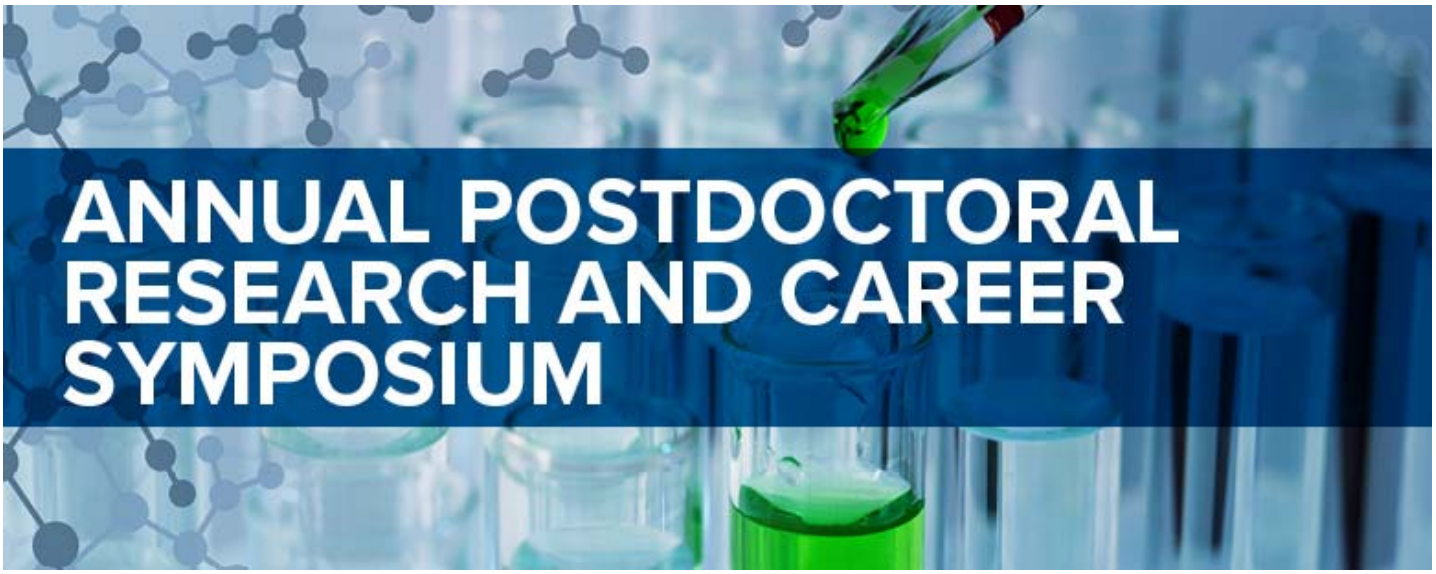

November 8, 2018

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Argonne National Laboratory Postdoctoral Research and Career Symposium

November 8, 2018

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Illinois Science and Technology Coalition

Materials Development, Inc.

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2018 Postdoctoral Research and Career Symposium
November 8, 2018

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2018 Postdoctoral Research and Career Symposium
November 8, 2018

Agenda

8:00 AM — Continental Breakfast and Registration (TCS Conference Center)

MORNING SESSION

9:00 AM — Welcome Remarks from Suresh Sunderrajan, Interim Associate Laboratory Director, Energy and Global Security Directorate

9:15 AM — Keynote Address by Peter Fiske, Director -Water Energy Resilience Research Institute (WERRI) - Lawrence Berkeley National Lab

10:00 AM — Poster Session A and Free Networking

NETWORKING LUNCH

11:30 AM — Networking Lunch (company exhibitors and representatives from diverse career paths will have a chance to talk with postdocs in small groups)

AFTERNOON SESSION

1:30 PM — Poster Session B and Free Networking

3:00 PM — Career Panel Discussion

4:00 PM — Presentation of Poster Awards and Closing Remarks from Stephen K. Streiffer Associate Laboratory Director, Photon Sciences, and Director of the APS

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2018 Postdoctoral Research and Career Symposium
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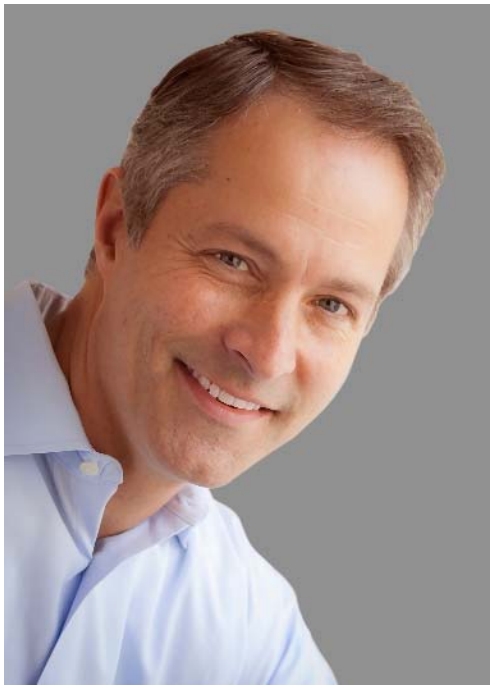
2018 Keynote Address



Dr. Peter Fiske, Director of the Water-Energy Resilience Research Institute (WERRI) at Lawrence Berkeley National Laboratory

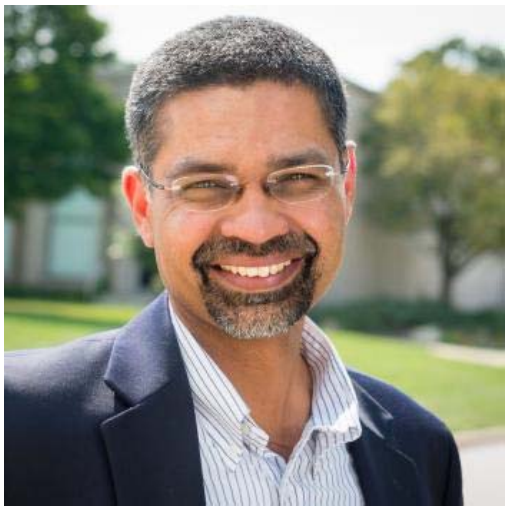
Dr. Peter S. Fiske is the Director of the Water-Energy Resilience Research Institute (WERRI) at Lawrence Berkeley National Laboratory. WERRI's goal is to orient and align the water-related research programs at LBNL to address critical gaps in the reliability, efficiency and sustainability of water-energy systems in California and the nation.

Prior to joining LBNL, Fiske was the Chief Executive Officer of PAX Water Technologies, Inc. from 2008 until January, 2017 when it was acquired by UGSI Inc. in an all-cash transaction. PAX Water pioneered the use of biomimicry to develop innovative and energy efficient technologies for the water industry. PAX Water won a number of national water industry awards and its iconic Lily impeller technology was featured in a major design exhibit at the New York Museum of Modern Art in 2008.

Fiske is also a frequent writer and lecturer on the subject of career strategy, entrepreneurship and leadership for scientists and engineers. He has been a keynote speaker or guest lecturer at some of the leading R1 universities in the United States. He is a founding faculty member of the Department of Energy's I-Corps Program. He is the author of Put Your Science to WORK!, numerous articles for the American Association for the Advancement of Science's career website ScienceCareers.org, and presently writes an occasional column in the journal Nature.

Prior to joining PAX Water, Fiske was co-founder of RAPT Industries, Inc., a pioneer in the field of plasma processing of optics and semiconductors. Fiske spun the company out of Lawrence Livermore National Laboratory where he was a staff scientist.

Welcome Remarks Speaker



Suresh Sunderrajan, Interim Associate Laboratory Director, Energy and Global Security Directorate Argonne National Laboratory

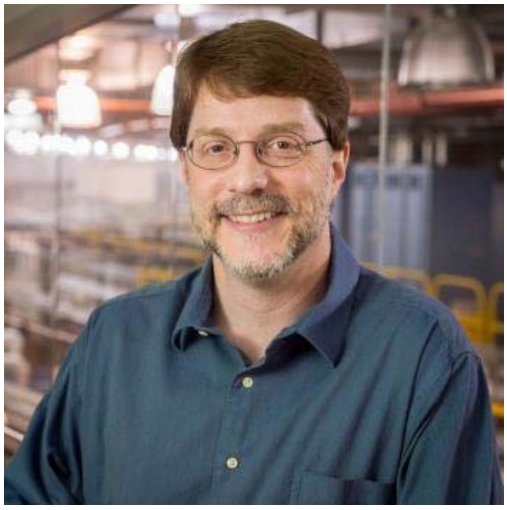
Dr. Suresh Sunderrajan is the interim Associate Laboratory Director for the Energy and Global Security Directorate. He leads a team that applies crosscutting expertise in science, engineering, and technology to develop solutions to challenging problems related to energy, manufacturing, and global security. Previously, he served as Associate Laboratory Director of Argonne's Science and Technology Partnerships and Outreach Directorate, which works with the laboratory's research directorates to develop strategies that sustain and expand the lab's relationships with industry, academia, government, and other sectors. Prior to starting at Argonne, Suresh was at United Technologies Corporation, where he served as Director of Innovation Business Development, the Corporate Intellectual Property monetization organization — responsible for patent and technology licensing, patent sales, and new business incubation opportunities. Before working at United Technologies Corporation, Suresh was a serial entrepreneur, part of the founding teams for four different start-ups.

Suresh also worked at the International Copper Association where he supervised several globally-dispersed early stage technology commercialization activities; at Eastman Kodak Company, where he led the commercialization of several generations of photographic imaging supports, the creation of a silver nanomaterials-based antimicrobial business, and was a Director with the Corporate Venture Capital group; and at Union Camp Corporation (International Paper) where, as a Senior Process Engineer, he led the first alkaline conversion of a coated board machine in the United States.

He holds more than 30 U.S. patents and received the Distinguished Inventor Award at Eastman Kodak. He is a Certified Licensing Professional. Suresh earned his PhD in Chemical Engineering at North Carolina State University, Raleigh and an SM in Management and Engineering from Massachusetts Institute of Technology.

Closing Remarks Speaker

Stephen K. Streiffer, Associate Laboratory Director, Photon Sciences, and Director of the APS

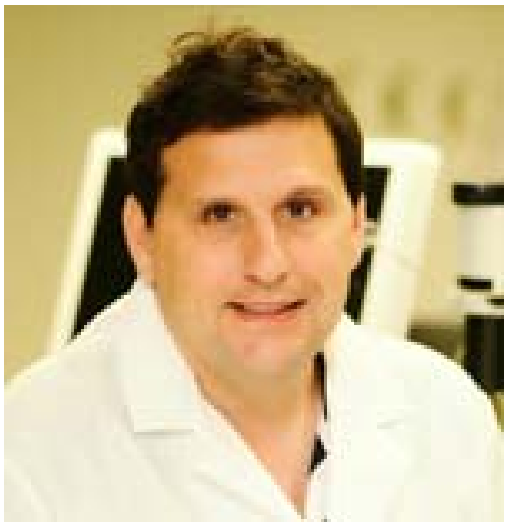


Stephen Streiffer is the Associate Laboratory Director for Photon Sciences at Argonne. The Photon Sciences directorate consists of the X-ray Science, Accelerator Systems and Advanced Photon Source Engineering Support divisions, which comprise the Advanced Photon Source (APS); and the Argonne Accelerator Institute.

The APS is the brightest source of high-energy X-rays in the Western Hemisphere and is used to study the structures of materials and processes at the atomic scale. It is also the largest scientific user facility in the North America, with more than 3,500 users visiting each year. He has also served as interim director of Argonne's Center for Nanoscale Materials, a national user facility that provides capabilities explicitly tailored to the creation and characterization of new functional materials on the nanoscale. The center's portfolio includes research on electronic and magnetic materials and devices, nanobio interfaces, nanofabrication, nanophotonics, theory and modeling, and X-ray microscopy. Dr. Streiffer's scientific expertise is in nanostructured complex oxides and in structural characterization of materials particularly using transmission electron microscopy and X-ray scattering techniques.

His research program include the development of novel concepts for integration of oxide heterostructures, establishing a fundamental understanding of polar interfaces, and exploring how these interfaces may be manipulated to influence electronic and chemical function.His active research projects focus on utilizing in-situ synchrotron X-ray methods to probe chemical vapor deposition of complex oxides as well as phase transformations and nanoscale size effects in ferroic thin films. He is also currently involved in in-situ synchrotron X-ray studies of the synthesis of InGaN heterostructures as part of an effort to expand the basic understanding of materials for energy-efficient solid state lighting. He has authored or co-authored more than 150 scientific publications and holds one patent.

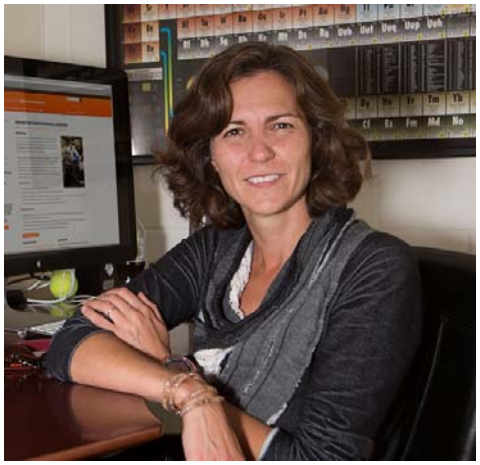
Academic Table



Walter Henne, Associate Professor of Chemistry at Governors State University

Walter Henne is an Associate Professor of Chemistry at Governors State University. He received his Ph.D. in Chemistry from Purdue University with a special focus in Bio-Analytical Chemistry and Chemical Biology. His current research interests center around the use of low molecular weight, high affinity ligands/probes for the development of targeted drug therapies and medical diagnostic assays. Areas span infectious disease, cancer and inflammatory disorders. He is the author of more than 20 peer-reviewed research papers, patents and has received several awards for excellence in teaching. Walter has mentored several Argonne postdocs through the academic search process.

Career Panelists



Dr. Ksenija Glusac, Associate Professor of Chemistry at the University of Illinois at Chicago with a joint position in the Chemical Sciences and Engineering Division at the Argonne National Laboratory

She obtained her B. Sc. from University of Belgrade, Serbia (Mentor: Prof. Radomir Saicic) and Ph.D. from University of Florida (Mentor: Prof. Kirk S. Schanze). After postdoctoral studies at Stanford University (Mentor: Prof. Michael Fayer), Ksenija started her independent research career at Bowling Green State University in 2006, where she was also a member of the Center for Photochemical Sciences. In 2015, Ksenija performed research as a visiting professor at the University of Michigan, in collaboration with Prof. Stephen Maldonado). In 2017, she took a joint position as the associate professor at the University of Illinois at Chicago and a principal scientist at the Argonne National Laboratory.

Ksenija studies conceptually new photo- and electro-catalysts relevant to energy storage and solar fuel applications. In specific, she investigates molecular models for earth abundant structures, which are expected to lead to a new generation of inexpensive and nontoxic materials. Ksenija's research interests are centered around the following themes: (i) electrocatalytic oxygen evolution and reduction reaction by heteroatom doped carbon nanomaterials; (ii) photocatalytic CO2 reduction by biomimetic NADH analog catalysts; (iii) excited-state hydroxide ion release and its application in photobased-driven chemical and polymerization reactions. Ksenija is a recipient of BGSU Outstanding Young Scholar Award, 2012 NSF CAREER Award, ACS PRF Postdoctoral Fellowship and 2002 Jones Award for Creativity and Originality.

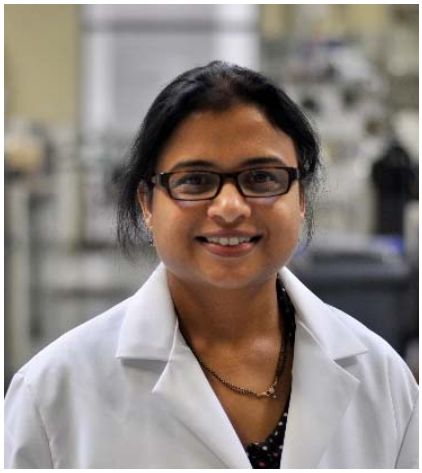
Dr. Joe Bernstein, Senior Director, Financial and Grant Services, UChicago

Dr. Joe Bernstein is the Senior Director, Financial & Grant Services, for the University of Chicago Division of the Humanities and serves as a University of Chicago Inclusion in Practice, Hearing One Another, and Safe Space diversity and inclusion program facilitator. In addition, he is concurrently pursuing his MBA from the University Of Chicago Booth School Of Business. Previously, Joe earned his AB in Physics from the University of Chicago in 1996, MS in Physics from the University of Kentucky in 1998, and PhD in Astronomy & Astrophysics from the University of Michigan in 2008 (MS 2002). Joe then worked as a postdoctoral researcher and communications professional at the U.S. Department of Energy's Argonne National Laboratory until 2013. Subsequently, he managed a graduate career advising team at the University of Chicago and then co-founded H-CORE, LLC, in 2014. Joe went on to work in a financial planning capacity at Northwestern Mutual

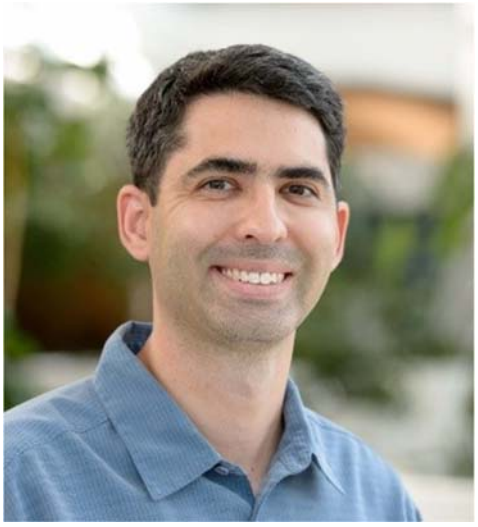
before returning to the University of Chicago in 2016 to launch his career in higher education financial administration.

Joe served as the Graduate Employees Organization Grievance Committee Chair and a Student Conflict Resolution Panelist at the University of Michigan. He founded the Talk to Joe the Astronomer education and public outreach program in 2008 and served as the 2011 Outreach Committee Chair for the National Postdoctoral Association. Joe has also been a public outreach volunteer at the Adler Planetarium and volunteer advocate with Rape Victim Advocates in Chicago. In addition to serving on the University of Chicago Sexual Misconduct Advisory Board, he has coached teams in the Hyde Park Kenwood Legends urban youth baseball organization. Joe is originally from the Texas Hill Country and makes his home on the South Side of Chicago.

Dr. Shalaka Shinde, Senior Scientist, Oil-Dri Corporation of America



Dr. Shalaka Shinde recently joined Oil-Dri in the role of Senior Research Scientist as part of the newly created Laboratory for Applied Microbiology. Dr. Shinde's research experience includes the study of micro-nutrients and the impact of fungi and bacteria on plant growth. She graduated from West Virginia University in 2012, where her research focused on plant mycorrhizal interaction using genetic, physiological and transcriptional studies. After graduation, Shalaka spent the next 5 years at Argonne National Lab working to understand the molecular mechanism of plant and microbe interactions using OMIC's tool.



Dr. Jonathan Logan, Scientist, Alcorix Co.

Dr. Jonathan Logan is a Scientist at Alcorix Co., where he develops X-ray optics for the synchrotron X-ray community using innovative microfabrication approaches. He has a Ph.D. in physics from the University of Chicago (2013), and was a postdoctoral scientist at the Hard X-ray Nanoprobe beamline at Argonne investigating epitaxial, magnetic thin films using focused X-rays (2014-2017). He developed a strong interest in entrepreneurship while participating in the Polsky I-Corps and DOE Energy I-Corps programs. He enjoys the varied nature of his work at a small company, which includes innovation, device fabrication, grant writing, computer simulations, customer discovery, and even webpage development.

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Poster Abstracts

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Poster Abstracts

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A-1

TCR-pMHC Bond Length Controls TCR Ligand Discrimination

Combined XPS-UPS Study of Conduction and Valence Band Offsets for Al 2 O 3 /HfO 2 High-k Dielectric Nanolaminates Grown on Single-crystal GaN and Ga 2 O 3 (010) by Atomic Layer Deposition

David J. Mandia[1], Bahadir Kucukgok[1], Maximillian Gebhard[1], Jian Liu[2], Jacob H. Leach[3], Angel Yanguas-Gil[1], Jeffrey W. Elam[1]

[1]Applied Materials Division, Argonne National Laboratory, Lemont, Illinois, USA
[2]Department of Chemistry, Northwestern University, Evanston, Illinois, USA
[3]Kyma Technologies, Inc., Raleigh, North Carolina, USA

The search for adequate binary metal oxide dielectric nanolaminates (NLs) to prevent degradation of power semiconductor devices is ongoing and involves the atomic layer deposition (ALD)-growth of a variety of binary metal oxide combinations. In the present work, we explore the ALD growth of amorphous (x)HfO_2/(y)Al_2O_3 NLs on Si (with native SiO_2 layer) substrates and then on both GaN and Ga_2O_3 single crystals. A variety of samples ranging from their homogeneous mixtures to HfO_2 or Al_2O_3-rich NLs are assessed before and after a thermal annealing by spectroscopic ellipsometry (SE), XAS techniques such as X-ray photoelectron spectroscopy (XPS) and X-ray absorption fine structure (EXAFS) measurements in order to elucidate the structural evolution of the NL at the GaN (or Ga_2O_3)-NL interface. By quantifying the HfO_2 incorporation throughout the Al_2O_3 layer and using the programmable nature of ALD to alternate layers of the HfO_2 and Al_2O_3 in an $(AB)_x$-$(CD)_y$ fashion, the influence of HfO_2 mobility within Al_2O_3 layer on the NL dielectric constant can be verified unequivocally. EXAFS is a powerful tool for determining the local coordination environment of the Hf at the GaN or Ga_2O_3(001)-HfO_2 interface and, at low super cycle numbers (sub-nm scale), the ultimate stability of the NLs can be probed and optimized such that the bulk material properties are retained. Finally, via a modified Kraut's method [1], Ultraviolet photoelectron spectroscopy (UPS) is used to obtain the valence band maximum of the GaN and Ga_2O_3 substrates and combined with the high-resolution XPS data for the Hf and Ga shallow core-level photoelectrons ejected from the thin HfO_2/Al_2O_3 overlayer in order to assess the conduction band offset (CBO) at the film-substrate heterojunction. Probing the insulator properties imparted by the high-k overlayer on the wide bandgap semiconductor surfaces of GaN and Ga_2O_3 is crucial in order to understand and prevent the degradation problem in Ga_2O_3/GaN-based power semiconductor devices. Moreover, photoluminscence (PL) studies of the coated and pristine samples will corroborate the effect of the bulk defect concentration on the conduction/valence band properties of the material.

[1] E.A. Kraut, R.W. Grant, J.R. Waldrop, S.P. Kowalczyk, Phys. Rev. Lett. 44, 1620 (1980).

A-3

Real Time Observation Of Binder Jetting Printing Process Using High-Speed X-Ray Imaging

Niranjan D. Parab[1], John Barnes[2], Cang Zhao1, Ross Cunningham[3], Kamel Fezza[1], Anthony Rollett[3], and Tao Sun[1]

[1]X-ray Science Division, Argonne National Laboratory, Argonne, IL 60439
[2]The Barnes Group Advisors, Pittsburgh, PA 15143
[3]Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA 15213

A high-speed synchrotron X-ray imaging technique was used to investigate the binder jetting additive manufacturing (AM) process. A commercial binder jetting printer with droplet-on-demand ink-jet print-head was used to print single lines on powder beds. The printing process was recorded in real time using high-speed X-ray imaging. The ink-jet droplets showed distinct elongated shape with spherical head, long tail, and three to five trailing satellite droplets. Significant drift was observed between the impact points of main droplet and satellite droplets. The impact of the droplet on the powder bed caused movement and ejection of the powder particles. The

depth of disturbance in the powder bed from movement and ejection was defined as interaction depth, which is found to be dependent on the size, shape, and material of the powder particles. For smaller powder particles (diameter less than 10 μm), three consecutive binder droplets were observed to coalesce to form large agglomerates. The observations reported here will facilitate the understanding of underlying physics that govern the binder jetting processes, which will then help in improving the quality of parts manufactured using this AM process.

A-4

Comparison of Different Modeling Approaches of Distributed Energy Resources for Bulk Electric System Reliability Studies

Rojan Bhattarai[1], Amirthagunaraj Yogarathinam[2] and Ning Kang[1]

[1]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
[2]School of Electrical Engineering and Computer Science, Pennsylvania State University, University Park, PA 16802

The increasing penetration of Distributed Energy Resources (DER) in the distribution system not only creates operational problems on the distribution system itself, but they may also impose challenges on the reliability of bulk electric system (BES). Under the high DER penetration scenario, proper modeling of DER along with their protection and control functionalities is essential to ensure accurate reliability impact analysis of the BES. Two approaches of modeling DER in the distribution system are discussed – aggregated and detailed modeling approaches. Aggregated DER modeling approach is compared with the detailed modeling approach in terms of their performance for the BES reliability impact analysis. The comparison studies are performed on a representative Transmission & Distribution (T&D) combined system, featuring the Kundur Two-Area system on the transmission system side and the IEEE 34-node test feeders on the distribution system side. Even though the aggregated modeling approach has computational advantages over the detailed modeling approach, the results obtained show that the parameters of the aggregated DER modeling should be well calibrated to capture the distributed nature of DER and the variations in their protection and control settings.

A-5

Electrochemical Corrosion of Alloyed Nuclear Waste Form

V.K. Gattu[1], W.L. Ebert[1], and J.E. Indacochea[2]

[1]Chemical and Fuel Cycle Technologies, Argonne National Laboratory, Argonne, IL 60439
[2]Civil and Materials Engineering, University of Illinois at Chicago, Chicago, IL 60607

Argonne-developed electrochemical method was applied to measure the corrosion behavior of waste forms. Developmental studies conducted during the past several years have led to a mechanistically-based model for predicting long-term corrosion kinetics for iron-based alloys and the laboratory testing protocol to parameterize that model.

Potentiodynamic (PD) scans and Potentiostatic (PS) tests were performed to characterize the corrosion behavior. Surfaces of the electrodes were characterized by SEM/EDS before and after the electrochemical tests to compare and identify the active-passive phases. Solutions collected during and at the end of the PS tests were analyzed using inductively-coupled plasma mass spectrometry (ICP-MS). Analytical functions were derived for modeling the Eh and pH dependence in the degradation model. Surface stabilization corresponding to the Eh-pH stability regions of passivating oxides decreases corrosion rates by ~100X. Finally, Equivalent circuit models of EIS responses can provide confidence in using measured electrochemical kinetics to model waste form performance.

A-6

Evaluating and Optimizing Kernels on OpenCL FPGA Platform for Energy-efficient High- Performance Computing

Zheming Jin[1]

[1]Leadship Computing Facility, Argonne National Laboratory, Argonne, IL 60439

Compared to central processing units (CPUs) and graphics processing units (GPUs) which have fixed architectures, field-programmable gate arrays (FPGAs) offer reconfigurability and promising performance and energy efficiency. With these FPGA-based heterogeneous computing systems, programming standards have emerged to facilitate transformation of algorithms from standard systems to heterogeneous systems. Open Computing Language (OpenCL) is a standard framework for writing programs that execute across various heterogeneous computing platforms. Investigating the characteristics of kernel applications with emerging OpenCL-to-FPGA development flows is important for researchers, who have little hardware development experience, to evaluate and adopt the FPGA-based heterogeneous programming model in a laboratory. In this poster, I will focus on the evaluations and optimizations of a variety of OpenCL kernels on an Arria10-based OpenCL FPGA platform. The experimental results show that FPGAs are promising heterogeneous computing components for energy-efficient high-performance computing.

A-7

Comparison of Graphite Materials for Fast-Charging Capability in Lithium-Ion Batteries

Joel Kirner[1], Yan Qin[1], Xin Su[1], Linghong Zhang[1], Yangxing Li[2], Wenquan Lu[1]

[1]Chemical Sciences & Engineering Division, Argonne National Laboratory, Argonne, IL 60439
[2]Central Research Institute, Huawei Technologies Co., LTD, Longgang District, Shenzhen, 518129, China

Fast-charging capability in lithium-ion batteries (LIBs) is highly desirable in order to assuage “range anxiety” for electric vehicle consumers. In state-of-the-art LIBs, the ability to safely fast-charge is limited by polarization at the graphite anode, which can result in dangerous lithium-metal plating. In this work, we analyze and compare the fast-charging capabilities of a series of graphite samples from commercial suppliers. Electrochemical data from the different graphite anodes in full-cell batteries is interpreted with the help of characterization data of the raw materials in order to improve understanding of structure-function relationships.

A-8

In-Situ Visualization of Extreme-Scale Cosmological Simulations using Point Sprites

Sergei Shudler, Silvio Rizzi, Joseph Insley, Thomas Uram

Leadership Computing Facility Division, Argonne National Laboratory, Lemont, IL 60439

As the HPC world moves towards extreme-scale systems with highly asymmetrical FLOPs to IO bandwidth ratio, in-situ analysis has the potential to reduce the prohibitive amounts of data simulations write to disk for post-hoc analysis. In-situ techniques aim to analyze scientific data whilst the application is running and the data is still in memory. The goal is to minimize expensive data movements or, at least, filter parts of it. One prominent example for a highly scalable simulation is HACC (Hardware/Hybrid Accelerated Cosmology Code), a particle-based cosmology code that aims to improve our understanding of the universe structure and, in particular, dark matter and dark energy. Previous study has shown that using point sprites visualization for particle-based simulation offers both high-fidelity results and better performance. In this work, we take a step further and use point sprites visualization in situ, thereby allowing users to inspect the results on the fly. Moreover, we plan to further

investigate the benefits of integrating HACC with general in-situ and data analysis frameworks.

A-9

$BaFe_2S_3$: Turning An Insulator Into A Metal – A Local Probe Magnetic Study

Philipp Materne[1], Wenli Bi[1,2] , Jiyong Zhao[1], Michael Y. Hu[1], Maria Lourdes Amigó[3], Silvia Seiro[3], Saicharan Aswartham[3], Bernd Büchner[3], and E. Ecan Alp[1]

[1]Argonne National Laboratory, Lemont, IL, USA
[2]University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA
[3]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany

BaFe2S3 is a quasi one-dimensional Mott insulator that orders antiferromagnetically below ~125 K. The application of pressure induces a transition to a metallic state, and superconductivity emerges. The evolution of the magnetic behavior on increasing pressure has up to now been either studied indirectly by means of transport measurements, or by using local magnetic probes only in the low-pressure region. Here, we investigate the magnetic properties of BaFe2S3 up to 9.9 GPa by means of synchrotron 57Fe Mössbauer spectroscopy experiments, providing the first local magnetic phase diagram. The magnetic ordering temperature increases up to 185(5) K at 7.5 GPa, and is fully suppressed at 9.9 GPa. The low-temperature magnetic hyperfine field is continuously reduced from 12.9 to 10.3 T between 1.4 and 9.1 GPa, followed by a sudden drop to zero at 9.9 GPa indicating a first-order phase transition. The pressure dependence of the magnetic order in BaFe2S3 can be qualitatively explained by a combination of a bandwidth-controlled insulator-metal transition as well as a pressure enhanced exchange interaction between Fe-atoms and Fe 3d-S 3p hybridization.

A-10

Effects of Ions and Temperature at the Water/Silica Interface Probed by Sum Frequency Generation Spectroscopy

Kaitlin Lovering[1], Keng Chou[2], and Allan Bertram[2]

[1]Chemical Science Engineering Division, Argonne National Laboratory, Argonne, IL 60439
[2]Department of Chemistry, University of British Columbia, Vancouver, BC V6T 1Z4

The mineral/aqueous interface is pervasive in marine, terrestrial, and atmospheric environments. In the atmosphere, the presence of insoluble aerosols can promote the formation of ice in clouds. The phase of the cloud changes its lifetime and albedo and the interactions that occur at mineral/water interfaces affect the earth's radiative budget. Consequently, understanding these interfacial interactions is important for climate models. However, surfaces and interfaces are the minority component in most systems and are difficult to study. Under the electric dipole approximation, Sum Frequency Generation (SFG) Spectroscopy is only allowed in non-centrosymmetric systems, such as interfaces, and can provide molecular level information of interfacial interactions. Using SFG, we are able to directly probe how the structure of water changes at the silica surface as temperature and ion concentration are varied. We find that while there are significant specific ion effects at the surface at room temperature, the ions may not have a significant effect on the surface freezing process.

A-11

Computational Studies of Aldol Condensation over MgO Catalyst Surfaces

Mingxia Zhou, Larry A. Curtiss, and Rajeev S. Assary

Material Science Division, Argonne National Laboratory, Argonne, IL 60439

Biomass conversion in biomass utilization requires efficient and economical catalysts. The search of optimal

catalyst requires timely and costly catalyst design, synthesis, and test steps. Therefore, it needs the theoretical study to understand quantitative influence of catalyst-surface structures and their molecular level interaction with solvent and biomass derivatives such as ketones to optimize new catalysts for the production of energy-dense and longer chain distillates. The density functional theory calculations were performed to compute the thermodynamic and kinetic feasibility of 2-pentanone and 3-pentanone aldol condensation over MgO (100) surface. Based on the computed thermodynamics (reaction energies) and kinetics (energy barriers), the energetic spans are about 1.3 eV for both 2-pentanone and 3-pentanone aldol condensation on MgO(100) surface, while dehydration step is the rate-limiting step. In addition, a catalyst model Mg(OH)2 was built for Gaussian calculations to study the role of water. The computed results show that the presence of water can reduce the energy barrier of the rate-limiting step by about 0.28 eV and 0.17 eV for 2-pentanone and 3-pentanone aldol condensation, respectively.

A-12

High-Temperature Stable TiAlN Weak Absorber for SolarThermoPhotoVoltaics

Nari Jeon[1], Dave Mandia[1], Stephen Gray[2], Jonathan Foley[3], and Alex B. F. Martinson[1]

[1]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439
[2]Nanoscience and Technology Division, Argonne National Laboratory, Argonne, IL 60439
[3]Department of Chemistry, William Paterson University, Wayne, NJ 07470

Affordable solar cell technology is presently limited to less than 35% efficiency due to the wide breadth of energies that are incident upon the earth's surface: 5 to 0.5 eV, which includes ultraviolet, visible, and infrared. One alternative approach to greater solar conversion efficiency without this fundamental limit utilizes a near perfect absorber coupled to a selective emitter with much narrower bandwidth: 1.2 to 0.5 eV, only a small slice of the infrared spectrum. Selective emitter technology is currently limited by loss of
spectral selectivity of thermal emission due to material and nanostructure degradation at high temperatures. We demonstrate improved thermal stability for simple yet selective planar emitters that maintain excellent selectivity at 1200 °C for up to 6 hours. We propose novel structures with record selectivity via computational optimization that leverage critical coupling between a weak absorber and Bragg reflector (BR). One such structure, fabricated by plasma-enhanced atomic layer deposition (PEALD) of TixAl1-xN and refractory oxides, is evaluated with respect to long-term thermal stability, oxidation, interfacial diffusion and crystallization.

A-13

Structural Dynamics at Bismuth-Ionic Liquid Interfaces during Electrochemical Reduction of CO_2

Jonnathan Medina-Ramos

CSE Division, Argonne National Laboratory

Bismuth (Bi) electrodes are highly efficient and selective platforms for CO2 reduction to CO, when used in acetonitrile solutions containing an imidazolium ionic liquid (IL) such as 1-butyl3- ethylimidazolium triflate ([BMIM]OTf). The reduction of CO2 to CO involves the transfer of two electrons (2e−) and two protons (2H+) to the CO2 molecule. Electrochemical and theoretical results prove that imidazolium cations such as [BMIM]+ serve as both proton donors and cocatalytst during CO2 reduction at the Bi−IL solution interface. This poster presents the results of in situ X-ray reflectivity measurements carried out at the APS, which demonstrate that Bi electrodes also undergo significant structural changes in solutions containing [BMIM]+, under potentials that coincide with the onset of CO2 reduction. Using well-ordered Bi (001) thin films (~ 6nm-thick) in solutions containing [BMIM]+, we observed that native bismuth oxide (Bi2O3) gets reduced into metallic Bi0 as the potential is scanned negatively from open circuit (~−0.3 V vs. Ag/AgCl). Furthermore, at potentials preceding the onset of CO2 conversion (i.e. near −1.5 V vs. Ag/AgCl) the Bi (001) film's reflectivity unexpectedly begins to drop, with a ~60% decrease achieved near −1.9 V, a potential at which CO2 is reduced to CO. This decrease in Bi (001) reflectivity is triggered by changes in both coverage and film thickness, and it is driven by strong

interactions between the negatively charge Bi surface and adsorbed [BMIM]+ cations. Remarkably, an almost complete recovery of the Bi (001) reflectivity takes place during a subsequent anodic scan. Herein, we discuss the implications that the structural evolution of Bi electrodes have on the mechanism of CO2 reduction at the Bi-IL interface, and the outcome of ReaxFF and DFT calculations intended to model this phenomenon.

A-14

Atomically Thin Layers of Graphene-Mos2 Solid Lubricants to Minimize Friction in Steel-DLC Contacts

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Recent demonstration of two dimensional (2D) materials ability to minimize friction to unmeasurable levels (superlubricity) and reduce wear at macroscale loads and speeds propelled research further in the direction of translating the nanomaterials ability to industrially relevant material combinations such as steel and diamond-like-carbon (DLC) material pair. In this study, we have used 2D materials i.e. graphene, MoS2 and a combination as a solid lubricant to minimize friction and wear in steel contacts coupled with Hydrogenated DLC. Unidirectional sliding friction tests conducted at different loads and speeds under dry nitrogen conditions shows a reduction in friction (16x) and wear (29x). Investigation of the surface morphology of the material pairs and the wear debris in TEM indicates that the amorphous carbon mixed with graphene layers resulted in low friction and wear.

A-15

Reducing Cost of Lithium-Ion Batteries Through Techno-Economic Analysis and Supply Chain Optimization

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The drive towards large-scale commercialization of electric or hybrid electric automobiles is challenged by high battery prices. In this work, cost contributing components – ranging from manufacturing to the supply chain operations are studied to explore avenues that enable reduction of overall battery cost. A major focus is on developing process and economic models to identify production and supply chain routes that reduce costs of materials, manufacturing, and overall battery pack. On one hand, detailed techno-economic models are developed to estimate the cost and energy required to produce battery materials, e.g. cathodes (NCM, LMO) [1] and electrolytes (LiPF6) [2]. On the other hand, process models are developed to increase the speed and reduce cost for solvent removal [3] and recovery during electrode manufacturing. Detailed analysis is performed to identify factors for reducing the cost of operations and improving the quality of product. In this poster, a collage of results will be presented highlighting the key learnings and outcomes from the aforementioned studies. The results will show the impact of various process and economic parameters on the overall battery cost. The poster will conclude with a discussion on the lessons learned, and the future outlook.

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[2] Susarla, N., Ahmed, S., Estimating cost and energy demand in producing lithium hexafluorophosphate for Li-ion battery electrolyte. To be submitted to Journal of Power Sources.
[3] Susarla, N., Ahmed, S., Dees, D.W., Modeling and analysis of solvent removal during Li-ion battery electrode drying. Journal of Power Sources, 2018. 378: p. 660-670.

A-16

Closed Loop Modeling of the APS-Upgrade Orbit Feedback Control System

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Orbit stabilization to 10% of the expected small beam sizes for APS Upgrade (APS-U) requires pushing the state of the art in fast orbit feedback control, both in the spatial domain and in dynamical performance. We are building a Matlab/Simulink fast orbit feedback system model to guide decisions about APS-U fast orbit feedback system implementation and to provide a test bench for optimal-control methodologies and orbit correction algorithms applicable to the APS-U. A transfer function model was built from open-loop frequency-response and step-response measurements of the present APS and subsequently validated against closed-loop measurements. A corresponding model for APS-U fast orbit feedback was generated by substituting measured responses of APS-U prototype corrector magnets and power supplies into this same model. Simulated closed loop attenuation responses for different latencies are compared against measurements. Stabilizing PID gains are designed using model and predicted dynamic performance is validated.

A-17

Search for New Physics Beyond the Standard Model

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The discovery of the Higgs boson at the Large Hadron Collider (LHC) at Geneva, Switzerland completes the Standard Model (SM) describing particle interactions. The years ahead will be an exciting time for the particle physics community to search for new physics beyond the SM (BSM). However, as the LHC delivers more and more data, we will either see the emergence of BSM physics at a much higher energy scale, or we will be forced to scrutinize deeper into massive experimental data to understand whether the SM breaks down at LHC-accessible energies. This will impose significant challenges on experiments, which need employ better detector technologies with higher radiation tolerance and better resolution and timing, and develop advanced analysis techniques, such as deep machine learning, for data processing. This presentation will discuss some ongoing R&D activities, aiming to enhance the performance of the ATLAS experiment with a series of upgrade activities planned.

A-18

On-Track Measurements of Road Load Changes in Two Close-Following Vehicles: Methods and Results

Michael Duoba, and Alejandro Fernandez Canosa

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As emerging automated vehicle technology is making advances in safety and reliability, engineers are also exploring improvements in energy efficiency with this new paradigm. Powertrain efficiency receives due attention but also impactful is finding ways to reduce driving losses in coordinated driving. Efforts focused on simulation to quantify road load improvements require a sufficient amount of background validation work to support them. This study uses a practical approach to directly quantifying road load changes by testing the coordinated driving of two vehicles on a test track at various speeds and vehicle time gaps. Axle torque sensors were used to directly measure the load required to maintain steady-state speeds while following a lead vehicle at various gap distances.

Test methods to obtain relatively robust results, considering the challenges of track testing in real-life conditions (wind, weather, temperature changes, etc), were explored. We found that total road load was reduced by 10-12% at an optimum gap time of 0.25 to 0.4 seconds. Challenges that were encountered included less repeatability of load measurements at short gap distances and powertrain mode switching (from a hybrid vehicle). This study will provide the framework for further investigations in coordinated driving road load with track testing methods.

A-19

Joint ptycho-tomography reconstruction through alternating direction method of multipliers

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Argonne National Laboratory

We present the extension of ptychography for three-dimensional object reconstruction in a tomography setting. We describe the alternating direction method of multipliers (ADMM) as a generic inversion framework to efficiently solve the nonlinear optimization problem. In this framework, the ADMM breaks the joint approach into two well-defined subproblems: ptychographic phase retrieval and tomographic reconstruction. Hence, it allows us to use existing state-of-the-art algorithms for each subproblem. Further, we show that the proposed joint approach is more robust to noise than conventional methods, voids the existing requirements on probe overlap, and thus can allow faster scanning of large volumes.

A-20

Uncertainty Quantification in the Calculation of Phase Diagrams for Materials Design

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The calculation of phase diagrams (CALPHAD) approach provides critical information for the design of new materials [1], including the volume fractions, compositions and energies of the stable phases at macroscopic composition, temperature, and pressure (X-T-P). With the widespread adoption of the CALPHAD method, the materials design community quickly realized that the accuracy of CALPHAD predictions vary widely in X-T-P space due to experimental error, model inadequacy and unequal data coverage. In response to this need, researchers have developed frameworks to quantify the uncertainty of the parameters in thermodynamic property models and propagate it to the predicted phase diagram [2, 3]. In all previous studies, this representation was limited to uncertainty intervals on the phase boundaries of binary systems. In this work, we propose a suite of tools that leverages samples from the multivariate distribution of model parameters to represent uncertainty in forms well suited to materials design tasks. These include representations of the distribution of phase diagram morphologies, the distribution of invariant points and the dependence of phase stability and the distributions of phase volume fraction, composition activity and Gibbs energy on X-T-P location - irrespective of the total number of components.

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B-1

Ultrafast Electron Microscopy User Facility at Argonne National Laboratory

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Transmission electron microscopy (TEM) is capable of sub-nanometer resolution and is one of the most important tools in materials science. Traditional TEM has been limited to studying static or slowly evolving systems. Ultrafast electron microscopy (UEM) utilizes a pump-probe laser system in addition to a standard TEM, generating photoelectrons at the cathode and optically exciting material dynamics at the specimen. Real-space imaging of transient material behavior with femtosecond time-resolution and nanometer spatial-resolution is possible with UEM and opens the door to studying physical phenomena not previously accessible. The new UEM user facility at Argonne National Laboratory will have the first operational UEM with both direct-electron camera and energy-filtering capabilities in the US. A tunable wavelength ultrafast laser and an adjustable laser repetition rate allow for a large experimental parameter space. Structural, chemical, and electronic information can simultaneously be studied. Current research directions include quantum materials, plasmon-phonon coupling, and phonon-defect Interactions.

[1] Zewail, A. H. Four-Dimensional Electron Microscopy. Science 2010, 328, 187-193.

B-2

High Resolution, Large Field-of-view Imaging with Electron and X-ray Ptychography

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Ptychography is an emerging technique for imaging materials at the nanoscale. Unlike traditional microscopes whose resolution are often limited by optical lens, ptychography use computer algorithms to reconstruct object's structure from scanning diffraction patterns. Using a scanning transmission electron microscope and a state-of-the-art pixel array detector, we recently demonstrated a record-breaking 0.39 angstrom resolution on a twisted bilayer of two-dimensional molybdenum sulfide [1]. This technique allows us to image the bonding of every individual atom with unprecedented precision, while using a minimal flux of damaging electrons. At Advanced Photon Source, we have developed several X-ray ptychography instruments to study a variety of materials such as biological tissue, energy materials, and electronic chip. With fast data acquisition, we are capable of imaging computer chips with over 1-millimeter field-of-view at 10 nm resolution. Ptychography can also be combined with tomography to recover the 3D structure of large objects.

[1] Y. Jiang et al. Nature 559 343–349 (2018).

B-3

Precision Magnetic Field Calibration for the Muon g-2 Experiment at Fermilab

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The Muon g-2 Experiment at Fermilab (E989) has been designed to determine the muon anomalous magnetic moment to a precision of 140 parts per billion (ppb), a four-fold improvement over the Brookhaven E821 measurement. Key to this precision goal is the determination of the magnetic field of the experiment's muon

storage ring to better than 100 ppb.

The magnetic field is measured and monitored by nuclear magnetic resonance (NMR) probes, which are mounted on a trolley and pulled through the muon storage region when muons are not being stored. These trolley probes are calibrated in terms of the free-proton Larmor precession frequency ω p by a specially-constructed NMR calibration probe. In E821, the uncertainty in the field measurement was 170 ppb, of which 50 ppb was due to the calibration probe. In E989, these uncertainties will be reduced to 70 ppb and 35 ppb, respectively. To meet these stringent requirements, a new specially-designed probe called the "plunging probe" has been built which will be used to calibrate the trolley probes. This poster will present the design, fabrication, and testing of the plunging probe, along with the calibration procedure that is executed during the experiment.

B-4

Dynamics of Emergent Vortices in Swarms of Magnetic Rollers

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Ensembles of strongly interacting particles driven out-of-equilibrium by an external periodic forcing often develop nontrivial collective dynamics. Active magnetic granular materials proved to be an excellent model experimental systems to explore emergent behavior and out-of-equilibrium self-assembly phenomena.

Ensembles of magnetic micro-particles (diameter ~150 μm), immersed in water and sediment on the bottom surface of the container turn into rollers when energized by a single-axis homogeneous alternating magnetic field applied perpendicular to the surface supporting the particles. The rolling motion emerges as a result of spontaneous symmetry breaking of the particle rotations in external field in a certain range of excitation parameters. Experiments reveal a rich collective dynamics of magnetic rollers: flocking, spontaneous formation of steady vortices and rich roller vortex dynamics have been observed. Emergent roller vortices can spontaneously switch their chiral state (direction of rotation) and do not require a confinement to form and exist. We reveal the capability of certain non-active particles to pin the vortex and manipulate its dynamics. Building on our findings, we demonstrate the potential of magnetic roller vortices to effectively capture and transport inert particles at the microscale. Our work suggests new approaches and techniques for manipulation of active granular materials.

The research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

B-5

Application-aware Node Resource Management for Energy Efficiency

Sridutt Bhalachandra, Kamil Iskra, Swann Perarnau and Pete Beckman

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Power is increasingly the limiting factor in High Performance Computing (HPC) at Exascale and will continue to influence future advancements in supercomputing to mitigate large operating costs and carbon footprints. The Argo project is a DOE initiative for designing a modular operating system/runtime for the next generation of supercomputers while leveraging their hierarchical nature with a key focus on power management. At a system level, a Global Resource Manager (GRM) monitors power across the entire machine and distribute power budgets across the jobs. Inside each job, this power budget is then distributed to nodes, according to application characteristics and node availability. Finally, on each node, a Node Resource Manager (NRM) is in charge of enforcing the power budget while trying to maximize performance or improve energy efficiency through several resource management policies. Increasing variability in current HPC systems along with the growing complexity

in supercomputing applications necessitate sophisticated power control schemes that are application aware. We present a bulk synchronous parallel (BSP) application-aware power policy with de-coupled monitoring and control that identifies critical path across application phases to dynamically adapt power. Our preliminary single node results show up to 15% energy reduction across a variety of HPC applications.

B-6

Directed Crystal Nucleation and Growth of Blue Phase by Chemically Patterned Surfaces

Xiao Li

University of Chicago

Topological defects in blue-phases liquid crystals (LCs) can be self-assembled into three dimensional cubic crystalline structures, representing unique ordered states of matter among the other LCs. However, polycrystalline, platelet and multi-domain topological defects of blue-phase LCs are difficult to overcame with current methods. And past studies of polycrystalline BPs were challenged by grain boundaries between randomly oriented crystalline nanodomains. This presentation will describe a chemically patterned surface that allows blue-phase LCs to be directed self-assembled upon the alternative planar/homeotropic (P/H) stripe pattern surface and into the uniform monodomain structure. The resulting blue-phases are single crystal, are oriented and guided with the underlying substrate and can be created over arbitrarily large areas. Meanwhile, the processes that mediate crystal nucleation and growth and the transformation between crystal structures having different lattice symmetries are of fundamental importance to a wide range of scientific disciplines. By using the single crystals of liquid crystal blue-phases with a controlled orientation, we study the liquid analog of a crystal-crystal transformation. In contrast to traditional atomic crystals, the transitions that arise in blue phases take place over sub-micron length scales. They do, however, occur in a diffusion-less manner, with characteristics that are eminiscent of traditional martensitic transformations in atomic crystals. Our results provide a potential avenue to fully exploit the electro-optical properties of blue phases, which have been hindered by the existence of grain boundaries.

B-7

Utilizing Static Auto-ignition Measurements to Estimate Intake Air Condition Requirements for Compression Ignition in a Multi-Mode Engine – Application of Chemical Kinetic Modeling

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A multi-mode operation strategy, wherein an engine operates compression ignited at low load and spark ignited at high load, is an attractive way of achieving better part-load efficiency in a light duty spark ignition (SI) engine. Given the sensitivity of compression ignition operation to incylinder conditions, one of the critical requirements is accurate control of intake charge conditions – pressure (P), temperature (T) and equivalence ratio (φ), for achieving stable combustion and enable rapid mode-switches. This poster presents correlating ignition delay data under various engine-relevant operating conditions (P,T,φ) to combustion phasing and stability data obtained from a modern SI engine operated in compression ignition mode. Chemical kinetic models are utilized to estimate the ignition behavior towards enabling reduced-order approaches for engine combustion control. The calculated auto-ignition behavior for multi-component surrogates of five co-optima research gasoline blends provides insight into the impact of chemical composition covering ACI relevant operating conditions. Both static and variable volume simulations explain the existent role of engine dynamics on controlling combustion phasing. Finally, the trends are compared against those of experimental measurements from a RCM and further discussions regarding fidelity requirements for use of chemical kinetic mechanisms as a tool for predicting engine combustion phasing are made.

B-8

A scalable Gibbs energy minimization model for solvent extraction systems

Chukwunwike Iloeje

Argonne national Laboratory

The emergence of clean energy technologies in which rare earth elements provide critical functionality has increased the demand for these materials, with important implications for supply security. Recycling rare earths provides an option for diversifying their supply sources. While solvent extraction is a proven technology for rare earth separations, its application often requires extensive trial-and-error experimentation. We introduce an alternative screening approach, based on Gibbs energy minimization for predicting extraction equilibria in hydrometallurgical systems, and illustrate its applicability to the design and optimization of rare earth separations, with explicit consideration for mixtures sourced from Nickel Metal Hydride (NiMH) batteries.

B-9

Large-Scale Optimization Algorithm for Linear Equality Constrained Minimization

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This exposition describes two large-scale trust-region optimization methods for linear equality constrained general non-linear, non-convex objective functions. The proposed methods exploit shifted low-rank representations of Hessian matrix approximations. The structure of these matrices is used to develop algorithms that compute feasible iterates which simultaneously minimize quadratic approximations of the original non-linear objective functions. The main advantages of the proposed methods are fast computational times, and applicability to large problems.

B-10

Atomic Layer Deposition Of Co/Pt Multilayer Films For Perpendicular Magnetic Anisotropy

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Smaller, Faster and Efficient" are the key words describing the ever increasing need of data-storage industry.[1] This demand has brought about a shift from longitudinal recording in magnetic media to perpendicular recording, where magnetic bits are perpendicular to the plane of the recording media instead of being in the same plane. Significantly higher storage density is obtained with perpendicular magnetic recordings utilising materials demonstrating perpendicular magnetic anisotropy (PMA). Strong PMA is usually observed in ultrathin films of ferromagnetic metals like Co and Fe forming alloys with heavy metals like Pt, Pd, Au and Ta.[2] Of them Co/Pt alloys and multilayer structures are probably the most widely investigated system for understanding the PMA origin and behaviour.
In this work, we utilise atomic layer deposition (ALD) of Co/Pt multilayers. Bis(N-t-butyl-N'-ethylpropanimidamidato)cobalt(II) and hydrogen precursors are used for Co ALD while Trimethyl(methylcyclopentadienyl)platinum(IV) and water are used as precursors for Pt deposition. Pt/[(Co/Pt)/Pt stacks are grown using alternate cycles of Co and Pt. QCM, HRTEM and XPS analysis of the multilayer stacks are utilised to study the interfaces of the multilayer films. SQUID measurements show a change in anisotropy between pure Co and Co/Pt multilayer films.

References:
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B-11

Reliability Benchmarking of Wide Bandgap Power Devices

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The demand for high-power electronics in Military high-density power applications, satellite communications, high-frequency radar operation, aerospace, electric vehicles, and all electric warships, has increased dramatically in recent years, which placed an extraordinary pressure on wide bandgap (WBG) power devices [1]. The smaller footprint, lower weight, higher-temperature operation, lower power losses, higher operating frequency compared Si-based devices have made WBG power devices excellent candidate for AC-DC converters and inverters used for those applications [2]. But lack of reliability information for SiC and GaN power devices, prevents the widespread use of WBG power devices.

SiC and GaN power MOSFETs are the key components for the high-power electronics and power modules. We have tested 1200 V SiC power MOSFETs and 600 V GaN power MOSFETs. In this study we have developed, demonstrated protocols to test reliability of WBG power MOSFETs against thermal aging and bias temperature instability. Static characteristics of power MOSFETs were used as the dictating factor to understand degradation of power MOSFETs due to the variation of various environmental stressors. We have developed protocols for material defect analysis in order to understand root cause of device failure. For GaN power MOSFETs, we have performed in-situ and ex-situ neutron radiation reliability testing. At last, we have performed statistical analysis for numerous power devices which were fabricated by different manufacturers.

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B-12

Room Temperature Production of Lithium Metal Thin Film via Electrodeposition

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Lithium (Li) metal is highly attractive material for use in primary and rechargeable batteries due to its high theoretical specific capacity (3860 mAh/g), low density (0.534 g/cm3) and the lowest negative electrochemical potential (3.040 V vs. standard hydrogen electrode). Current production methods for lithium metal involve high temperature electrolysis (ca. 500 ˚C) of a eutectic mixture of lithium chloride (LiCl) and potassium chloride (KCl), and following refining. Here, we present a cost-effective room-temperature electrodeposition process, including the optimization of process parameters and conditions to produce a thin layer of lithium metal onto copper substrate, from an aqueous lithium source through a lithium-ion conducting separator. Through control of process parameters, the process can yield uniform, densely packed dendrite-free lithium metal nanorods with aspect ratios up to 100 (diameter ca. 350 nm and length ca. 35 μm). Room-temperature methods for producing high quality lithium metal eliminate energy-consuming reaction and reduce the steps in the current manufacturing process, thus drastically reducing the manufacturing cost of the final product. Our lithium metal deposition process provides precise control over lithium morphology during deposition and growth, which is expected to improve battery performance as a result of uniform lithium metal stripping during battery discharge.

B-13

Development of a Tribocorrosion-Bioreactor to Study Cell Response to Degradation Products – Initial Pilot Tests

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Metallic orthopedic implants in total joint replacement face the problem of wear and corrosion. The mechanisms behind it with consideration of the biological environment are not fully understood. The aim of this work is to develop a test-rig with cell cultures directly exposed to wear and corrosion products from joint replacement materials. The challenge of the initial pilot studies is to generate enough degradation products to trigger cell response.

The test rig, operating inside a CO2 incubator, has a lever-arm to load the metallic samples and a three-electrode configuration for potential control. The tribological set-up is based on a ball-on-flat configuration (alumina-on-CoCrMo) with reciprocating sliding motion. The lubricant is cell culture medium.

Tribocorrosion tests according to a 2-level 3-factor design of experiments with center point generated a calibration response surface, which allowed to define the influence of motion amplitude, applied load and electrochemical potential on the amount of metal released from the CoCrMo-discs. The average total mass was 0.115-1.64 mg. According to literature, the corresponding obtained concentration range of released metal is able to cause a decrease in cell viability.

The developed test apparatus permits studies on the effect of freshly released metal wear and corrosion products on cells. The chemical composition and reactivity of freshly released metal wear may differ greatly from stable wear products typically used in cell culture studies.

B-14

Automating the Algorithm Selection in MPI Collectives

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The MPICH/MPI library supports different collective algorithm implementations and selects the most appropriate among them using a static threshold based the number of transferred bytes. Nevertheless, this simplistic selection strategy may not work efficiently on all the systems, leading to suboptimal performance. Collective operations being widely used across a large number of applications, there is a need to address performance inefficiencies caused by the static selection logic. In this work we focus on analyzing different collective algorithms in MPI_Allgather and observe what parameters (e.g., transferred bytes, number of nodes and number of processes per node) affect the overall performance. We find that an algorithm selection logic that only uses the number of transferred bytes is not sufficient and other parameters, such as number of nodes and processes per node, should also be considered. This observation is dynamically captured into a closed form expression while collecting and using the topological information. This yields to a tailored selection of the most suitable algorithm for a given configuration, ultimately resulting in optimal performance. We plan to extend this analysis to other collectives in MPICH/MPI and expand the automation of the selection logic to extract architecture dependent parameters for better customized MPICH/MPI collective algorithm selection tuning.

B-15

Scale up of advanced fuel cell catalysts

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In the last few decades, a variety of advanced fuel cell electrocatalysts with controlled size, shape, composition, morphology, and improved catalytic activities in half-cell testing condition have been developed using wet chemistry synthesis methods. However, their performance in real world device have been rarely tested because of the difficulty to produce larger quantity of uniform, high quality nanocatalysts. In this poster, I will show our recent efforts in scaling up advanced fuel cell catalysts. A multi-layer Pt-skin PtNi nanoparticle electrocatalyst has been successfully scaled up from tens of milligrams to several grams per batch with improved activities over commercial Pt/C catalyst in both half-cell and device conditions. Our recent effort to remove restraints associated with batch processes lead us to develop a continuous flow synthesis platform. Our approach to accelerate the transition of nanomaterials to manufacturing will be discussed.

B-16

The Water-Energy Nexus: Electrodeionization for Energy Efficient Water Supply

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Water and energy are two vital resources that are intrinsically linked since water supply is energy intensive, and energy production requires water. In fact, thermoelectric power plants account for ~40 percent of total water withdrawals in the United States. As the amount of available freshwater declines, competition for water resources increases, and this has driven the thermoelectric power sector to consider alternative sources. These non-traditional source waters pose new and unique challenges regarding water quality because they contain complex mixtures and undesirably high concentrations of specific constituents. Thus, the development of energy efficient water purification technologies is an emerging challenge that must be addressed to ensure sustainable and resilient water and energy supplies.

Cooling water systems are particularly sensitive to certain mineral salts including silica due to its scaling potential, and this will limit the number of water reuse cycles in cooling tower operations. Typical methods for silica control are chemical intensive and/or are highly dependent on influent water quality. As an alternative, electrodeionization (EDI) is an energy efficient method that utilizes ion exchange phenomena and an applied electric field to drive ionic separation. This work focuses on the adaptation and implementation of EDI technology to enable the use of non-traditional water sources for cooling water applications.

B-17

Local hybrid density functional theory for heterogeneous systems

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Correctly capturing electron-electron interactions in a theory is the key for describing the optoelectronic properties of heterogenous materials. We propose a local hybrid functional within the density functional theory framework. This functional is derived by considering the screening of Coulomb interactions in a dielectric background. We also propose a finite field approach to compute the dielectric property of materials in a self-consistent way using the local hybrid density functional theory. We have implemented the whole theory in Qbox code and validated it

on various types of systems, including bulk materials (both 2D and 3D), interfaces (Si/α-Si3N4, Si/H2O), and surface (H-Si). It produces dielectric constant and band structure for these systems in agreement with experiment.

B-18

Evaluating the Impact of High-Bandwidth Memory on MPI Communications

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Modern HPC clusters include accelerators such as GPGPUs and many integrated core processors. These components are often equipped with high-bandwidth on-package memory (HBM) offering higher aggregated bandwidth than standard DRAM has but substantially less capacity. Although many studies have shown how to exploit this new memory technology for boosting an application's performance, no study has explored the potential benefits, and the associated capacity constraints, of HBM for MPI communications.

We fill this gap by carrying out a fine-grained evaluation of HBM usage in MPI using Knights Landing MCDRAM. Our contribution is twofold. First, we analyze the most common communication mechanisms offered by MPI, such as PT2PT and RMA, and for each of these we consider the effect that different memory placement strategies of internal MPI library objects has on performance; Second, we introduce capacity constraints and consider the impact that moving different MPI objects to MCDRAM has on the total memory budget. Our analysis shows that although MCDRAM can improve MPI communication performance, this improvement comes at the cost of higher memory usage. Since HBM is a scarce resource we also provide a list of recommendations that can help users decide what MPI objects to place in MCDRAM to achieve the best performance possible.

B-19

Data Acquisition with Cuda for the Muon g-2 Experiment at Fermilab

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A data acquisition system using Nvidia Tesla K40 GPUs is being used to accelerate the rate of data acquisition for a new particle physics experiment at Fermilab. A new measurement of the anomalous magnetic moment of the muon is being performed. The most recent measurement, performed at Brookhaven National Laboratory and completed in 2001, shows a 3.6 standard deviation discrepancy with the standard model value of g-2. The new measurement will accumulate 21 times those statistics, measuring g-2 to 140 ppb and improving the uncertainty by a factor of 4 over that of the previous measurement. The data acquisition system for this experiment must have the ability to create deadtime-free records from 700 μs muon spills at a raw data rate 20 GB per second. Data is processed online in a layered array of networked commodity processors with 28 GPUs working in parallel to perform a fast recording of the muon decays during the spill. The GPU processing code is written in Cuda and achieves a factor of 100 in data reduction by processing each digitized sample in a parallel thread. A Cuda-based Monte Carlo simulation was also used to prototype the system and set design parameters. Data taking for the experiment is underway, and will run for two years.

B-20

Physics of Superconducting Photon Detectors: Overview and Energy Down conversion Model

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Superconducting detectors allow for significant improvements in sensitivity, speed, and frequency range for a wide variety of photon-sensing applications. Among a number of current and planned deployments in many areas of science including astrophysics and high-energy physics, X-ray Transition Edge Sensors (TESs) are now being developed for use in the Argonne Advanced Photon Source (APS) beamline. Even though the microscopic physics is relatively well established, there remain several poorly understood and difficult to model aspects of superconducting device behaviour. One recent area of progress concerns the interaction between photons and superconducting quasiparticles in thin films. Calculating the exact changes in superconductor properties (resistance, inductance, temperature) due to the absorption of light requires a model of how absorbed photon energy is converted into quasiparticles and phonons. This energy downconversion process has an associated "efficiency" which determines the performance of the detector. At low temperatures in thin superconducting films operating as resonators, our numerical model and experimental results show the detector responsivity and noise are therefore dependent on the device geometry, signal frequency, and readout power, in addition to the temperature [1,2]. This is particularly relevant for Kinetic Inductance Detectors (KIDs), and microwave resonators used for superconducting qubit readout.

[1] T. Guruswamy, D. J. Goldie, and S. Withington, "Nonequilibrium superconducting thin films with sub-gap and pair-breaking photon illumination", Superconductor Science and Technology 28, 054002 (2015).
[2] P. J. de Visser, S. J. C. Yates, T. Guruswamy, D. J. Goldie, S. Withington, A. Neto, N. Llombart, A. M. Baryshev, T. M. Klapwijk, and J. J. A. Baselmans, "The non-equilibrium response of a superconductor to pair-breaking radiation measured over a broad frequency band", Applied Physics Letters 106, 252602 (2015).

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2018 Postdoctoral Research and Career Symposium

November 8, 2018

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