopy (SERS) of single living cells and, for the first time, demonstrated that SERS can be used for real time monitoring of cell response to external stimulus. At Argonne, Vitol extended her research to magnetic nanomaterials for cancer treatment. She elucidated the mechanisms of magneto-mechanically induced apoptosis of brain cancer cells and developed hybrid thermally responsive nanomicelles for magnetically-assisted drug delivery. Vitol holds a Bachelor's degree in Optical Engineering from St. Petersburg University of Fine Mechanics and Optics (St. Petersburg, Russia) and Master's and PhD degrees from Drexel University. Her PhD thesis was recognized with Best Doctoral Dissertation award in 2010.

Erin Broderick, Senior R&D Engineer, UOP—A Honeywell Company

Erin Broderick graduated from the University of Illinois, Urbana-Champaign in 2006 with a BS degree in Chemistry. During her time at UIUC, she worked in Professor Eric Oldfield's group synthesizing organic compounds with anti-cancer activity. Broderick continued her education at the University of California, Los Angeles and graduated with a PhD in inorganic chemistry. Her graduate research with Professor Paula Diaconescu involved the synthesis of organometallic complexes for use as catalysts. Following her graduate work, Broderick returned to Illinois to perform research in the homogeneous catalysis group at Argonne National Lab. For the past three years, Broderick has been working in the Exploratory Group at UOP, a Honeywell Company.

Research Plenary
Argonne National Laboratory—Mission, Vision and Innovation

This session provides an overview of Argonne's research missions and themes through presentations by the Deputy Laboratory Director for Programs and four postdoctoral researchers representing each of our four Laboratory Directorates

Dr. Al Sattelberger, Deputy Director for Programs, Argonne National Laboratory

Alfred P. Sattelberger is the Deputy Laboratory Director for Programs at Argonne National Laboratory. He is responsible for the management and integration of the laboratory's science and technology portfolio, strategic planning, and the Laboratory Directed Research and Development (LDRD) program. Sattelberger has been at Argonne since 2006 and has served as the

Associate Laboratory Director (ALD) for Physical, Biological and Computing Sciences, ALD for Physical Sciences, ALD for Energy Engineering and Systems Analysis, and Interim ALD for Applied Sciences and Technology.

Sattelberger obtained a PhD in inorganic chemistry from Indiana University and was a National Science Foundation Postdoctoral Fellow at Case Western Reserve University. Prior to joining Argonne, he was a faculty member in the Chemistry Department at the University of Michigan and a staff member at Los Alamos National Laboratory. at Los Alamos, he held several scientific management positions and was named a Senior Laboratory Fellow in 2005. His personal research interests span actinide coordination and organometallic chemistry, fundamental technetium chemistry, metal-metal bonding and catalysis. He is a Fellow of the American Association for the Advancement of Science (AAAS) and of the American Chemical Society (ACS), the chair of the Chemistry Section of the AAAS, a past chair of the Inorganic Chemistry Division of ACS, a member of DOE's Nuclear Energy Advisory Committee (NEAC), and chair of the Fuel Cycle Subcommittee of NEAC. He holds faculty appointments at Northwestern University and the Harry Reid Center for Environmental Studies at the University of Nevada, Las Vegas. He also lectures occasionally at the University of Chicago.

Sébastien Boisvert, PhD, Director's Fellow,
Mathematics and Computer Science Division
Representing the Computing, Environment and Life Sciences Directorate

Sébastien Boisvert is a Director's Fellow (his project is entitled "Accelerating key workflows in genomics with the actor model") at Argonne National Laboratory (since October 2014; Postdoctoral Appointee from April 2014 to September 2014) where he works with passionate people under the guidance of Professor Rick Stevens in the Computing, Environment, and Life Sciences (CELS) Directorate. He is working on novel actor algorithms to solve grand challenges in metagenomics -- such as the Department of Energy (DOE) Joint Genome Institute (JGI) Great Prairie Soil Metagenome Grand Challenge. He currently works on a distributed metagenome assembler called Spate that is entirely defined in terms of actors. His research also involves designing and implementing a distributed actor compute engine called Thorium for computational biology that can run on various platforms such as Mira at the Argonne Leadership Computing Facility (ALCF). He received a BSc degree in Biotechnology from Université de Sherbrooke (Québec, Canada) in 2008. He also received a MSc degree in Physiology-Endocrinology in 2010 from Université Laval (Québec, Canada) and a PhD degree in the same discipline from the same institution in 2014. His doctoral work was on distributed metagenome assembly using message passing with Professor Jacques Corbeil and Professor François Laviolette.

Canan Uckun, PhD, Postdoctoral Appointee, Energy Systems Division
Representing the Energy and Global Security Directorate

Canan Uckun is a postdoctoral appointee at Argonne National Laboratory since 2012. During her postdoctoral experience, she has been involved in a wide range of projects including power systems modeling, hydro power optimization, and demand response through dynamic pricing of electricity and building technologies. Currently, she works on power systems modeling using stochastic programming in the presence of renewable generation, system level analysis of grid-level energy storage as part of Lab-Directed Research and Development, analysis of global helium markets, and financial transactions for buildings. She has BS and MS degrees in Industrial Engineering from Marmara University and Koc University, Istanbul, Turkey. She also holds a PhD degree in Business and an MBA degree from the University of Chicago, Booth School of Business.

Doga Gursoy, PhD, Postdoctoral Appointee, X-Ray Science Division Representing the Photon Sciences Directorate

Doga Gursoy received the B.Sc. and M.Sc. degrees in electrical engineering from the Middle East Technical University in 2004 and 2007, respectively, and PhD degree in the same field from the Graz University of Technology in 2010. His dissertation was on developing computational methods for optimal data acquisition for near-field electromagnetic and optical tomography systems targeting biomedical applications. After graduation, he joined University of Houston, where he has primarily focused on the modeling and computational aspects of energy-resolving x-ray detection and imaging systems. Since 2013, he is working as a postdoc at the X-Ray Science Division of Argonne National Laboratory. He has been developing tomographic image reconstruction methods for various x-ray imaging techniques. He is interested in multimodal imaging and inverse problems, and the associated algorithms.

Brandon R. Long, PhD, Postdoctoral Appointee, Chemical Sciences and Engineering Division, Representing the Physical Sciences and Engineering Directorate

Brandon R. Long is a postdoctoral appointee in the Electrochemical Energy Storage Department of the Chemical Sciences and Engineering Division at Argonne National Laboratory, where he investigates novel cathode materials for advanced Li-ion batteries. He received his PhD in chemistry from the University of Illinois at Urbana-Champaign in 2012. Long's doctoral studies focused on the electrochemical and spectroscopic study of semiconductors for Li-ion anodes as part of the Energy Frontier Research Center, The Center for Electrical Energy Storage–Tailored Interfaces that is administered by Argonne.

2014 Postdoctoral Research and Career Symposium

Poster Abstracts

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Biology and Environmental Science

A-1

Carbon Budgeting in Plant Microbial Interaction during Nutrient Stress

Desai, Shalaka and Frank Collart

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Symbiotic relationships influence survival and productivity in forest ecosystems and consequently affect ecosystem carbon- nutrient cycling. In addition to fungal associations, some bacteria can also play a major role in nutrient uptake and plant protection from pathogens. Many strains of *Pseudomonas fluorescens* are characterized as mycorrhizal helper bacteria (MHB) based on their ability to promote mycorrhizal formation and enhance plant productivity in low nutrient soils. To better understand the role of these MHB-plant associations, we examined the impact of several *P. fluorescens* strains (WH6, SBW-25, Pf0-1, and PF-5) on the *in vitro* growth of aspen seedlings at control versus low concentrations of nitrogen (4mM versus1mM) and phosphorous (1.5mM versus 20µM). Control and nutrient limited seedlings were grown with and without the MHB on vertical petri-plates in controlled environmental conditions. While growth rate and morphology were assessed as primary indicators of plant health, number of leaves, plant shoot height, root length and root structure such as branching pattern and rootlets, were also evaluated weekly.

A-2

Brodifacoum Interaction with Membranes and Tissue Distribution

Marangoni, M. Natalia[1], Michael Martynowycz[2], Ivan Kuzmenko[3], Trudy Bolin[3], Tianpin Wu[3], Sophie Gleber[3], Lydia Finney[3], Stefan Vogt[3], David Gidalevitz[2], and Douglas Feinstein[1]

[1] Department of Anesthesiology, University of Illinois at Chicago, Chicago, IL 60612
[2] Department of Physics and Center for Molecular Study of Condensed Soft Matter, Pritzker Institute of Biomedical Science and Engineering, Illinois Institute of Technology, Chicago, IL 60616
[3] Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439

Brodifacoum (BDF) is a highly lethal long-acting anticoagulant poison widely used as rodenticide. Due to its potency, widespread availability, and fast topical absorption, it poses a potential threat as a chemical weapon. BDF has a very long half-life and interacts with lipophilic substances. We aim to elucidate for the first time, BDF interaction with lipid membranes and map tissue distribution using x-rays of its Br atom. Results on constant pressure isotherms on DPPC Langmuir monolayers showed that BDF causes area changes typical of a rapid insertion followed by a gradual monolayer collapse. Follow-up studies include Atomic Force Microscopy, X-ray Reflectivity, and Grazing Incidence X-ray Diffraction on different monolayer models. Using X-ray Fluorescence Microscopy (XFM) in tissues, we spatially resolved BDF signal along common in-situ elements indicative of cellular homeostasis. We also tested the effects of a novel antidote on the chemical state of BDF in tissues using X-ray Absorption Fine Structure (XANES). After treatment, preliminary spectra results showed changes in BDF chemistry typical of a shift from organic to inorganic form. Future studies include XFM, XANES and micro-XANES in several tissues to test treatment efficacy. This is the first time a synchrotron is used to test BDF and antidote effects.

A-3

Lab-on-a-Chip: Microfluidic Live-Cell Assay for Islets of Langerhans for Human Transplant

Mendoza-Elias, Joshua E.[1,2], **Mohammad Nourmohammadzadeh**[1,2], **Yuan Xing**[1,2], **David T. Eddington**[1,2], **José Oberhozer**[1,2], **and Yong Wang**[1,2]

[1] Department of Surgery, University of Illinois at Chicago, Chicago, IL 60612
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Islet transplantation has been emerging as promising therapy for Type I diabetes mellitus (T1DM) and is the only therapeutic that can achieve glycemic control without the need for exogenous insulin. Transplanting islet cells is a minor surgical procedure with low morbidity, mortality, and cost. However, an obstacle to realizing this goal is a lack of an islet potency index as required by the U.S. Food and Drug Administration (FDA) biologics licensing, as well as a more complete understanding of the physiological mechanisms governing islet and beta-cell physiology. Recently, the University of Illinois at Chicago (UIC) has developed a microfluidic platform that can mimic *in vivo* islet microenvironments through precise and dynamic control of perifusing culture media and oxygen culture levels; all while measuring functionally relevant factors including intracellular calcium levels, mitochondrial potentials, and insulin secretion. By developing an understanding of the physiology and pathophysiology of islets we can be more enabled to develop strategies that promote optimization and ultimately improve the success of islet transplantation and as well as open new clinical avenues. The article then concludes presenting initial findings from studies seeking to develop an islet potency test.

A-4

Linking Virus-Host Interactions and Nutrient Biogeochemistry in the Open Oceans: A Model Systems Approach

Mukherjee, Maitreyee

University of Chicago

Half of global photosynthesis occurs in the oceans, accomplished in large part by unicellular microbes. Two of the most important players are the autotrophic picophytoplankton *Prochlorococcus* and *Synechococcus*. Viruses infecting these and other microbes are also extremely abundant, estimated at 10^{30} total viruses in the oceans, and are predicted to be responsible for the lysis of about 20% of the microbial biomass in the sea. Hence viral lysis likely contributes significantly to global nutrient cycling, though incorporating viral infection dynamics into global biogeochemical models remains a major challenge. In addition to lysis, viruses may also influence biogeochemistry by manipulating the metabolism of their hosts. For example, P-acquisition (*phoA*) and P-transport genes (*pstS*) are encoded in the genomes of phages infecting marine cyanobacteria, raising the questions of whether these genes are expressed during infection, how they contribute to P uptake during an infection, and how much they contribute to viral production. In this study, we have used laboratory-based model systems to study the effects of nutrient limitation (P in this case) on viral adsorption, infection and lysis rates. Our model system involve marine *Synechococcus* strain WH7803 and two phages that infect this strain: Syn9 and SSM1. Using one step growth assays, quantitative PCR, infectivity assays, gene expression analysis during infection, transcriptomics and proteomics, we aim to address some of the basic questions mentioned above related to virus-host interaction dynamics in the global oceans, and their contribution to global nutrient cycles.

A-5

Bio-MEMS for 3D Encapsulated Islet Culture under Hypoxia

Nourmohammadzadeh, Mohammad[1,2], Hamidreza Nourmohammadzadeh[3], Joshua E. Mendoza-Eliasa[1,2], Yuan Xing[1,2], James J. McGarrigle[2], Kevin Kavalackal[4], Nicholas Jacus[5], Peter DeWeirdt[5], Priyanka Kadari[6], José Oberholzer[1,2], and Yong Wang[1,2]

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[2] Department of Surgery/Transplant, University of Illinois at Chicago, Chicago, IL 60612
[3] Department of Civil Engineering, Sirjan University of Technology,Sirjan, Kerman, Iran 78169
[4] Department of Neuroscience, University of Illinois at Chicago, Chicago, IL 60607
[5] New Trier High School, Winnetka, IL 60093
[6] Hinsdale Central High School, Hinsdale, IL 60521

Islet microcapsulation is a promising technique to avoid immunosuppression. However, hypoxic stress is one of main factors for the function loss of microencapsulated islets and. A three-layer microfluidic chip was designed with integrated O_2 controller to investigate the microcapsulated islet behavior under various O_2 concentration using simultaneous multiparametric assay in response to glucose and KCL. Fluid flow simulation was performed to verify the hydrodynamic principles [1]. The device can load 100 encapsulated islets less than 1min with 99% efficacy. The unique integration of the gas modulation allowed for rapid membrane-diffused oxygenation of individual islet's at the microscale level. $[Ca^{++}]$ of microencapsulated islets to 25mM glucose were O_2 dependent and were inhibited by hypoxia. Hypoxic concentrations decreased $[Ca^{++}]$:8.19%±2.5 in 10%O_2, 3.57%±1.18% in 5%O_2, and 1 70%±0 64 in 1%O_2. Similarly, mitochondrial potential changes were also inhibited in O_2 dependent manner (21-10-5-1%): 17.23%±3.13, 8.83%±3.53, 6.40%±2.56, and 4.09%±1.37 [2]. The mean NAD(P)H change increase in response to 25mM glucose was 6.43%±4.05. Under 1%O_2, the NAD(P)H level was significantly inhibited. Moderate hypoxia (10 and 5% O_2) also depressed NAD(P)H levels (10%O_2: 4.65% ± 2.17 and 5%O_2: 4.79% ± 2.84).

References

1. M. Nourmohammadzadeh, M. Rahnama, S. Jafari, "Microchannel flow simulation in transition regime using lattice Boltzmann method," Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, **226**(2), 552-562, 2012.
2. M. Nourmohammadzadeh, J.F. Lo, M. Bochenek, J.E. Mendoza-Elias, Q. Wang, Z. Li, L. Zeng, M. Qi, D.T. Eddington, J. Oberholzer, Y. Wang, "Microfluidic array with integrated oxygenation control for real-time live-cell imaging: effect of hypoxia on physiology of microencapsulated pancreatic islets," Analytical Chemistry, **85**(23), pp. 11240-9, 2013.

A-6

Enhancing Reaction-Based Contaminant Transport Model to include Radionuclides with Long Decay Chains

Wang, Cheng[1]*, Charley Yu[1], and Gour-Tsyh Yeh[2]

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*wangcheng@anl.gov
[2] Department of Civil and Environmental Engineering, University of Central Florida

This paper presents a physics-based watershed-scale model with integrated hydrology/hydraulic and water quality transport submodels and its enhancement to include radionuclides with long decay chains. The numerical model comprises three modules for river networks, land surface, and subsurface system, respectively. The surface modules are capable of simulating coupled fluid flow, sediment transport, and reactive chemical transport in river networks and surface runoff, whereas the subsurface module is capable of simulating the same coupled processes as in the surface modules except the sediment transport. The radionuclide transport module considering parent decay and progeny ingrowth for both surface and

ground water are under development and will be incorporated into the RESRAD-OFFSITE code. The capability of this general model can be easily extended by including a set of reactions for simulating certain contamination processes. The continuity, momentum, mass balance equations, mixed equilibrium and kinetic equation for biogeochemical reactions, and kinetic equations for ingrowth and decay, are employed as governing equations and the Finite-Elements Scheme is used to solve the governing equations numerically. Two example problems are presented, including a hypothetical simulation of complex geochemistry in groundwater where Uranium and $Fe(OH)_3$ are involved in 40 geochemical reactions and the simulation of U238 decay chain.

Chemistry and Biochemistry

A-7
Inverted Pendant Drop Method for X-Ray Absorption Spectroscopy of Solutions

Bera, Mrinal K. and Mark R. Antonio

Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439

X-ray absorption spectroscopy is an invaluable tool in probing coordination environments of targeted elements in all forms of matter. Due to low escape depths of electrons compared to x-ray photons, x-ray absorption measurements done by measuring total electron yield (TEY) and x-ray fluorescence (XRF) together can provide both interfacial and bulk coordination environments. We present a simple and inexpensive system design for collecting simultaneously TEY and XRF signals from an inverted pendant drop of electrolyte solutions. The concept was tested with four aqueous solutions of rare earth elements—cerium and europium—with identical pH and concentrations. The x-ray absorption near edge structure (XANES) and the extended x-ray absorption fine structure (EXAFS) data obtained from the solutions show remarkable differences in their TEY and XRF responses. The differences directly indicate variations of the Ce^{3+} and Eu^{3+} coordination environments near air-water interfaces compared to the bulk solutions. Simultaneous surface and bulk sensitivities, low volume requirements ~1 ml of solutions, and quick alignment procedures of the set-up make it attractive and distinct from the conventional way of collecting X-ray absorption measurements from solutions.

A-8
Salty Water from First Principles

Gaiduk, Alex P.[1], François Gygi[2], and Giulia Galli[1]

[1] Institute for Molecular Engineering, The University of Chicago, IL 60637
[2] Department of Computer Science, University of California, Davis, CA 95616

Why does ice float on water? How do salts dissolved in water modify the pristine liquid structure and its electronic properties? These are just two of the many deceivingly simple questions regarding the structure and properties of water and aqueous solutions that are yet to be answered. First-principles molecular dynamics provides information about the microscopic structure of liquids, complementing measurements and helping to interpret experimental data. Most existing first-principles simulations of salts in water have been performed using gradient- corrected approximations, which are affected by the self-interaction error. Such approximations tend to give hydrogen bonds that are too strong at ambient conditions and make liquid water overstructured. In this work, we employ the non- empirical hybrid functional PBE0 to study the structure and electronic properties of water and 1 M solutions of Na^+ and Cl^- ions. We show that, in addition to predicting a more realistic structure of water, hybrids greatly improve the description of the

electronic properties of solutions. We also show that Na^+ has little effect on the properties of aqueous Cl^-, justifying the use of an "infinite dilution model", in which only Cl^- ions are added to water, while Na^+ is replaced by the uniform background compensating charge.

A-9

Shift-and-Invert Parallel Spectral Transformations: Density Functional Based Tight- Binding Applications

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The quest to discover and synthesize novel materials with ever growing complexity forces us to study larger simulations with more reliable electronic structure methods. Extreme scale computing enables us to push these limits further and further with the cost of tailoring the methods and algorithms for the architecture of emerging supercomputers. Density-functional based tight-binding method (DFTB) is one of the promising methods to perform very large-scale simulations with a reliable accuracy for suitable systems. The computational bottleneck in DFTB simulations is the matrix diagonalization step. With conventional dense eigensolvers, this step has a cubic scaling for the computational time and a quadratic scaling for the memory requirement. Shift-and-Invert Parallel Spectral Transformations (SIPs) method can reduce these scalings by using the sparsity of these applications. SIPs is based on the PETSc framework and built on top of a spectrum- slicing solver in SLEPc library. We demonstrated the capabilities of SIPs using DFTB applications on metallic single-wall carbon nanotubes, diamond nanowires, and crystal diamonds of varying sizes. We reached up to a matrix size of 512,000 by 512,000 for the nanotube and utilized up to 266,144 cores. We have found that one can obtain 60% of the eigenpairs in a few tens of seconds for any size of the problem, provided there is enough computational power that scales at worst quadratically with the system size.

A-10

Radical-Radical Well-Skipping Reactions Are Important in Biofuels Flame Chemistry

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There is a long history of developing chemical kinetic models to predict the combustion chemistry of petro-derived and alternative fuels. The reliability of such models is dependent on the accuracy of the elementary reaction rate constants assembled in such models and the inclusion of the important reaction pathways. In the present study, a variety of biofuel flame experiments have been simulated. Radical-radical reactions that were previously not considered in literature combustion models were theoretically characterized and were found to have a significant effect on flame model predictions. Preliminary flame simulations indicate that stable fuel-radicals can build up to substantial concentrations. Therefore, an important sink for fuel-radicals in flames can be bimolecular reactions of these with dominant flame-radicals (H, CH_3, OH, etc.). We have theoretically characterized the reactions of H-atoms and CH_3 radicals with the relatively stable radicals of ethanol (CH_3CHOH) and methylformate (CH_2OCHO). Under low-to-ambient pressure conditions, well-skipping to molecular/radical products and direct abstraction are the predominant pathways. Inclusion of these well-skipping and abstraction reactions in flame models has a pronounced effect on the prediction of combustion intermediates and

consideration of these mechanistic pathways is essential for the development of predictive combustion models.

A-11

Porous Organic Polymer Supported Single-Site Copper: Synthesis, Catalysis, and Comparison with Homogeneous System

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Porous organic polymers (POPs) are highly crosslinked, microporous, amorphous materials, usually constructed from various organic building blocks using strategies like cross-coupling, condensation, 'click' chemistry, and alkyne or nitrile trimerization. Apart from their application in gas storage and separation, metallation of POPs provides single-site metal centers that are excellent catalysts for several energy related transformations. Compared to homogeneous analogs, these catalysts are far superior in terms of activity, stability, and most importantly selectivity. A redox active catechol-functionalized POP (catPOP) material with single-site Cu^{I}/Cu^{II} centers has been developed and established as an efficient and selective catalyst for aerobic alcohol oxidation under mild conditions. Coordination chemistry and redox property of the copper centers within this heterogeneous support are remarkably different from their homogeneous counterpart.

A-12

Aqueous Light-Driven Hydrogen Production by Ru-Ferredoxin-Co Hybrid Complexes

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Artificial photosynthetic complexes have been developed to perform light-driven hydrogen production, but these complexes have limited stability in aqueous solution and neutral pH. Herein we have developed a protein-based artificial photosynthetic hybrid system which enables a native electron transfer protein, ferredoxin to act as an electron transfer scaffold from a ruthenium photosensitizer and a molecular cobaloxime catalyst. This system performs photocatalysis to produce 320 total turnovers in a period of 6-8 hours. Electron transfer within the complex has been investigated by EPR and transient optical spectroscopy. The complex undergoes oxidative quenching of the Ru PS and forms a Ru(III) species, and then transfers electrons through the ferredoxin [2Fe-2S] cluster to form a Co(I) species in 130 µs. This demonstrates that a protein can stabilize a molecular catalyst in solution to develop a functional hydrogen production system capable of proton-coupled electron transfer.

A-13

The Effect of Oxygen Partial Pressure during Synthesis on the Electrochemical Performance of $Li_xNi_{0.158}Mn_{0.68}Co_{0.162}O_2$ (x = 1.25, 1.45) Cathodes

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Lithium-, manganese-rich, nickel-manganese-cobalt (LMR-NMC) oxides are of great interest for use in a new generation of high capacity lithium ion batteries targeting plug-in hybrid (PHEVs) and electric vehicles (EVs) applications. In this study, LixNi0.158$M_{n0.68}Co_{0.162}O_2$ cathode materials were prepared under four different oxygen partial pressures ranging from 1 atm to 2×10^{-3} atm. The oxygen partial pressure used in the synthesis showed strong effect on the electrochemical performance but almost no effect on the voltage fade of LMR-NMC materials. In general, an oxygen-rich environment produced cathode materials with higher capacity and better cyclability. We found that lithium content was more important than oxygen partial pressure in terms of effect on the properties of the material.

Nanomaterials

A-14

Ion Transport Controlled by Nanoparticle-Functionalized Membranes

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From ion-channels embedded in lipid bilayers to water treatment facilities to fuel cells, membrane-based separation processes are ubiquitous in nature and find widespread usage in many applied technologies. Despite significant differences over a wide range of length scales, one of the key, and common, features for optimizing a membrane's transport and selectivity properties is the well-specified control of molecular interactions in confined geometries. In this talk, I will outline a versatile new approach for the functionalization of membranes using ligands adsorbed to the surface of nanoparticles. Introducing some of the same charged groups as those found in advanced membrane technologies such as carboxyl and amine groups in reverse osmosis membranes, variations in the ligand terminal group are used to influence and control ionic transport. Further functionality exploiting the ligands as binding sites is demonstrated for the introduction of sulfonate groups and a modification to the membrane charge density. These results are then extended to smaller dimensions by systematically varying the underlying pore diameter. The resulting nanoparticle-functionalized membranes have selective transport characteristics that compare well with other emergent membrane technologies such as carbon nanotubes[1] while maintaining one of the highest permeabilities for ionic-separation membranes to date[2].Leveraging the flexibility by which by which ligated nanoparticles can be synthesized, these results open up exciting possibilities for a number of functionalized components that have been chemically adsorbed onto the surfaces of nanoparticles, and for the first time, describe a means by which to deliver this functionality to the all-important regime of porous materials.

References

1. Fornasiero, F., et al., PNAS, **105**, 17250-17255 (2008)
2. Humplik, T., et al., Nanotechnology **22**, 292001 (2011)

A-15

Extraordinary Wear Resistance of Single and Few Layer Graphene

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Graphite as a macro-scale solid lubricant has been widely studied and has been used in industry for more than 40 years. It is well known that bulk graphite works the best in humid environments, but fails to provide low friction and wear in inert, dry, or vacuum environments.

In this study, we demonstrate a distinct wear/friction behavior of graphene from that of bulk graphite (HOPG). We show that in case of sliding steel surfaces, few layers of graphene works equally well as a solid lubricant in both humid and dry environments. In fact, we observed that the reduction in wear of steel surfaces is as much as 4 orders of magnitude while friction is cut down by factors of 4 to 5. Such marked friction and wear reductions are attributed to the low shear and highly protective nature of the graphene, which conformally coats the underlying surface and prevents tribo-corrosion when present at sliding contact interfaces. Furthermore, we demonstrate that the lifetime of few-layer graphene extends up to 50,000 cycles, when tested in hydrogen environment. This opens up a new avenue for the use of graphene as a solid lubricant in various practical applications.

A-16

Sequential Infiltration Synthesis (SIS) for Advanced Lithography

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Sequential infiltration synthesis (SIS), related to atomic layer deposition (ALD), involves gas phase molecular assembly reactions and has been recently demonstrated for the purpose of hardening various polymeric lithography resists towards subsequent etching and for block copolymer (BCP)-assisted inorganic nanostructure templating. SIS precursors such as trimethylaluminum (TMA) and water (the same precursors used for Al_2O_3 ALD) react directly with the patterned resist layer within an ALD chamber operating in semi-static mode. Our current works involve inorganic materials pattern transfer by SIS lithography using sub-30 nm BCP self- assembled structures. These patterned inorganic nanopatterns can be directly used in devices or can be used for further substrate etching. Although SIS can dramatically enhance pattern transfer relevant to device applications, the complex processes involved in SIS are not clearly understood. Understanding the chemistry underlying SIS is necessary to ensure a high degree of perfection in large-scale lithography, and in this purpose, we have performed *in situ* Fourier Transform Infrared (FTIR) spectroscopy during SIS on different homopolymers to illustrate the knowledge of SIS precursor–polymer functional group interaction.

A-17

X-ray Scattering from Optically Trapped Nanoparticles

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A major barrier to applying coherent x-ray diffraction imaging to freestanding micro- and nano-scale objects is their tendency to freely move within the intense beam from synchrotron source. Typically such objects must be securely bonded to a substrate, which can alter their internal structures. While the forces moving such particles are not completely understood, we believe optical tweezers may be a solution. Optical tweezers provide a unique method to control small particles, ranging from several microns to tens of nanometers. Using optical techniques, these laser trapped particles can be manipulated and forces on the objects in the trap can be measured. Combined with phase modulation techniques, optical traps with different geometries and polarization can be generated, resulting in an accurate orientation of anisotropic particles [1,2]. We have built an apparatus of dynamic holographic optical tweezers which is compatible with x-ray diffraction imaging at beamline-34 of APS. In August we are going to test the x-ray diffraction from optically trapped micro-and nano-particles of both materials and biological sample origin with the goal of eliminating the barrier to studies of freestanding objects due to uncontrolled sample drifts. By observing the Bragg peaks, we can determine and optimize the stability of trapped particles. Then we will use coherent x-ray diffraction imaging[3] to image a freestanding sample explicitly selected by the user for the first time.

References
1. Zijie Yan, Julian Sweet, Justin E. Jureller, Mason J. Guffey, Matthew Pelton, and Norbert F. Scherer, 2012. "Controlling the Position and Orientation of Single Silver Nanowires on a Surface Using Structured Optical Fields," ACS Nano, **6** (9), 8144- 8155.
2. Zijie Yan, Justin Jureller, Julian Sweet, Mason Guffey, Matthew Pelton, Norbert F. Scherer, 2012. "Three-Dimensional Optical Trapping and Manipulation of Single Silver Nanowires," Nano Letters, **12** (10), 5155-5161.
3. Mark A. Pfeifer, Garth J. Williams, Ivan A Vartanyants, Ross Harder, and Ian K. Robinson. 2006. "Three-Dimensional Mapping of a Deformation Field inside a Nanocrystal." Nature, **442** (7098), 63–66.

A-18

Active Electrocatalysts of Unique Surface Properties Prepared by Electrochemical Deposition

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Methods for achieving maximum utilization of Pt have been extensively pursued in the synthesis of electrocatalysts, owing to both the high cost and the great catalytic activities of Pt for a range of chemical reactions that are essential to renewable energy technologies, such as fuel cells and water electrolyzers. In this presentation, electrochemical deposition of Pt from NaCl- supported electrolytes will be reported as an alternative means to prepare electrocatalysts of ultrahigh Pt utilization. Of particular interest is the deposition of ultrathin Pt films, whose thickness can be controlled precisely at monolayer level. Deposition conditions for growing ultrathin Pt films on Au, Ni, W, and WC will be provided. The nucleation and growth mechanisms of Pt thin films will be discussed by illustrating the transport of Pt ions to the electrode surface and its subsequent charge transfer at the electrode surface. The high activity of Pt thin films grown on Ni and WC supports will be shown in catalyzing hydrogen evolution

reaction (HER). Also, the effect of surface intermixing and segregation on their HER activity will be presented.

A-19

Novel Bulk and Surface Structures for High Capacity Lithium-Ion Battery Cathodes

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Lithium-ion batteries are playing an increasingly ubiquitous role in society. The successful commercialization of battery technology has triggered further efforts to expand the use of lithium-ion chemistries to large-scale applications including all-electric and hybrid-electric vehicles and smart grids. Despite these technical accomplishments, large-scale vehicle electrification–especially affordable, long-range EV's and PHEVs–will require batteries with approximately three times the current energy densities at about one third of the current cost per kWh. Therefore, further breakthroughs in scalable energy storage are necessary before the full benefits of vehicle electrification can be realized. We will discuss novel synthesis routes to incorporate stabilizing spinel components into layered-layered, composite electrode structures. The spinel component, containing 25% transition metals in lithium layers, may serve as a stabilizing unit against structural transformations inherent in layered-layered cathodes. Furthermore, unique surface architectures, based on atomic layer deposition (ALD) of metal fluorides, will be presented.

A-20

Complex Oxide Nanomembrane Systems

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Nanomembranes (NMs) are nanoscale-thickness sheets of single-crystalline materials that are freestanding, flexible, compliant, and transferrable. The unique mechanical properties of NMs make them suitable for (1) strain engineering, the controlled introduction or relaxation of elastic strain to alter fundamental properties of materials; and (2) materials integration, joining dissimilar materials through NM bonding to create novel interfaces or multifunctional devices. NMs made of perovskite-structured complex oxide materials are particularly interesting because we can investigate the large structural variations associated with changes in ionic/electrical conduction, ferroelectric domain structure, or catalytic activity as a function of strain in freestanding or transferred NMs of such materials. We show here that we can combine dissimilar materials with oxide NM synthesis through the release of single-crystalline oxide thin films from the original growth substrate. By measuring structural changes in ferroelectric NMs with *in-situ* synchrotron x-ray techniques, we monitor changes in strain, polarization, and structural phase as a function of chemical environment and temperature. Our oxide NM synthesis technique represents a significant advancement in materials integration and provides a useful way for probing fundamental materials properties in freestanding thin films.

A-21

Controlling Nanoscale Light-Matter Interactions with Microelectromechanical Systems

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The possibility to confine light to a volume beyond the diffraction limit and the ability to manipulate and enhance localized electromagnetic fields surrounding metallic nanostructures is driving the surge of research in metallic nanostructures and plasmonics. One of the critical limitations to the development of this field is the lack of robust, repeatable approach for active control of the optical coupling between plasmonic excitations. Micro-electro-mechanical systems (MEMS) are an ideal platform for reproducibly controlling the interaction between nanostructures because they provide fast, stable and precise control of their geometry and arrangement in a continuous manner for a large range of distances. We have fabricated Au plasmonic nanostructures on low- stress, low-index aluminum oxide platforms and have integrated them on to custom designed and fabricated MEMS devices that can be electrostatically actuated. Dark-field spectroscopy is used to measure the spectral characteristics and we have observed plasmonic resonance of the coupled particles and wavelength shifting of the resonance with changes in the dimer gap facilitated by MEMS actuation. This wavelength tuning demonstrates nanoparticle interaction in the near- and far-fields. Simulations using 3D finite-difference time-domain (FDTD) show good correspondence to the experimental results. This is a first demonstration of controllable plasmonic tuning of a nanoparticle system using a compact MEMS device, which allows for repeatable measurement of the spectral characteristics on any standard dark-field microscope-spectrometer.

A-22

Proteins at Interfaces

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How fast do proteins transport charges across lipid membranes? Can smart proteins used as molecular tools deliver drugs across physiological barriers? How does a cell penetrating peptide insert into cells?– These are questions I have been excited about to answer. To this end, I have worked in different teams in which we used and developed highly sensitive vibrational optical spectroscopies tailored to analyze molecular interfaces. I used surface-enhanced Raman and infrared absorption spectroscopy with monolayer sensitivity, in combination with electrochemistry. We engineered thin metal layers to provide the required plasmonic enhancement and to induce charge transfer onto which protein and biomimetic lipid layers were assembled. Questions about charge transfer kinetics in membrane-bound redox complexes could be answered. As a postdoc, I applied sum frequency generation to study the structural behavior of cell-penetrating peptides used in drug delivery systems at different interfaces. Inspired by the ability to study complex biological monolayer systems, I am currently implementing surface-enhancement to 2D IR spectroscopy, a delicate method promising to reveal ultrafast dynamics in molecular monolayers. The poster will present my projects and demonstrate how I transferred and combined ideas to create new approaches in order to access proteins at interfaces.

A-23

Enhanced Colloidal Stability of Titania Nanofluids via Surface Modification

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Nanofluids are liquids that are engineered by stably dispersing functional nanomaterials into the base fluids. Advanced thermo-physical properties of nanofluids including, but not limited to thermal and electrical conductivity, diffusivity, heat transfer, specific heat, density and viscosity can be utilized in many industrial applications. One of the main challenges in nanofluid engineering is achieving high concentration of nanomaterial in suspension without dramatic increase in viscosity. Most studies on nanofluids have only reported on nanoparticle loadings between 0.1 and 10 wt% because of viscosity limitation, whereas the objective of this study was to obtain stable nanofluids with loading of titania (TiO_2) nanoparticles higher than 10wt%.

To achieve high suspension stability and low viscosity a simple one-step surface modification procedure was used to functionalize the titania nanoparticles with sulfonate groups. Modified nanoparticles were characterized with scanning electron microscopy and thermogravimetric analysis. The nanofluids with concentrations up to 50wt% were prepared from modified TiO_2 nanoparticles which showed excellent colloidal stability and only moderate viscosity increases (<50% increase at 30wt %). The effects of the surface modification on the nanofluid properties were further assessed through using a variety of particle sizes (5 to 100nm) and characterization of resulting thermal conductivities and viscosities at different temperatures.

A-24

Stepwise and Epitaxial Growth of DNA-Programmable Nanoparticle Superlattices

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Many researchers are interested in developing methods for rationally assembling nanoparticle building blocks into periodic lattices. These superlattices could in principle be used to create designer materials with properties useful for optics, biomedicine, energy, and catalysis. DNA is a particularly attractive ligand for the programmable assembly of nanoparticles, as synthetically tunable variations in nucleotide sequence enable precise superlattice engineering. However, these superlattices are typically formed in solution as polycrystalline materials, making device integration challenging. Here we show that a stepwise growth process can be used to systematically study and control the evolution of a bcc crystalline thin-film comprised of DNA-functionalized nanoparticle building blocks on a complementary DNA substrate. Importantly, the judicious choice of DNA interconnects allows one to tune the interfacial energy between various crystal planes and the substrate, and thereby control crystal orientation and size in a stepwise fashion using chemically programmable attractive forces. We further demonstrate epitaxially superlattice growth on lithographically patterned templates, eliminating grain boundaries and enabling fine control over orientation and size. This work will be important for the development of on-chip material platforms that take advantage of the periodicity and/or controlled density of the inorganic core, such as optical metamaterials, photonic crystals and heterogeneous catalysts.

A-25

Charge Gradient Microscopy for Surface Polarization Charges Imaging

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Charge Gradient Microscopy (CGM) is expected to be a strong tool in dynamic mapping bound surface charges, e.g., ferroelectric domain switching[1,2]. During this presentation, I will show that we can create an unscreened surface of periodically poled lithium niobate (PPLN) locally in ambient with no or little influence to the polarization charges underneath. Subsequently, we investigate the adsorption kinetics of external screening charges on the ferroelectric surface as a function of time. To further understand the screening charges contribution to the CGM signals, we used a patterned AFM probe to isolate the current signals from bound and screening surface charges. We will present a model to explain the screening surface charge removal and the interaction with the AFM probe during the CGM scans in ferroelectric domain and domain wall imaging.

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References
1. S. Hong, S. Tong, W.I. Park, Y. Hiranaga, Y. Cho, and A. Roelofs, Proc. Natl. Acad. Sci. U.S.A., **111**, 6566–6569, (2014)
2. J.M. Gregg, A. Kumar, Nature, **510**, 481–482 (2014)

Energy

A-26

Analysis of Techno-Economic Feasibility and Fuel-cycle GHG Emissions for Synthetic Fuel Production via Electrochemical CO_2 Reduction and Fischer-Tropsch Process

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Electrochemical reduction of CO_2 is a potential viable pathway for producing renewable synthetic fuels. This study analyzes the techno-economic feasibility and fuel-cycle greenhouse gas (GHG) emissions for a proposed system that converts CO_2-released from fossil fuel-burning power plants to diesel fuel via electrochemical reduction of CO_2 to CO and the Fishcer-Tropsch process. The current performance levels of CO_2 electrolyzers and Fischer-Tropsch process were used to compute critical metrics for evaluating the performance of the system, including (i) cost, (ii) fuel-cycle GHG emissions, and (iii) energy efficiency. The synthetic fuel cost and well-to- gate GHG emissions are currently about 3 times those of petroleum fuels. A sensitivity analysis indicated under optimistic circumstances (e.g., projected performance of electrolyzers), fuel produced via this pathway is likely to remain at least 50% more expensive than fossil

fuels, and a modest reduction in GHG emissions can be achieved. Key findings include that synthetic fuels from CO_2 reduction currently is not economically competitive with petroleum fuels. Fuel-cycle CO_2 emissions of synthetic fuels depend on carbon intensity of electricity and can be significantly improved with better technologies and system configurations. Other CO_2 utilization pathways can be explored and analyzed using the framework and analytical tools in this study for better system design and directing fundamental research.

A-27

Understanding Reactivity of Phenothiazine-Based Redox Shuttles in Lithium-Ion Batteries

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Redox shuttles are electro-active molecules added to lithium-ion batteries for the purpose of protecting against overcharge. Development of new redox shuttles is centered on functionalization of a handful of redox-active cores that exhibit overcharge protection. Even so, few redox shuttle candidates protect for extended periods of time, and at present, the failure mechanisms are not well understood. In this study, we incorporated phenothiazine-based redox shuttles into coin cells; following the failure of each cell, we characterized its contents in order to identify the decomposition products of the redox shuttle within. Decomposition mechanisms were proposed and explored via experimental and computational methods.

A-28

Atomic Layer Deposition of Metastable β-Fe_2O_3 via Isomorphic Epitaxy for Photo-Assisted Water Oxidation

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Solar-to-hydrogen energy conversion is regarded to be an integral component in the future renewable energy infrastructure. Photo-assisted electrochemical (PEC) water splitting is one possible route towards a viable solar-to-hydrogen conversion process. Of the candidate PEC water splitting photoanode materials, hematite (α-Fe_2O_3) remains one of the most promising because of its suitable bandgap for solar absorption, terrestrial abundance, and stability in aqueous. However, sluggish water splitting kinetics and poor charge transport properties continue to limit its application. Other iron oxide phases are either difficult to synthesize in useful forms or have failed to demonstrate appreciable photoactivity. Here, we investigate the alternative bixbyite-phase of iron(III) oxide (β-Fe_2O_3), synthesized via isomorphic epitaxial stabilization using atomic layer deposition (ALD).

X-ray diffraction measurements and Raman spectroscopy verify the formation of β-Fe_2O^3 thin films with cube-on-cube epitaxy with respect to the low-index epitaxial ITO/YSZ templates. As- grown films are largely crystalline phase-pure and photoactive. While absorption characteristics and overall PEC activity of the β-phase thin films are similar to that of the α phase, β-Fe_2O^3 exhibits lower photocurrent onset potential and a smaller bandgap. These properties indicate potential advantages that β-phase photoanodes may ultimately hold over hematite for water splitting applications.

A-29

Exciton Management in Organic Photovoltaic Multi-Donor Energy Cascades

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Significant advances in organic photovoltaic (OPV) device technology over the past decade demonstrate its practical viability due to ultralow cost on large area, lightweight and flexible substrates. Power conversion efficiencies (PCE) now exceed 12% for multijunction OPV cells [1,2]. There are several recipes demonstrated that improve the exciton harvesting in a single heterojunction OPV cell, for example by blending donor and acceptor to promote efficient exciton dissociation, by incorporating exciton blocking layers at anode and/or cathode side. Here we present another promising approach using a three stage energy cascade donor structure [3]. These so-called "energy cascades" drive exciton transfer from the anode to the dissociating interface while reducing exciton quenching and allowing improved overlap with the solar spectrum. Our cascade device structure is as follows:

glass/indium-tin-oxide/D1/D2/D3/C_{60}/BPhen (4,7-diphenyl-1,10-phenanthroline)/Ag,

where donors are D1=diphenyltetracene, D2=rubrene, and D3=tetraphenyldibenzoperiflanthene [4]. The donor materials were chosen on the basis of their optical energy gaps follow D1>D2>D3 so that D1 blocks excitons from quenching at the anode, D2 transfers excitons to D3 and D3 contributes to the photocurrent due to its strong absorption at visible wavelengths, while also determining the open circuit voltage when paired with the fullerene acceptor. PCE of the cascade solar cell is twice that of bilayer devices. This improvement is due to a significant increase in photocurrent along with an increase in open-circuit voltage and fill factor. We analyze the transfer and blocking properties of this structure based on photoluminescence and modeling of the exciton distributions in the donor thin films.

References
1 Xiaozhou Che, Xin Xiao, Jeramy D. Zimmerman, Dejiu Fan, and Stephen R. Forrest, Advanced Energy Materials, DOI: 10.1002/aenm.201400568 (2014).
2. M. Peach, http://optics.org/news/4/1/36 (2013).
3. Cody W. Schlenker, et al., *Chemistry of Materials* **23** (18), 4132-4140 (2011).
4. Olga L. Griffith and Stephen R. Forrest, *Nano Letters* **14** (5), 2353-2358 (2014).

A-30

Toward Advanced Exciton Charge Separation with Metal-Organic Framework Films

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Metal-organic frameworks (MOFs) have been shown to possess interesting properties that may prove beneficial for efficient solar energy conversion schemes. For example, light harvesting MOF crystals have been prepared which exhibit ultrafast energy migration.[1] This fast energy migration is hypothesized to be facilitated by the spatial separation of chromophores and the anisotropy of the crystals. To take advantage of this anisotropy in solar energy conversion, porphyrin-based MOF films were grown in a controlled and oriented fashion on a conductive substrate using the layer-by-layer method (LBL), where individual components of the MOF are introduced to the substrate one at a time. This self-limiting method

has been show to produce uniform films for which the orientation can be controlled through selective functionalization of the substrate.[2] Thickness and absorption measurements allowed us to deduce that the porphyrins are oriented perpendicular to the substrate in 2D sheets. Comparing absorption and electrochemical characterization allowed us to determine that all porphyrins were reversibly accessible electrochemically. Integration into a pseudo-solar cell shows that voltage can be generated and current can be collected from the MOF film. This work represents a promising first step of employing precisely controlled and oriented MOFs in solar energy conversion schemes.

References
1. Son, H.-J.; Jin, S.; Patwardhan, S.; Wezenberg, S.J.; Jeong, N.C.; So, M.; Wilmer, C.E.; Sarjeant, A. a.; Schatz, G.C.; Snurr, R.Q.; Farha, O.K.; Wiederrecht, G.P.; Hupp, J.T., *J. Am. Chem. Soc.*, **2013**, *135*, 862.
2. Zacher, D.; Yusenko, K.; Bétard, A.; Henke, S.; Molon, M.; Ladnorg, T.; Shekhah, O.; Schüpbach, B.; de los Arcos, T.; Krasnopolski, M.; Meilikhov, M.; Winter, J.; Terfort, A.; Wöll, C.; Fischer, R. a., *Chem. Eur. J.*, **2011**, *17*, 1448.

A-31

CFD Simulation of Gasoline Compression Ignition

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Gasoline compression ignition (GCI) is a low temperature combustion (LTC) concept that has been gaining increasing interest over the recent years owing to its potential to achieve diesel-like thermal efficiencies with significantly reduced engine-out nitrogen oxides (NO_x) and soot emissions compared to diesel engines. In this work, closed-cycle computational fluid dynamics (CFD) simulations are performed of this combustion mode in an effort to understand effects of model settings on simulation results. The CFD model is evaluated against experimental results corresponding to a low load start of injection (SOI) timing sweep. The model is then exercised to investigate the effect of SOI on combustion phasing with constant intake valve closing (IVC) conditions and fueling over a range of SOI timings. Simulation results indicate that there is an optimum SOI timing which results in the most stable combustion. Advancing injection with respect to this point leads to significant fuel mass burning in the colder squish region, leading to retarded phasing and ultimately misfire for earlier SOI timings. On the other hand, retarding injection beyond this optimum timing results in reduced residence time available for gasoline ignition kinetics, and also leads to retarded phasing.

A-32

Spatial and Chemical Control of Substitutional Intermediate Band Materials: Toward the Atomic Layer Deposition of $V_{0.25}In_{1.75}S_3$

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Intermediate band solar cells (IBSC) have the potential to reach efficiencies 20% larger than traditional single-junction devices. $V_{0.25}In_{1.75}S_3$ theoretically has nearly ideal properties for an IBSC, but only powders of it have been created so far. Here we present $V_xIn_yS_z$ thin films grown by atomic layer deposition (ALD), which gives us control over uniformity, stoichiometry, and crystallinity. Our initial studies focused on ALD of In_2S_3 via alternating pulses of a novel indium(III) amidinate precursor and hydrogen sulfide. Oxygen-free, crystalline films of In_2S_3 were deposited with a band gap near 2.0 eV and

reasonable electronic properties. Once this deposition recipe was developed, pulses of a novel vanadium(III) amidinate precursor were included. Film growth was studied *in situ* using quartz crystal microbalance while varying the deposition conditions. By varying the ratio of indium, sulfur, and vanadium precursor pulses, we could vary the stoichiometry of the films. UV-Vis-NIR measurements indicate a large absorption peak at a smaller energy than the indium sulfide band gap. The peak increases as the vanadium content of the film increases. Control over crystallinity and electronic properties has also been observed.

A-33

Studying the Structural and Electronic Configurations during Photocatalytic Activation of O_2 at a diiron(II) Complex.

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Several mono and carboxylate-bridged diiron nuclear enzymes are critical in activating dioxygen in various biological processes such as DNA synthesis, hydrocarbon metabolism and cell proliferation [1]. Iron-containing enzymes such as cytochrome P450, peroxidases, catalases and methane monooxygenase (MMO) have been shown to activate dioxygen by using two electrons and protons to produce iron (IV) oxo intermediates [2-4]. The remarkable efficiency of these enzymes is often attributed to the formation of these iron(IV) cations which serve as active oxidants in enzymatic reactions and are able to attack the C-H bonds of a wide range of hydrocarbon substrates [5]. It is widely postulated that ferryl-oxo species are key intermediates in the mechanism of cytochrome P450 and MMO. However due to the complexity of the protein environments in biological iron enzymatic systems[1], monitoring the structural changes occurring during dioxygen activation is a complex undertaking. This project serves to study the light driven activation of a well characterized artificial analogue of an diiron MMO enzyme, (μ-peroxo) (μ-carboxylato) diiron(III) complex, $[Fe_2(\mu\text{-}O_2)(N\text{-}EtHPTB)(\mu\text{-}PhCO_2)]^{2+}$ in a chromophore/diiron complex assembled unit. Such types of assemblies provide new avenues for study of catalytic reaction mechanisms. They are promising examples of artificial molecular systems leading to dioxygen activation as visible light is efficiently absorbed at the chromophore, and light energy is in turn converted into a chemical potential via an electron relay through charge accumulation processes at the iron metal center. Formation of high valent iron peroxo species have been shown by UV-Vis, EPR and Resonance Raman spectroscopy as well as x-ray spectroscopic analysis. XANES and EXAFS revealed formation of an iron peroxo species with different coordination number and formation of a peroxo bridge.

References

1. Do LH, Hayashi T., Moenne-Loccoz P, & Lippard S.J. (2010) Carboxylate as the Protonation Site in (Peroxo) diiron(III) Model Complexes of Soluble Methane Monooxygenase and Related Diiron Proteins. *J.Am.Chem.Soc.* **132**:1273-1275.
2. Kotani H, Suenobu T., Lee Y-M., Nam W, and Fukuzumi S. (2011) Photocatalytic Generation of Non-Heme Oxoiron(IV) Complex with Water as an Oxygen Source. *J.Am.Chem.Soc.* **133**:3249-3251.
3. Lawrence Que J (2007) The Road to Non-Heme Oxoferryls and Beyond. *Acc.Chem.Res.* **40**:493-500.
4. Fukuzumo S., Kishi T., Kotani H., Lee Y-M, and Nam W. (2010) Highly efficient photocatalytic oxygenation reactions using water as an oxygen source. *Nat. Chem.* **3**:38-41.
5. Krebs C., Fujimori D.G., Walsh C.T., & J. Martin Bollinger J. (2007) Non-Heme Fe(IV)-Oxo Intermediates. *Acc.Chem.Res.* **40**(7):484-492.

A-34
Simulation of $LiFePO_4$ Nanoparticle Microstructure with a Coupled Phase-Field, Elasto-Mechanics and Surface Tension Model

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The microstructure of $LiFePO_4$ nanoparticles, of interest as a high discharge rate cathode material for rechargeable batteries, is studied using a multiphysics phase-field model. Spinodal decomposition is coupled with elasto-mechanics and surface tension, yielding alternating strips of Li-rich and Li-poor phases at low temperatures. The material is highly anisotropic in terms of elastic constants, surface energies, Li mobility and lattice mismatch between phases. The microstructure influences (dis)charge performance and can induce mechanical failure due to stresses. Phase separation appears to depend on the size of the particle, as nanoparticles exhibit greater stability of the homogenous phase as compared to larger cathode particles.

This work explores the cause and behavior of the striping mechanism, as it depends on coupled spinodal decomposition, anisotropic stress and surface tension. The transition from nanoparticle to bulk behavior is also examined.

Physics and High Energy Physics

A-35
Prototyping the SuperCDMS Active Neutron Veto

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SuperCDMS SNOLAB is a Generation 2 dark matter experiment that employs cryogenic, high-purity germanium and silicon crystals to search for interactions of Weakly Interacting Massive Particle (WIMP) dark matter with nuclei. We are currently developing designs for an organic scintillator veto to reject neutron elastic scatter events, one of the primary expected backgrounds for the experiment. I will show progress and early results from a small-scale prototype consisting of 15L of linear alkylbenzene scintillator, doped with 30% trimethylborate to enhance thermal neutron capture, and read out by wavelength-shifting fibers and silicon photomultipliers.

A-36
Performance of the ATLAS Fast TracKer (FTK)

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The existing ATLAS three tier trigger system reduces the event rate from 40 MHz to ~400 Hz, at the LHC design luminosity of 10^{34} $cm^{-2}s^{-1}$. After the upgrades of Long Shutdown 2, the LHC will deliver luminosities beyond the original design specification. The increasing luminosity will lead to larger event sizes and will require more sophisticated trigger algorithms to reduce backgrounds and maintain bandwidth limitations. These issues are most difficult to handle for the Level-2 trigger system. The

ATLAS Fast TracKer (FTK) is a hardware trigger designed to operate at the full Level-1 accept rate of 100 KHz and provide high quality tracks to the Level-2 trigger system. FTK performs track reconstruction in custom electronics with massive parallelism of associative memories and FPGAs. An overview of the FTK system design is presented along with R&D prototype progress of the individual components. Recent results on the performance impact for important physics areas including b-tagging, lepton isolation, and primary vertex finding will be shown from ATLAS MC simulation studies for different LHC luminosities.

A-37

Geant4 Simulation Studies for Improving Hadron Calorimeter Energy Resolution

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The next generation of lepton collider detectors (ILC, CLIC, Muon Collider) will emphasize precision for all sub-detector systems. The best hadron calorimeters have ($\Delta E/E$) ~50%/$\sqrt{E}$ for single particles, 70%-100%/ $\sqrt{E}$ for jets. What's wrong with hadrons? One benchmark: distinguish W and Z vector bosons in their hadronic decay mode. This requires a di-jet mass resolution better than the natural width of these bosons and hence a jet energy resolution better than 3%. For hadron calorimetry this implies an energy resolution a factor of at least two better than previously achieved to date by any large-scale experiment. Requires new ideas and concepts. We present a Geant4 simulation study done in understanding various parameters that affect the hadron sampling calorimeter energy resolution.

A-38

The Evolution of the Region of Interest Builder in the ATLAS Experiment at CERN

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ATLAS is a multipurpose particle detector at the Large Hadron Collider (LHC) at CERN designed to record the products of proton collisions. Given their high interaction rate (1GHz), selective triggering in real time is required to reduce the rate to the experiment's data storage capacity (1KHz). To meet this requirement, ATLAS employs a combination of hardware and software triggers to select interesting events for physics analysis. The Region of Interest Builder (RoIB) is an integral part of the ATLAS detector Trigger and Data Acquisition (TDAQ) chain where the coordinates of the region of interests identified by the first level trigger (L1) are collected and passed to the High Level Trigger (HLT) to make a decision. While the current custom RoIB operated reliably during the first run of the LHC, it is desirable to have the RoIB more operationally maintainable in the new run, which will reach higher luminosities with an increased complexity of L1 triggers. Our group is responsible for migrating the functionality of the multi-card VME based RoIB into a single PCI-Express card in a commodity PC. We have been exercising the software and firmware routines for reading out data in order to optimize our rates and understand our memory and CPU limitations.

A-39

Development of LBNE Photon Detector Front End Electronics

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The LBNE (Long-Baseline Neutrino Experiment) is the next generation accelerator-based neutrino oscillation experiment planned in US. The experiment will use a new muon-neutrino beam sent from Fermi National Accelerator Laboratory and will detect electron-neutrino appearance and muon-neutrino disappearance using a Liquid Argon TPC located at a distance of 1300 km at Sanford Underground Research Facility in South Dakota. The primary physics goal of the LBNE is a definitive determination the neutrino mass hierarchy, determination the octant of the neutrino mixing angle θ_{23}, and precise measurement of *CP* violation in neutrino oscillation. Neutrino interaction in LAr result in charged particles producing ionization and scintillation light signals. Dedicated photon detection (PD) system is under design for use in the LBNE LArTPC far detectors. The PD is designed to capture ultraviolet scintillation light that occurs when excited atoms in the liquid argon decay back to the ground state. These photons have a wavelength of 128 nm. Two processes contribute to producing prompt (decay constant 6 ns) and late (decay constant 1.6 μs) light components. By measuring the time of arrival of the photons, as well as the pulse height, the PD system can provide a time zero reference for the reconstruction of the event, as well as help identify the spatial coordinates of the event by triangulating between different photon detector elements in the detector. In addition the detection of scintillation light may be used as a trigger for the TPC. Measurement of the late light that arises from triplet states, which can be useful as a particle identification tool. The PD system must shift the wavelength of the scintillation light in order to use affordable photo-detectors. The baseline design couples wavelength-shifter coated ultraviolet transmitting acrylic to 3 mm2 silicon photo-multipliers (SiPMs). By detecting scintillation light we aim to improve event reconstruction capabilities and efficiently separate neutrino events from background. The signal out of the SiPMs is a charge or current pulse. The PD electronics must receive the SiPM signal, and digitize it to measure the time of arrival and also the pulse height. The SiPM response is quantized to measure integer number of photo-electrons, which is then used in the determination of the spatial location of the event. This presentation will describe requirements, implementation, and tested performance of the prototype front-end electronics to be used in PD system in LArTPC of LBNE.

A-40

Complex Scalar Dark Matter in a B-L Model

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In this work, we implement a complex scalar dark matter (DM) candidate in a $U(1)_{B\text{-}L}$ gauge extension of the Standard Model. The model contains three right-handed neutrinos with different quantum numbers and a rich scalar sector, with extra doublets and singlets. In principle, these extra scalars can have vacuum expectation values (V_Φ and V_ϕ for the extra doublets and singlets, respectively) belonging to different energy scales. In the context of $\zeta \equiv V_\Phi << V_\phi$, which allows one to obtain naturally light active neutrino V_Φ masses and mixing compatible with neutrino experiments, the DM candidate arises by imposing a Z_2 symmetry on a given complex singlet in order to make it stable. After doing a study of the scalar potential and the gauge sector, we obtain all the DM-dominant processes concerning the relic abundance and direct detection. Then, for a representative set of parameters, we find that a complex DM with mass

around 200 GeV, for example, is compatible with the current experimental constraints without resorting to resonances. However, additional compatible solutions with heavier masses can be found in vicinities of resonances. Finally, we address the issue of having a light *CP*-odd scalar in the model showing that it is safe concerning the Higgs and the Z_μ-boson invisible decay widths, and also astrophysical constraints regarding energy loss in stars.

A-41

Design and Fabrication of Prototype 6 cm X 6 cm Microchannel Plate Photodetector with Bialkali Photocathode for Fast Timing Applications

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Planar microchannel plate-based photodetector with bialkali photocathode is capable of fast and accurate time and position resolutions. A new 6 cm x 6 cm photodetector production facility was designed and built at Argonne National Laboratory. Small form-factor MCP-based photodetectors completely constructed of glass were designed and prototypes were successfully fabricated. Knudsen effusion cells were incorporated in the photocathode growth chamber to achieve uniform and high quantum efficiency photocathodes. The thin film uniformity distribution was simulated and measured for an antimony film deposition, showing uniformity of better than 10%. Several prototype devices have been fabricated with the described system. A typical prototype device with bialkali photocathode exhibits time-of-flight resolution of ~ 27 psec and differential time resolution of ~ 9 psec, corresponding to spatial resolution of ~ 0.6 mm.

A-42

Development of a 4 K Laser STM for Photophysical Studies at the Atomic Scale

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A detailed understanding of the optical and photo-physical properties of single molecules/atoms at relevant length scales is critically important for the development of molecular electronics and organic photovoltaic devices. In order to extend these studies in a stable environment, we are developing a 4 K Laser Scanning Tunneling Microscope (4K-Laser-STM) with integrated high-numerical-aperture (NA) optics behind and above the sample based on the Pan-style STM scanner. Using slip-stick inertial piezo steppers, the sample stage can be coarsely translated in X and Y directions, and, for optical experiments, a three-axis inertial lens stage can align the high-NA optics to focus laser excitation to and from photon collection at the tip-sample junction. The STM is cooled by a liquid helium bath surrounded by a liquid nitrogen jacket for operation near 4 K. Two separate ultrahigh vacuum chambers are used for sample preparation and STM measurements. The system has been tested successfully and will be commissioned soon.

Materials Science

A-43
Three-Dimensional Bragg Coherent Diffraction Imaging Using Polychromatic X-Rays

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Coherent x-ray diffraction imaging (CXDI) has been developed to obtain three-dimensional images of various types of specimens at the nanoscale [1,2]. CXDI performed in the Bragg geometry has been employed to examine strain and deformation field distributions inside crystals [3,4]. There has been much effort to enhance the capability of the CXDI by seeking to overcome current spatial limitations and experimental constraints [5-6]. However this technique requires significant time to perform three-dimensional scans making it incompatible with most time-resolved studies.

In this study, we propose a new approach for CXDI with the goal of obtain three-dimensional images as well as internal strain distribution on short time scales using a polychromatic beam. Because polychromatic coherent x-rays produce multiple projections of coherent diffraction patterns at the same time, this approach takes advantage of rapid measurements without scanning samples. This innovative approach may provide opportunities for real time measurements and time-resolved three-dimensional imaging on isolated or extended crystalline samples. The broadband coherent x-rays illuminated the sample and the coherent x-ray diffraction patterns were collected with an area detector. The setup for this technique and preliminary results taken at the 34ID-E beamline of the Advanced Photon Source will be discussed.

References
1. J. Miao et al., *Nature* 400, **342** (1999).
2. M. Pfeifer et al., *Nature* 442, **63** (2006).
3. I. Robinson et al., *Nature Materials* **8**, 291 (2009).
4. W. Cha et al., *Nature Materials* **12**, 729 (2013).
5. S. Hruszkewycz et al., *Nano Letters* **12**, 5148 (2012).
6. S. Hruszkewycz et al., *Physical Review Letters* **110**, 177601 (2013).

A-44
Resonant Tunneling of Fluctuation Cooper Pairs

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Superconducting fluctuations have proved to be an irreplaceable source of information about microscopic and macroscopic material parameters that could be inferred from the experiment. According to common wisdom, the effect of thermodynamic fluctuations in the vicinity of the superconducting transition temperature, T_c, is to round off all of the sharp corners and discontinuities, which otherwise would have been expected to occur at T_c. Here we report the current spikes due to radiation-induced resonant tunneling of fluctuation Cooper pairs between two superconductors which grow even sharper and most pronounced upon approach to T_c. This striking effect offers an unprecedented tool for direct

measurements of fluctuation Cooper pairs' lifetime, which is key to our understanding of the fluctuation regime, most notably to nature of the pseudogap state in high temperature superconductors. Our finding marks a radical departure from the conventional view of superconducting fluctuations as blurring and rounding phenomenon.

A-45

Towards Large Scale First Principles Modeling of Nanomaterials for Energy Conversion Research

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The availability of computational resources, scaled up to the petascale, has opened the challenging opportunity to simulate materials whose size is comparable to the one actually probed by experiments. In this context, accurate electronic structures are typically needed in order to build predictive capabilities that can be employed to design new materials with customized properties made more efficient using principles revealed by basic science. Density functional theory (DFT) is widely used as a first principle tool to simulate the structural and electronic properties of materials. Typical limitations of DFT with semilocal functionals can be overcome by considering hybrid functionals and manybody perturbation theory (MBPT) based corrections. However the use of these strategies for large systems, able to take into account for instance the role of disorder, defects, interfaces or quantum confinement, has been strongly limited by the computational cost of the simulations. In this poster we present the implementation of a new hybrid functional scheme for condensed systems and discuss both method and code development for MBPT simulations of large systems. The simulations of the quasiparticle electronic structure of systems relevant for photovoltaics and photocatalysis are presented and the parallel performance of the developed code is discussed.

A-46

Synchrotron X-Ray Studies of Thin Film Solid Oxide Fuel Cell Cathodes

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Solid oxide fuel cells (SOFCs) are a scalable, fuel-flexible, and efficient technology for energy conversion. However, several materials design and efficiency challenges still limit their performance. In particular, the oxygen reduction reaction at the cathode is known to be a rate-limiting step in the energy conversion process. To improve SOFC performance, it is crucial to gain a better fundamental understanding of the reduction reaction mechanism and its relation to changes in the cathode structure and composition during cell operation.

Synchrotron measurements at the Advanced Photon Source have provided unique insight into the oxygen reduction reaction. In the current work, the oxygen exchange reaction in strontium- and cobalt-doped lanthanum ferrite (LSCF), a common cathode material, was studied *in situ* using thin films deposited on a YSZ electrolyte substrate. Oxygen exchange coefficients at the cathode surface and the cathode/electrolyte interface were obtained by studying changes in the cathode oxygen vacancy concentration in response to an applied electrochemical bias. Vacancy concentration changes were

calculated by using synchrotron x-ray diffraction to measure changes in the film's lattice parameter, which increases with increasing oxygen vacancy concentration. This technique was used to study the effect of atmospheric H_2O and CO_2 on the LSCF oxygen exchange performance.

A-47

Ultraprecision Surface Monitoring during Growth of InGaN on GaN

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Ultrahigh-precision control of interface flatness, thickness and composition in the heterostructure of InGaN/GaN is becoming increasingly important for the realization of InGaN-based light emitting diodes (LEDs) with the best performance and the highest efficiency. In this poster, we propose new tools for *in situ* monitoring during metalorganic vapor phase epitaxial growth at the atomic level [1].

The tool is the grazing-incidence x-ray reflectivity measurement system, for which atomic-level roughness resolution is obtained because of the short wavelength of x-rays. In addition, x-ray reflectivity is also sensitive to the density of valence electrons in each atom. Therefore, we can measure *in situ* the atomic-level surface roughness and composition in real time. The surface roughening of the epilayer as a function of growth time was calculated from the continuous *in situ* XRR curve. The growth rate, critical thickness $h_{c(r)}$ for surface roughening, and roughening rate were obtained. We observed two critical points at which the x-ray intensity corresponds to the roughness change. The first critical point shows the roughening without lattice relaxation, and the second point indicates the lattice relaxation caused by the generation of defects. The experimental critical thickness $h_{c(r)}$ of the $In_{0.11}Ga_{0.89}N$ epilayer analyzed from the continuous *in situ* XRR curve was about 14.87 nm.

References
1. Guangxu Ju, Shingo Fuchi, Masao Tabuchi, Hiroshi Amano, and Yoshikazu Takeda: Continuous in situ X-ray reflectivity investigation on InGaN epitaxial growth by metalorganic vapor phase epitaxy, Journal of Crystal Growth (Elsevier) Vol. **407**, pp. 68–73 (2014).

A-48

Fragment Approach to Density Functional Theory Calculations of Large Systems

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Ab initio electronic structure simulations have been used extensively over the past few decades to improve our understanding of the behavior and properties of materials. In particular, density-functional theory (DFT) has become the method of choice due to its excellent balance between accuracy and efficiency. However, standard implementations of DFT scale cubically with the number of atoms and so algorithms must be designed with reduced scaling in order to allow simulations of realistic (large) systems of technological importance. One such code is BigDFT, which has been designed for massively parallel machines and recently expanded to include a linear-scaling approach. This approach uses an adaptive localized basis set, which is itself represented in an underlying wavelet basis set and thus retains all the

benefits of wavelets such as systematic convergence, while also presenting some new advantages. In particular the basis functions can be reused between closely related systems, resulting in further computational savings and facilitating a fragment based approach. This fragment approach is particularly suited to the explicit treatment of solvents and the calculation of charge transport parameters. We will present details of the fragment approach in BigDFT, highlighting an example in each of these two application areas.

A-49

Time-Dependent Ginzburg-Landau Equations and Vortex Dynamics Simulations on GPUs

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Most energy applications of superconductivity, such as electric power transmission over superconducting cables or powerful magnets, require low energy dissipation in high-temperature superconductors. Restricting the mobility of the vortices carrying magnetic field in the superconducting material by pinning them with admixed inclusions or confining their motion geometrically can minimize dissipation. We present modern simulation results of the time-dependent Ginzburg-Landau equation for large-scale mesoscopic superconductors, like narrow superconducting strips and nano-patterned superconductors. In particular, we discuss the case of nano-scale extended pinning inclusions, whose geometry has a non-trivial influence on the current-voltage characteristics. The required large-scale simulations were made possible with recent GPU computing techniques.

A-50

A Theoretical Perspective on the Photocatalytic Water Splitting Properties of Cobalt Oxides

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Cobalt oxides have found common use as cocatalyst materials for photocatalytic water oxidation. We investigate the role defects play in altering the quasi-particle gap and the absolute position of the valence and conduction bands in the phases of cobalt oxide relevant to water oxidation, cobalt oxyhydroxide (CoOOH) and the cobalt oxide spinel (Co_3O_4). We evaluate the valence band alignment between the cobalt oxide phases to assess their relative oxidative strength and find that on an absolute scale both phases are favorably positioned with respect to the water oxidation potential and are positioned at less oxidizing potentials than the valence bands of the prototypical photoanode materials they are coupled with (e.g., ZnO and WO_3). We make use of the nonempirical self-consistent hybrid functional we recently developed for condensed matter systems, which yields macroscopic dielectric constants and band gaps in excellent agreement with experiment. This self-consistent hybrid functional provides a more affordable means to obtain similar high accuracy results as the expensive many-body perturbation techniques.

Mathematics and Computer Science

A-51
A Method for the Estimation and Detection of Individual Solar Oscillations

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The study of the systematic oscillations of the Sun, or solar modes, has led to better understanding of the Sun's inner structure and dynamics. Estimates of individual mode frequencies are desirable as inputs for solar inversion models and have been obtained in the literature using either least-squares models fit to spectrum estimates or directly to Fourier-transformed helioseismic data. Recent studies have concluded that solar modal structure remains coherent past turbulence in the convection zone and imprints its signatures on the solar wind and the interplanetary magnetic field fluctuations [2], so data from these sources can be expected to contain several hundreds of modes in very short bands in frequency. Estimation of modal parameters from these data pushes the limits of conventional spectrum-based approaches. An alternative parametric approach described here uses maximum likelihood estimation on a simple Lorentzian model with four parameters: A, the integrated power of the mode, a the damping constant, f0 the center frequency and s2 the noise power. Assuming a Gaussian process model, the likelihood can be simplified using a Karhunen-Loève expansion where the associated eigenvalues and eigencoefficients have convenient analytic expressions [3]. This method may also be of interest for modeling terrestrial free oscillations.

References
1. J. Christensen-Dalsgaard. Helioseismology, **74**:1073–1129, 2002.
2. D.J. Thomson, L.J. Lanzerotti, F.L. Vernon, III, M.R. Lessard, and L.T.P. Smith. Solar modal structure of the engineering environment. Proc. IEEE , **95**:1085–1132, 2007.
3. H.L. VanTrees, K. Bell, and Z. Tian. Detection, Estimation, and Modulation Theory, Part I: Detection, Estimation and Filtering Theory. 2nd edition, 2013.

A-52
Distributed Generation for Energy-Efficient Buildings: A Mixed-Integer Multi-Period Optimization Approach

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We study a two-stage mixed-integer program with application in distributed generation for energy-efficient buildings. This challenging problem is beyond the capacity of current solvers, because the second-stage problem contains a large number of binary variables. By exploiting periodicity structure in daily, weekly, seasonal, and yearly demand profiles, we develop a column generation approach that significantly reduces the number of binary variables, consequently, rendering computationally tractable problems. Furthermore, our approach provides bounds with provable performance guarantees.

Synchrotron

A-53
Measuring Cavitation in Fuel Injection Systems Using Synchrotron X-Rays

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Reducing emissions and increasing the efficiency of Diesel engines is a critical factor in meeting our future energy and transportation needs, and improving air quality. To achieve these goals, diesel engine manufacturers are moving to higher fuel injection pressures and smaller injector holes. Doing so leads to a new problem; hydrodynamic cavitation of the fuel inside the injector due to rapid changes in pressure and velocity. This can damage the injector and alters the structure of the fuel spray, affecting combustion and emissions. The problem is not fully understood, as cavitation is difficult to measure. Under the X-ray Fuel Spray project supported by the U.S. Department of Energy, we use brilliant x-rays from Argonne's Advanced Photon Source to shed light on the problem. X-ray phase contrast imaging allows us to observe cavitation occurring in real time in fuel injectors. X-ray radiography and fluorescent spectroscopy allow us for the first time to quantitatively measure the cavitation vapor distribution in plastic models, which can be directly compared to high-resolution simulations performed at Argonne's Laboratory Computing Resource Center. These tools give us a new insight into the fundamental fluid mechanics of cavitating flow, addressing an important engineering problem facing the U.S. automotive industry.

A-54
Molten Oxides above 2000K: From Silica to Uranium Dioxide

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Many oxides melt at temperatures above 2000K, which prevents study of the melt in an ordinary furnace. To access temperatures up to 3500K we use aerodynamic levitation and laser heating techniques, which minimize chemical contamination of the sample. One important recent study is that of Uranium dioxide (UO_2). UO_2 is the major fuel component for most nuclear power reactors in use today. Yet the 3140K melting temperature of UO_2 has severely limited study of the liquid phase. Here we studied hot solid and molten UO_2 with synchrotron x-ray diffraction and compare the measured structure and properties with molecular dynamics predictions. On melting, the average U-O coordination of the melt drops from 8 to 6.7(5) and molecular dynamics (MD) models refined to this low coordinated structure predict ~3 times higher U-U mobility compared to 8-coordinated melt arrangements.

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