Argonne NATIONAL LABORATORY

Annual Postdoctoral Research and Career Symposium

November 2, 2017

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Argonne National Laboratory Postdoctoral Research and Career Symposium

November 2, 2017

Co-sponsored by:

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2017 Postdoctoral Research and Career Symposium
November 2, 2017

Table of Contents

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2017 Postdoctoral Research and Career Symposium

November 2, 2017

Agenda

8:45 AM	Continental Breakfast and Registration (TCS Conference Center)

MORNING SESSION

9:00 AM	Welcome Remarks
9:15 AM	Keynote Address by Dr. Marius Stan, Senior Computational Scientist, ANL
10:15 AM	Poster Session A and Free Networking

NETWORKING LUNCH

11:45 AM	Networking Lunch (company exhibitors and representatives from diverse career paths will have a chance to talk with postdocs in small groups)

AFTERNOON SESSION

1:45 PM	Poster Session B and Free Networking
3:15 PM	Career Panel Discussion
4:15 PM	Presentation of Poster Awards and Closing Remarks
5:00 PM	Adjourn

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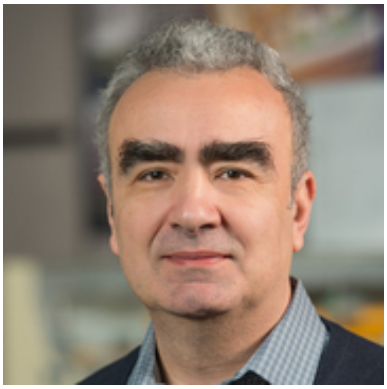
2017 Postdoctoral Research and Career Symposium
November 2, 2017

2017 Keynote Address

How to Get a Job After a Postdoctoral Appointment: Lessons from Soccer

Marius Stan, Argonne National Laboratory

Life as a postdoc is beautiful: exciting research, rewarding collaborations and a friendly work environment. Like most beautiful things, it comes to an end after two or three years. Then securing a permanent position at a national laboratory, in academia or in industry is a complex and often stressful endeavor that requires careful preparation. In addition to improving skills, teaming up, and being productive, it involves understanding leadership and management, securing funding and wisely timing the application moment. The author shares his experience as a former postdoc and current hiring manager and illustrates key concepts using video clips from soccer.



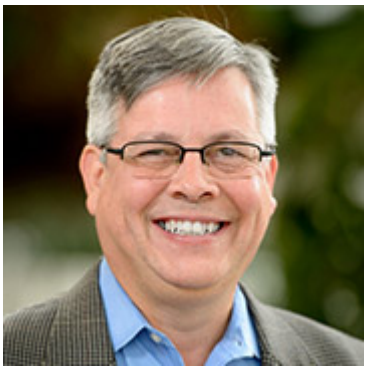
Dr. Marius Stan, Senior Computational Scientist and Leader of the Complex Physical Systems group in the Global Security Sciences division, Argonne National Laboratory.

Dr. Marius Stan is a Senior Computational Scientist and Leader of the Complex Physical Systems group in the Global Security Sciences division. The group uses artificial intelligence, machine learning, and multi-scale computer simulations to understand and predict properties of complex natural systems.

Marius was born in Romania and graduated with a B.S. in Physics from the University of Bucharest. In 1997 he received the Ph. D. in Chemistry from the Institute of Physical Chemistry of the Romanian Academy. The same year he joined Los Alamos National Laboratory in the US as a postdoctoral research associate. Shortly after that he was hired as permanent staff and created and led a research group on computational chemistry and physics of materials. In 2010, Marius joined Argonne National Laboratory as a Senior Computational Energy Scientist. He is also Adjunct Professor and Senior Fellow at the University of Chicago's Computation Institute and at the Northwestern-Argonne Institute for Science and Engineering.

Marius has extensively published in the scientific literature and is writing a book on "Models and Simulations of Materials" for Taylor & Francis. He is an avid soccer player and a published author of short-stories and poetry (in Romanian). You may also recognize him as Bogdan, the car wash owner, in the acclaimed TV series "Breaking Bad."

Welcome Remarks Speaker



Dr. John Quintana, Interim Deputy Laboratory Director for Operations and Chief Operations Officer, Argonne National Laboratory

John P. Quintana is the Interim Deputy Director for Operations and Chief Operations Officer at Argonne National Laboratory. Leveraging extensive experience in engineering, research, and management, Dr. Quintana works with leaders across the laboratory to continuously improve mission support services offered with high quality leadership, effectiveness, and efficiency.

Dr. Quintana's 10-plus years of experience at Argonne include six years as an associate division director in the Advanced Photon Source (APS), where he was responsible for the groups performing mechanical engineering design and mechanical maintenance, as well as radiation and experimental safety. He has served as Argonne's Deputy Chief Operations Officer since August 2011.

Dr. Quintana has published more than 50 peer-reviewed articles and holds a doctorate in materials science and engineering from Northwestern University and a bachelor's degree in mechanical engineering from the University of California at Berkeley.

Closing Remarks Speaker

Dr. Paul Kearns, Interim Director, Argonne National Laboratory

Paul K. Kearns is the interim director of the U.S. Department of Energy's Argonne National Laboratory. He is responsible for guiding development and implementation of the laboratory's strategic vision and leading Argonne to deliver outstanding performance in science and technology, operations, employee health and safety, and environmental protection. Dr. Kearns promotes a culture of innovation and collaboration within the laboratory and helps Argonne maintain strong strategic partnerships.

Dr. Kearns has nearly three decades of management experience, a strong background in science and engineering and extensive experience with the U.S. Department of Energy. He served six years as Chief Operations Officer for Argonne.

Dr. Kearns is a fellow of the American Association for the Advancement of Science, member of the American Nuclear Society and the Society for Conservation Biology, and served as a visiting professor in engineering and physical sciences at the University of Manchester in the United Kingdom. He holds a doctorate and a master's degree in bionucleonics and bachelor's degree in natural resources and environmental sciences, all from Purdue University.

Academic Careers Panelists

Prof. Eric Landahl, Associate Professor and Director of Physics Graduate Studies, DePaul University

Eric Landahl received his BA from the University of Chicago in 1994 in Physics, and his MS from DePaul University in 1996. He was an undergraduate co-op student at Argonne in the Accelerator Systems Division. He obtained his PhD from the University of California, Davis in Applied Science in 2001. His PhD thesis work was in the area of nonlinear electrodynamics.

From 2001 - 2003 he worked as an Assistant Research Engineer for the University of California, Davis, while located at the Stanford Linear Accelerator. He joined Argonne's Advanced Photon Source as a beamline scientist in 2003 and left in 2008 to join the Physics faculty at DePaul University where he is now Associate Professor and Director of Physics Graduate Studies. His current research interests are in time-resolved x-ray science.

Prof. Casey Larsen, Assistant Professor of Chemistry, Benedictine University

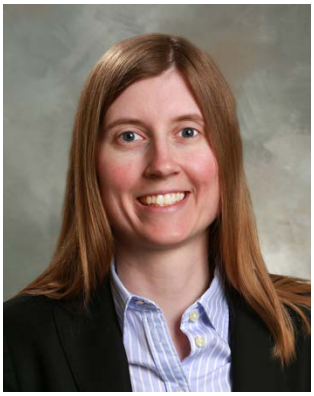
Casey Larsen is an Assistant Professor of Chemistry at Benedictine University in Lisle, Illinois. Her research interests are in synthetic organic and organometallic chemistry, and transition metal mediated catalysis, specifically in the development of homogeneous catalysts to allow for unique and selective transformations of organic molecules. She received a B.S. in Biology, with a minor in Chemistry, and an M.A. in Chemistry from San Diego State University. She received her Ph.D. in Chemistry from the University of California, San Diego in 2012.

Dr. Larsen was a Postdoctoral Appointee at Argonne National Laboratory in the Chemical Sciences & Engineering Homogeneous Catalysis Group from September 2013 to December 2014. Moving from sunny San Diego to chilly Chicago allowed Dr. Larsen to experience what winter really is, with sled and all. In her free time, Casey enjoys cooking and experimenting with food…. which is really just doing chemistry in the kitchen!

Prof. Sunshine C. Silver, Assistant Professor of Chemistry, North Park University, Chicago

Sunshine Silver is an Assistant Professor of Chemistry at North Park University in Chicago where she teaches a variety of undergraduate chemistry courses and is the adviser of the Chemistry Club. She is a bioinorganic chemist by training and received her Ph.D. in Biochemistry from Montana State University in the lab of Joan Broderick investigating Radical SAM enzymes. Sunshine spent about two and a half years as a Postdoctoral Appointee at Argonne National lab working with Lisa Utschig in the Solar Energy Conversion Group in the CSE division. Sunshine taught at Concordia University Chicago for two years and then joined the faculty at NPU in the fall of 2015. She is currently enjoying performing research with students on select metalloenzymes.

Non-Academic Careers Panelists



Dr. Erin Broderick, Senior R&D Engineer, Honeywell UOP
After completing her undergraduate degree and the University of Illinois at Urbana, Champaign, Erin performed her graduate work in inorganic chemistry at the University of California, Los Angeles where she worked with Dr. Paula Diaconescu on the synthesis and application of organometallic complexes. After graduate school, she obtained a post-doc at Argonne in the homogeneous catalysis group. Since 2012, Erin has worked in the exploratory research group at Honeywell UOP.

Dr. Steven Kraft, Senior Research Scientist, Cabot Microelectronics Corporation

Steven received his Ph. D. in Inorganic Chemistry from Purdue University in 2012 as a Robert R. Squires Fellow synthesizing and studying uranium organometallic compounds, and his B.S. in Chemistry from St. Norbert College in 2008. In early 2014, Steven 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 research scientist at Cabot Microelectronics Corporation developing products to polish materials for the semiconductor industry.

Dr. Carolyn L. Phillips, Data Scientist, Capitol One
Dr. Carolyn L. Phillips is a Data Scientist at Capital One, part of a technology team building a next generation customer matching platform that is designed to operate for millions of customers. Previously she was a Lead Data Scientist at a startup using machine learning to detect fraudulent and manipulative behaviors in the financial markets, a staff scientist at Argonne National Laboratory in the Mathematics and Computer Science Division, and a Fellow of the Computation Institute at the University of Chicago.

Dr. Phillips' research has focused on designing algorithmic solutions to find patterns in complex systems. Her research has covered topics from liquid crystals to superconductors, from nanoparticle clusters to quasicrystals, and from machine learning to study self-assembling crystals to algorithms for solving the mathematical filling problem.

She received a BS in Mathematics from MIT, a MS in Mechanical Engineering from MIT, and a MSME in Mechanical Engineering from the Naval Postgraduate Program. She received a PhD from the University of Michigan in Applied Physics and Scientific Computing as a Department of Energy Computational Science Graduate Fellowship. She then joined Argonne National Laboratory as the Aneesur Rahman Postdoctoral Fellow with a joint appointment in the Computational Institute at the University of Chicago.

Dr. Elina Vitol, Staff Scientist, 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 multibillion Fortune 500 corporation. Dr. Vitol is currently a Staff Scientist at Nalco – an Ecolab company. She is the technical lead for open innovation and technology transfer in the area of microbial control and monitoring for the global Ecolab/Nalco organization. She also serves as subject matter expert in optics-based analytical and diagnostic instrumentation, materials science and nanotechnology. Dr. Vitol is the recipient of the "Rising Star" award by Sensors magazine and Sensors Expo & Conference 2015. Sensors Expo and Conference is the leading industry event in North America exclusively focused on sensors and has emerged as one of the largest and most important gatherings of engineers and scientist involved in the development and deployment of sensor systems. "Rising Star" award recognizes an emerging engineer/sensor development leader under the age of 34 who is active within the sensors industry and whose efforts have already contributed to advancing sensor technology or sensor applications in commerce.

Prior to joining Ecolab in July 2013, Dr. 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, Dr. 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. Dr. 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.

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2017 Postdoctoral Research and Career Symposium
November 2, 2017

Poster Abstracts

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Posters Abstracts

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A-1
Polynomial Filtering for Large, Sparse SVD Computations

Jared L. Aurentz[1], Anthony P. Austin[2], and Vasileios Kalantzis[3]

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[2] Mathematics and Computer Science Division, Argonne National Laboratory, Lemont, IL, 60439
[3] University of Minnesota, Computer Science and Engineering Dept., Minneapolis, MN, 55414

Polynomial filtering is a well-established technique for computing a few eigenvalues of a large, sparse matrix, especially when those eigenvalues lie in the interior of the spectrum. We extend these techniques to handle singular value computations. We show that polynomial filters can be useful not only for interior singular value problems but also for extremal problems, especially when a large number of singular values are sought.

A-2
Field Scale Simulation of Axial Hydrokinetic Turbines in a Natural Marine Environment

Saurabh Chawdhary[1], Diyonsis Angelidis[2], Lian Shen[3], Fotis Sotiropoulos[2]

[1] Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439
[2] Department of Civil Engineering, Stonybrook University, Stonybrook, NY 11794
[3] Department of Mechanical Engineering, University of Minnesota, MN 55455

Marine and hydrokinetic (MHK) energy is a promising source or renewable energy. It has seen major development in the recent years with the first grid connected MHK plant already granted federal license in New York City's East River. However, existing technologies need fundamental research to enable efficient energy extraction from identified MHK sites. In this work, we employ a novel large eddy simulation (LES)-based framework to investigate the site-specific flow dynamics past MHK arrays in a real-life marine environment. The new generation unstructured Cartesian flow solver, coupled with a sharp interface immersed boundary method for 3D incompressible flows, is used to numerically investigate New York City's East River, where an array of MHK turbines is to be deployed as part of the Roosevelt Island Tidal Energy (RITE) Project. Multi-resolution simulations on locally refined grids are used to simulate the flow in a section of East River with detailed river bathymetry and inset turbines at field scale. The results are analyzed in terms of the wake recovery, overall wake dynamics, and the power produced by the turbines. These results will help develop design guidelines for the site-specific turbine array configuration.

A-3
Magnetism and ultrafast magnetization dynamics of Co and CoMn alloys at finite temperature

R. Chimata[1], E. K. Delczeg-Czirjak[1], A. Szilva[1], R. Cardias[1,2], Y. O. Kvashnin[1], M. Pereiro[1], S. Mankovsky[3], H. Ebert[3], D. Thonig[1], B. Sanyal[1], A. B. Klautau[2], and O. Eriksson[1]

[1] Department of Physics and Astronomy, Material Theory, University Uppsala, SE-75120 Uppsala, Sweden
[2] Faculdade de Física, Universidade Federal do Pará, Belém, PA, Brazil
[3] Department of Chemistry, University of Munich, Butenandtstrasse 5-13, D-81377 Munich, Germany

Temperature-dependent magnetic experiments such as pump-probe measurements generated by a pulsed laser have become a crucial technique for switching the magnetization in the picosecond time scale. Apart from having practical implications on the magnetic storage technology, the research field of ultrafast magnetization poses also fundamental physical questions. To correctly describe the time evolution of the atomic magnetic moments under the influence of a temperature-dependent laser pulse, it remains crucial to know if the magnetic material under investigation has magnetic excitation spectrum that is more or less dependent on the magnetic configuration, e.g., as reflected by the temperature dependence of the exchange interactions. In this paper, we demonstrate from first-principles theory that the magnetic excitation spectra in Co in fcc, bcc, and hcp structures are nearly identical in a wide range of noncollinear magnetic configurations. This is a curious result of a balance between the size of the magnetic moments and the strength of the Heisenberg exchange interactions, that in themselves vary with configuration, but put together in an effective spin Hamiltonian results in a configuration-

independent effective model. We have used such a Hamiltonian, together with ab initio calculated damping parameters, to investigate the magnon dispersion relationship as well as ultrafast magnetization dynamics of Co and Co-rich CoMn alloys.
Ref : Phys. Rev. B 95, 214417 (2017).

A-4
Room-temperature Blue Luminescence from Highly Electron-doped TiO_x Nanostructures on the Surface of $SrTiO_{3-\partial}$(001)

Seyoung Cook,[1] Richard A. Rosenberg,[2] Laurence D. Marks,[1] Dillon D. Fong[3]

[1] Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60202
[2] Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439
[3] Materials Science Division, Argonne National Laboratory, Argonne, IL 60439

The defect behavior and the associated physical properties of complex oxides can be altered at the surface where the oxygen coordination environment of the transition metal cation can differ significantly from the bulk via formation of near-stoichiometric surface reconstructions and highly non-stoichiometric surface phases. Here report on the observation of a relatively strong contribution to the blue luminescence from TiO_x nanostructures formed on the surface of $SrTiO_{3-\partial}$ (001) with a gradient of oxygen vacancies prepared by a DC-resistive heating process. Using a suite of soft X-ray spectroscopy including X-ray excited optical spectroscopy and scanning probe microscopy techniques, we systematically probe the evolution of the room-temperature blue light emission originating from the electrons doped by the oxygen vacancies. We find the dynamics of the blue luminescence can be explained by an Auger recombination process, which allows us to quantify the doped electron concentrations in the bulk and surface regions. The enhanced electron doping at the surface explains the two-component blue luminescence behavior, which is corroborated by observations of a space charge layer formation together with chemical and structural changes in the near-surface region.

A-5
Temperature-Dependent Optical Properties of Lead Halide Perovskite Nanocrystals

Benjamin T. Diroll,[1] Peijun Guo,[1] and Richard D. Schaller[1,2]

[1] Center for Nanoscale Materials, Argonne National Laboratory
[2] Department of Chemistry, Northwestern University

The temperature-dependent properties of all inorganic cesium lead trihalides and hybrid organic-inorganic methylammonium and formamidinium lead iodide nanocrystals are examined. Inorganic perovskite nanocrystals show strong temperature resilience instrumental in display technology and halide vacancy trapping and quenching of emission at high temperature. The low temperature properties of hybrid perovskite-type nanocrystals reveals the absence of typical phase transitions observed in bulk material, allowing the study of photophysical properties of solar-relevant material at cryogenic temperatures.

A-6
Precision Magnetic Field Calibration for the Muon g-2 Experiment at Fermilab

David Flay,[1]

[1] University of Massachusetts, Amherst, MA 01003, USA

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 will be 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 will be calibrated in terms of the free-proton Larmor precession frequency ωp 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 to be conducted during the experiment.

A-7
Electrochemical Corrosion of U -bearing HT9 Based Alloyed Nuclear Waste Form

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

[1] Nuclear Engineering Division, Argonne National Laboratory, Argonne, IL 60439
[2] Civil and Materials Engineering, University of Illinois at Chicago, Chicago, IL 60607

An electrochemical testing protocol is being developed to measure the corrosion behavior of waste forms made by alloying metallic fuel waste that remains after electrochemical processing of spent nuclear fuel with cladding hulls, contaminated hardware, and added trim metals. Understanding the corrosion mechanisms of host phases containing the radionuclides and a scientific basis for experimentally measured durabilities will provide confidence in long-term performance predictions. 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-8
Data Acquisition with GPUs for the Muon *g*-2 Experiment at Fermilab

W. Gohn for the Muon g-2 Collaboration

University of Kentucky, Lexington, KY

A new measurement of the anomalous magnetic moment of the muon, $a_\mu \equiv (g-2)/2$, is being performed at the Fermi National Accelerator Laboratory. 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 collected using 1296 channels of μTCA-based 800 MSPS, 12 bit waveform digitizers and processed in a layered array of networked commodity processors with 26 GPUs working in parallel to perform a fast recording of the muon decays during the spill. The system is controlled using the MIDAS data acquisition software package. Commissioning for Muon *g*-2 began in May 2017 and is ongoing, with full rate production slated to begin early next year.

A-9
Size-dependent electrocatalytic behavior of sub-nanometer copper clusters in the reduction of CO_2

Avik Halder[1], Rosalba Passalacqua[4,6], Siglinda Parathoner[4,6], Gabriele Centi[5,6], Eric. C. Tyo[1], Sönke Seifert[2], and Stefan Vajda[1,3,7,8]

[1] Materials Science Division, [2]X-ray Science Division, and [3]Nanoscience and Technology Division, Argonne National Laboratory, Lemont, Illinois 60439
[4] Department of Chemical, Biological, Pharmaceutical and Environmental Science, [5]Department of Mathematical and Computer Sciences, Physical Sciences, and Earth Sciences, [6]ERIC aisbl and CASPE (INSTM Lab. of Catal. for Sustainable Prod. & Energy), University of Messina, V.le F. Stagno d'Alcontres, 31-I-98166 Sant'Agata di MESSINA, Italy
[7] Department of Chemical and Environmental Engineering, School of Engineering & Applied Science, Yale University, New Haven, Connecticut 06520, United States
[8] Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637, United States

The study of the electrochemical behavior of size-controlled bare Cu nanoclusters has been performed to elucidate the redox behavior of sub – nm copper particles and the effect of CO_2 on them. Cu_5 and Cu_{20} cluster impregnated glassy carbon samples are prepared in high vacuum chamber by a combination of magnetron sputtering source (for producing pure clusters in gas phase), mass spectrometry and softlanding techniques. The average valence state and the chemical composition of the clusters are determined by grazing incidence X-ray absorption near edge structure (GIXANES) measurement. Simultaneous grazing incidence small angle X-ray scattering (GISAXS) results confirms that the naked clusters stay as isolated particles on the electrode surface. A custom made electrochemical setup has been used for sample investigation with highly sensitive square wave voltammetry (SWV) and cyclic voltammetry (CV) techniques.

C_{u20} nanoclusters show anodic redox processes occurring at much lower potential with respect to Cu_5 nanoclusters, which behave relatively similar to much larger Cu particles. However, Cu_5 nanocluster coordinate effectively CO_2 (hydrogen carbonate) in solution differently from Cu_{20} nanoclusters and larger Cu particles. This effect, rather than the redox behavior, is apparently connected to the ability of Cu_5 nanoclusters to reduce CO_2 under cathodic conditions at low overpotential. Although preliminary, these results provide rather exciting indications on the possibility to realize low overpotential electrocatalytic conversion of CO_2.

References:
[1] Passalacqua, R., Parathoner. S., Centi, G., Halder, A.*, Tyo, E. C., Yang, B., Seifert, S., Vajda, S. Electrochemical behaviour of naked sub – nanometre sized copper clusters and effect of CO_2. Catal. Sci. Technol. Vol. 6, 6977 (2016).

A-10
Precision Magnetic Field Measurement For The Muon g-2 Experiment

Ran Hong[1], Joseph Grange[1], and Peter Winter[1]

[1] High Energy Physics Division, Argonne National Laboratory, Argonne, IL 60439

The New Muon g-2 Experiment (E989) at Fermilab will measure the anomalous magnetic moment of muon aμ aiming at a precision of 140 ppb. This new experiment will shed light on the long-standing 3.5 standard deviation between the previous muon g-2 measurement (E821) at Brookhaven National Laboratory and the Standard Model calculation, and potentially discover new physics. The New Muon g-2 Experiment measures the precession frequency of muon in a uniform magnetic field, and the magnetic field experienced by the muons needs to be measured with a precision better than 70 ppb. We refurbished the in- vacuum trolley system that carries 17 nuclear magnetic resonance (NMR) probes to scan the magnetic field in the muon storage region. 378 NMR probes installed at fixed locations in the vicinity of the muon storage region monitor the field drift in between trolley measurements. The magnetic field is shimmed to high uniformity so that the root-mean- square fluctuation is less than 20 ppm. The current that generates the magnetic field is also regulated in situ based on the fixed-probe measurement to reduce its drift. In this presentation, an overview of the magnetic field measurement system and shimming effort is given.

A-11
The Flux and Cyclic Metabolic Processes of Urbanized Ecosystems

Michael Iversen[1]

[1] Department of Urban Planning and Policy, University of Illinois at Chicago, Chicago 60607

There exists an opportunity to investigate urban areas as analogous to ecosystems, thus allowing a complex, metabolic systems approach to be applied to the planning of coupled natural-human systems. Similar to how an ecologist studies natural environments within the hierarchal scale of an ecosystem, this novel approach is based on the investigation of urbanized areas as ecosystems onto themselves, or as urbanized ecosystems. Such an approach is scalable and transferable to neighborhood, community and regional applications. Towards this end, this research presents a methodology, Urbanized Ecosystems (UrbEcoSys), developed as a proof of concept application for the Village of Oak Park, Illinois. This community was first conceptualized as a complex, metabolic, and dynamic ecosystem, based on scoping, inventorying, and assessing its critical variables and relationships, as represented by the flux and cyclic processes of energy, materials, information and economic costs. This conceptualization allowed a more formalized level of inquiry in the form of a system model. Findings relative to baseline metrics were then assessed relative to their alignment with the village's overall vision and policy. The outcomes from this assessment were then used to support an informed decision- and policymaking process, prioritized within the municipal budget's allocation of finite resources.

A-12
Realization of Spectrally Selective Emitters Screened by Pareto Optimization for Thermophotovolatics

Nari Jeon[1], **Jonathan J. Hernandez**[2], **Stephen K. Gray**[3], **Alex B. F. Martinson**[1], **and Jonathan J. Foley IV**[4]

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[2] Union County College, Cranford, New Jersey, 07016, USA
[3] Nanoscience and Technology Division, Argonne National Laboratory, Argonne, Illinois, 60439, USA
[4] Department of Chemistry, William Paterson University, Wayne, New Jersey, 07470, USA

The broad band of solar spectrum limits single junction photovoltaic (PV) cells to the Shockley-Queisser limit of ~33%, mainly due to photons with energies below the bandgap and photons with energies above the bandgap, which suffer from thermal loss. A central idea of the solar thermophotovoltaics (STPV) is to spectrally tune the solar spectrum matched the bandgap of a target PV cell to minimize these losses. In STPV systems, concentrated sunlight is shined on thermal absorber with thermally contacting emitters, which emit the spectrally tuned spectrum. We proposed a new design of the emitters to tailor thermal emission by exploiting critical coupling between reflection in multi-layer dielectric stacks and absorption in weakly absorbing thin layer. Pareto optimization was utilized to select a small number of promising structures based on two conflicting figures of merits – spectral efficiency and spectral density. One of the simple structures of the proposed structures was experimentally realized. The multi-layer dielectric stacks of SiO_2/TiO_2 and weak absorber of $W\text{-}Al_2O_3$ alloys were fabricated by atomic layer deposition. The realized structures exhibit excellent thermal stability upon prolonged annealing at 1000 °C under inert atmosphere. The measured spectral efficiency and spectral density approached the ideal values of the fabricated structures.

A-13
Biophysical Investigation of the Dual Role of Choline Kinase α in Cancer

Stefanie Kall[1], **Kindra Whitlatch**[2], **Edward Delikatny**[3], **Thomas Smithgall**[2], **Arnon Lavie**[1]

[1] University of Illinois at Chicago, Department of Biochemistry and Molecular Genetics
[2] University of Pittsburgh, Department of Microbiology and Molecular Genetics
[3] University of Pennsylvania, Department of Radiology

Nearly every form of cancer subtype exhibits cells with an up-regulation of Choline Kinase α (ChoKα). Because of this observation, ChoKα has been a target in understanding the drivers of malignant transformation and

enzymatic regulation in cancerous cells and tumours. Research shows that small molecule inhibition of ChoKα renders cells senescent and prevents their rapid expansion; however, ablation of ChoKα via siRNA triggers apoptosis. This suggests that the role of ChoKα in malignancy is not limited to its enzymatic function. Here, we investigate an alternative scaffolding role of ChoKα that may have an impact on its behaviour in cancer cells. Additionally, we examine how an inhibitor that binds to a site not previously identified by other inhibitors may be effective in Phase I clinical trials due to its impact on this alternative role of ChoKα.

A-14
The Development Cu(I) Photosensitizer and Co(II)-poly(pyridyl) Proton Reduction Catalyst Modules and their Incorporation into Photosensitizer-Catalyst Assemblies

Lars Kohler[1], Dugan Hayes[1], Lin X. Chen[1], Karen L. Mulfort[1]

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The main goal of our work is the development of new modular systems for photocatalytic hydrogen production. Here, we will present recent work on 1) CuHETPHEN photosensitizer modules, 2) Co(II)-poly(pyridyl) catalyst modules and 3) their covalent linkage.

1) Cu(I)-bisphenanthroline complexes are known to have similar photophysical properties to $Ru(bpy)_3^{2+}$ but their relatively short lifetime limits their widespread use. The copper heteroleptic phenanthroline (CuHETPHEN) synthesis approach presents a means to enable synthetic diversity for linking electron donors, acceptors, and catalyst modules to Cu(I)diimine complexes. To that end, we are studying CuHETPHEN complexes containing either 2,9-dimesityl-1,10-phenanthroline or 2,9-bis(2,4,6-triisopropylphenyl)-1,10-phenanthroline as a blocking ligand. Different substituents on the second phenanthroline ligand can be used to vary the physical and photophysical properties. For example, the excited state lifetime can be tuned across two orders of magnitude up to 74 nanoseconds.

2 and 3) Recent work has focused on the synthesis of a new Co(II)-poly(pyridyl)macrocycle catalyst module that is highly active for aqueous proton reduction when photo-driven by $Ru(bpy)_3^{2+}$ using ascorbate as a sacrificial electron donor. We will present some mechanistic insight and catalytic efficiencies. Additionally, this macrocycle possesses the capability to covalently attach photosensitizer modules leading to a very stable new type of photosensitizer-catalyst assembly.

A-15
Study on Novel Reaction Pathway via Sparingly Solvating Electrolytes for Lithium-Sulfur Batteries

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DOE's energy storage hub (JCESR) is exploring "beyond lithium-ion" solutions that can attain important metrics (pack level energy density of 400 Wh/L, cost of $100/kWh) relevant to transportation applications. The lithium−sulfur battery has long been seen as a potential next generation battery chemistry for electric vehicles owing to the high theoretical specific energy and low cost of sulfur. However, even state-of-the-art lithium−sulfur batteries suffer from short lifetimes due to the migration of highly soluble polysulfide intermediates and exhibit less than desired energy density due to the required excess electrolyte. The use of sparingly solvating electrolytes in lithium-sulfur batteries is a promising approach to decouple electrolyte

quantity from reaction mechanism, thus creating a pathway towards high energy density.

Herein, we demonstrate that sparingly solvating electrolytes can fundamentally redirect the Li-S reaction pathway by inhibiting the traditional mechanism. The sparingly solvating electrolytes promote intermediate and short-chain PS during the first third of discharge, before disproportionation results in crystalline Li_2S and a restricted fraction of soluble PS which are further reduced during the remaining discharge. The results of this study will be presented in the meeting.

A-16
A Statistical Machine Learning Approach to Characterize the Parallel I/O Performance on a LUSTRE File System

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Parallel I/O performance is one of the prominent contributor to execution time variability of a job on large-scale HPC systems. This confounds the efforts to predict job performance for application optimizations, or scheduling among other things. In this work, we developed complementary metrics that take into account application and file-system characteristics to analyze the relationship between the job performance and the state of the file-system. We use data from different applications run with different I/O characteristics (POSIX/MPI-IO, Read/Write, etc.) and repeatedly run multiple times on EDISON system at NERSC.

We proposed a semi-automatic approach to partition the data into sub-groups based on Extra-tress regression. Then, robust variational Gaussian process regression (using Student-t likelihood) is used to obtain a predictive model for I/O time w.r.t the file-system side metrics for each of the sub-groups. The results show that the proposed approach has better predictive accuracy than other common machine learning methods. Also, the predictive accuracy of the sub-group based model is better than the case where a global model is fit to entire data and a separate model is fit to each application. Also, insights are drawn into the metrics that have a major impact on I/O performance for each sub-group.

A-17
Tailoring the Properties of Lead-Based Hybrid Perovskites for Photovoltaic Applications

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Lead halide hybrid perovskite semiconductors have emerged as attractive candidates for photovoltaic applications owing to their large absorption coefficients, easy synthesis and property tailoring via composition engineering. $MAPbX_3$ perovskites (where MA = Methylammonium and X = Br/Cl) were the subject of recent computational and experimental studies dealing with partial substitution of Pb with transition metal Co to obtain stable mid-gap states with tunable energy level. This paved the path towards a new class of multi-junction devices called intermediate band (IB) photovoltaics, which can theoretically surpass the Shockley-Queisser (S-Q) limit of solar conversion efficiency with additional absorption of sub-gap photons. In this work, we used Density Functional Theory to study several possible substituents (both transition and non-transition metals of suitable ionic sizes and valances) besides Co that can replace Pb in $MAPbX_3$ with a thermodynamic penalty similar to the thermal energy, and create desirable half-filled mid-gap states. We also studied the formation energies of external metal substitution and various intrinsic defects (such as vacancies and self-interstitials) in different charged states as a function of chemical potentials of constituent species, thus obtaining an understanding of the thermodynamic equilibrium growth conditions necessary for stabilizing any intrinsic or extrinsic defect. This exercise also helped identify charge transition levels created by the different substituents, which is important because such levels within the bandgap could correspond to energy state eigenvalues.

A-18
Suppression Of The Magnetism In CeFeAsO: Pressure Vs P-Substitution

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We investigated the suppression of the magnetic order due to the application of external pressure as well as As->P-substitution in CeFeAsO by means of conventional and synchrotron Mössbauer spectroscopy. By utilizing these local probes we can compare the influence and differences of pressure and P-substitution on a nanoscopic scale. CeFeAsO shows spin density wave magnetic order below ~145 K. We found that at low pressures and P substitution levels the suppression of the magnetic order is quantitatively equal but not at intermediate and higher pressures/levels. P- subsitution monotonically suppresses the magnetism to zero. At pressures up to 4.5 GPa the suppression is small (~20%) when an abrupt decrease to zero above 4.5 GPa occurs.

A-19
A Machine Learning - Genetic Algorithm (MLGA) Approach for Rapid Virtual Optimization Using High-Performance Computing

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A Machine Learning - Genetic Algorithm (MLGA) approach was developed to virtually discover optimum designs using training data generated from high-fidelity simulations. In the present work, a total of over 2000 sector-mesh computational fluid dynamics (CFD) simulations of a heavy-duty engine were performed. The engine being optimized was run on low-octane (RON70) gasoline fuel using a partially-premixed advanced combustion approach. A total of nine input parameters (or features) were varied, and the CFD simulation cases were generated by randomly sampling points from this nine-dimensional input space. The outputs (targets) of interest from these simulations included five performance and emission metrics. A robust superlearner approach was employed to build the ML model, where results from a collection of different ML algorithms were pooled together. Then, a stochastic global optimization genetic algorithm (GA) was used, with the ML model as the objective function, to optimize the input parameters based on a merit function constructed from the five targets. The results from the MLGA approach were found to be very close to a sequentially performed CFD-GA approach, where a CFD simulation served as the objective function. This study demonstrated the significant cost-savings potential of ML and high-performance computing with regard to design optimization.

A-20
Materials For Giant Spin Hall Device

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Spin-orbit coupling in metastable β-W generates spin-orbit torques (SOT) strong enough to switch between high and low resistive states in adjacent magnetic tunnel junction (MTJ) stack. Two different techniques to grow 5-20 nm thick β-W films by introducing either O_2 gas or N_2 gas during the deposition on SiO_2/Si or SiN/Si substrates is discussed. X-ray diffraction patterns, resistivities, X-ray photoelectron spectroscopy and X-ray reflectivity were utilized to determine phase, bonding information and thickness, respectively. These results demonstrate a reliable technique to fabricate β-W films up to 20 nm thick on bare Si, SiN and SiO_2, while providing insights that enable deposition of these films anywhere in the device stack.

Films with perpendicular magnetic anisotropy (PMA) can exhibit uniform magnetizations and higher thermal stability. Inserting a 1 nm Ta insert-layer between the CoFeB and W induces PMA which is confirmed by vibrating sample magnetometer and anomalous Hall voltage measurements. β-W(5)/Ta(1) channel and the adjacent CoFeB/MgO/Ta layers are patterned into a 100 nm wide Hall bar structures. In-plane current in β-W(5)/Ta(1) channel will create effective magnetic fields due to GSHE, which eventually switch an adjacent ferromagnetic metal. These effective field are analyzed by applying magnetic fields in various directions to quantify the effect.

A-21
High-Throughput Techniques Accelerating the Development of Fuel Cell Catalysts and Electrodes

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In proton exchange membrane fuel cells (PEMFCs), platinum is widely used as the catalyst material due to its high catalytic activity and stability, but the high cost of this precious metal is one of main barriers to widespread commercialization of this promising technology. The overall approach of this project is to accelerate the development of platinum group metal-free (PGM-free) catalysts by developing and utilizing high-throughput materials synthesis, characterization, and performance evaluation methodologies. In the materials characterization aspect of the project, a multi-channel flow double electrode (m-CFDE) cell has been designed and constructed for the simultaneous screening the catalytic activity of multiple samples using an aqueous hydrodynamic technique. In the performance evaluation aspect, the project involves the development and validation of a combinatorial membrane-electrode assembly and test system for determining the fuel cell performance of 25-electrodes simultaneously. In addition to synthesis and characterization of materials, the high-throughput methodology is also being applied to the fabrication of electrodes. An automated robotic catalyst ink dispensing system is being developed for precise deposition of nano-liter ink droplets across the m-CFDE glassy carbon electrodes and on the 25 segmented electrodes.

A-22
The Role of Machine Learning in Process-Structure-Property Relationships

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The development and deployment of new materials in industrial applications are notoriously sluggish. Processing-structure-property (P-S-P) relationships are critical in efforts to accelerate these efforts as they enable rapid bi-directional exploration of the materials design space. Machine learning (ML) techniques show great promise in aiding the creation of P-S-P relationships due to their impressive ability to capture complex functional relationships. This work presents the role of ML in the development of processing-structure (P-S) relationships to connect material composition and temperature to the existence of stable and meta-stable phases as well as structure-property (S-P) relationships to relate polycrystalline material microstructures to critical mechanical properties. Specifically, ongoing work is presented which demonstrates the use of Bayesian ML to select appropriate physics-based functional forms for thermodynamic quantities and to quantify their uncertainty in the Hafnium-Oxygen system. These improvements have direct application in increasing the reliability of CALculation of PHAse Diagrams (CALPHAD) results. Additionally, S-P relationships are developed to connect polycrystalline microstructures to their mechanical properties including elastic stiffness and yield strength through 2-point spatial correlations and dimensionality reduction techniques. Both studies demonstrate the promise of ML in the development of efficient and reliable S-P-S relationships.

A-23
Using Agent-Based Modeling to Enhance System-Level Real-time Control of Urban Stormwater Systems

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The ability to reduce combined-sewer overflow (CSO) events is an issue that challenges over 800 U.S. municipalities. Traditionally, mitigating CSO events has been carried out via time-intensive and expensive structural interventions such as retention basins or sewer separation, which are able to reduce CSO events, but are costly, arduous, and only provide a fixed solution to a dynamic problem. Real-time control (RTC) of urban drainage systems using sensor and actuator networks (e.g. retrofitting individual stormwater elements for sensing and automated active distributed control) has served as an inexpensive and versatile alternative to traditional CSO intervention. As more stormwater elements become retrofitted for RTC, system-level RTC across complete watersheds is an attainable possibility. However, when considering the diverse set of control needs of each of these individual stormwater elements, such system-level RTC becomes a far more complex problem. To address such diverse control needs, agent-based modeling is used such that each individual stormwater element is treated as an autonomous agent with a diverse decision making capabilities. Here, we present preliminary results and limitations of utilizing the agent-based modeling computational framework for system-level control of diverse, interacting stormwater elements.

A-24
Integrated Imaging and Multiscale Simulation to Investigate Lattice Deformations in Externally Stimulated Nanocrystals

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Investigating the temporal behavior of a diverse class of nanomaterials (such as core-shell nanoparticles, nanostructured catalysts, 2D materials, etc.) under conditions of external stimulation is crucially important for energy research. Recently, experimental techniques have evolved to conduct time-dependent lattice dynamics measurements in such systems. In particular, Bragg Coherent Diffraction Imaging (BCDI) has been used to directly image ultrafast lattice distortions in laser-heated nanocrystals. Furthermore, suitable simulation models prove to be an ideal foil to explore the underlying mechanisms behind the observed lattice deformations. With the convergence of time and length scales accessible by both experiments and simulations, we are now able to integrate experimental observations with classical molecular dynamics (MD) simulations and continuum finite element calculations to enhance the fundamental understanding of materials behavior under external stimulation.

Here, we demonstrate the machine learning and data driven approaches to integrate BCDI measurements with large-scale atomistic molecular dynamics simulations and finite element models to investigate lattice dynamics in externally stimulated nanocrystals. We will demonstrate the suitability of the workflow(s) as applied to a diverse class of materials systems and external stimulus. We show that direct comparisons between experiments and simulations are possible by using the appropriate level of theory or a combination of simulation techniques. In addition, the integrated experiment-informed simulation approach yields new insight into deformation mechanisms of nanomaterials that cannot be obtained and validated by either approach alone.

A-25

Understanding The Near-Threshold Single Photon Ionization Spectrum Of N_2 With (2+1') Resonance Enhanced Multiphoton Laser Spectroscopy

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The study of molecular photoionization can provide detailed information about how energy flows among the electronic, vibrational and rotational degrees of freedom in isolated, excited molecules. The near-threshold single photon ionization spectrum of N_2 has characteristic resonant structures resulting from autoionizing states. These states correspond to high vibrational levels of the b' $^1\Sigma_u^+$ state, Rydberg states converging to vibrationally excited levels of the X $^2\Sigma_g^+$ ground state of the ion, and Rydberg series converging to the electronically excited A $^2\Pi_u$ and B $^2\Sigma_u^+$ states of the ion. There have been a lot of debates surrounding the assignment of this complex photoionization spectrum, particularly involving the two intense features at 126100 cm^{-1} and 126500 cm^{-1} that resemble two towers of a cathedral. While there is agreement for the assignment of one of these towers, there is still considerable disagreement about the assignment of the second one. We have performed ultraviolet double-resonance experiments via the a'' $^1\Sigma_g^+$ level to probe transitions into this same energy region. We have succeeded in recording rotationally resolved spectra for a number of intermediate levels, and we are currently analyzing the results to see if we can provide insight into the assignment of the autoionizing resonances.

A-26

Intelligent Eco-Driving Strategy For A Hybrid Electric Vehicle in Highway Scenarios Based On Minimum Principle

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Increasing connectivity in passenger vehicles provides for a large amount of look-ahead information about driving conditions. An intelligent control algorithm is presented that takes advantage of this information to obtain the operation strategy for the powertrain of a parallel hybrid electric vehicle, in an uncongested highway cruising situation. In order to guarantee sufficient computational efficiency to meet future online requirements, the algorithm is based on Pontryagin's Minimum Principle. The whole driving/operation strategy is composed of a series of solutions to the optimal control sub-problem for each separate route segment. The control sequence computed offline is then evaluated in Autonomie. The simulation result shows 6% fuel savings compared to a baseline rule-based controller with no speed optimization.

A-27

Oxide Surface Modification for Single-Atom Catalyst Synthesis: Monodispersed Platinum Sites for Selective Hydrogenation-Dehydrogenation Reactions

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Recent advances in the area of single-atom catalysis (SAC) have generated strategies to access atom-efficient catalytic materials. The development of synthesis techniques with molecular-level control and the effective design of single-site supports have enabled precise downsizing of catalytic sites from bulk particles down to isolated metal atoms, and access to unprecedented reactivity and selective transformations, which are not easily achieved using bulk active sites. Additionally, SAC strategies have generated supported-but-homogeneous-in-function platform materials which are more amenable to characterization techniques; Hence, providing important insights into active site structure–activity relationships.

SAC is particularly challenging for sensitive and sintering-prone noble metals (e.g., Pd, Pt). Recent reports have shown that single-atom and/or pseudo-single Pd/Pt atom catalysts can be stabilized on defect sites on bulk oxides where the surface hydroxyl concentrations are significantly low. Here, we present the purposeful design of supports that enable the stabilization of single- atom/pseudo-single-atom catalysts for the selective hydrogenation of unsaturated organic functionalities. Our approach specifically focuses on the modification of oxide surfaces by installing cationic anchoring sites to stabilize single-atom and pseudo-single-atom Pt sites. The monodispersed Pt sites have been shown active for chemoselective reduction of polyfunctionalized nitroaryls, and selective, non-oxidative dehydrogenation of C3 to C4 alkanes.

A-28

Relative Solvating Power: Indicating the Shuttling Effect of Lithium Polysuflides in Lithium-Sulfur Batteries

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With its exceptionally high energy density (1675 mAhg-1) and extremely low cathode cost, lithium-sulfur (Li-S) batteries are a promising next-generation battery system whose applications include electric vehicles. Yet, the rapid capacity fading and low Coulombic efficiency of Li-S batteries impede its mass commercialization. The parasitic reactions of lithium polysulfides (LiPS), intermediates during the electrochemical reduction process of sulfur to lithium sulfide, are believed to be the major reasons for the fast capacity fading and low Coulombic efficiency. As a result, an in-depth understanding of the relationship between LiPS dissolution and the solvation state of electrolyte solvents is vital in developing efficient Li-S batteries.

Herein, we introduce the concept of relative solvating power, which can be determined by our newly developed internally-referenced DOSY NMR method, as an indicator for the degree of LiPS dissolution. The higher the relative solvating power of regular ether solvent to 1,3-dioxolane (DOL), the more severe will be the LiPS dissolution and the lower the Coulombic efficiency of the Li-S cell. Fluorinated ethers commonly demonstrate very low relative solvating power and thus reduce LiPS dissolution and enhance the Coulombic efficiency of the Li-S cell.

A-29

Morphologically-Directed Raman Spectroscopy for Characterization of Ingredient-Specific Particle Size Distributions in Nasal Spray Suspensions

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Morphologically-Directed Raman Spectroscopy (MDRS) has recently been developed for substance-specific particle size determination. This method combines microscopic imaging and Raman spectroscopy into one integrated platform. The technique characterizes the particles based on morphological parameters, identifies the chemical identity of the particles using Raman spectroscopy, and measures particle size using white light microscopy. While this method appears amenable for characterizing API-specific particle size for nasal suspension spray products, determination of the suitability of this method for marketed nasal suspension spray products, along with the ability to discriminate particle size differences in nasal suspension formulations, is under investigation. The purpose of this study was to develop a MDRS method to determine the particle size distribution of APIs in nasal spray suspensions. The selection of morphology filters (*e.g.*, aspect ratio, intensity mean and solidity) and chemical correlation score is critical to generate accurate and reliable data. This research provides important information regarding the suitability of the MDRS method for API-specific particle size evaluation of nasal suspension spray products. Overall, with a validated method, MDRS may be suitable for regulatory applications.

A-30
Simulations of Spray and Flow Variability in an Optical DISI Engine

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Modern internal combustion engines operate very close to their stability limits in order to maximize efficiency and minimize pollutant emissions. Variations from cycle to the next (also called cycle-to-cycle variations or CCVs) can have significant negative effects on the overall engine performance. These variations grow from small differences in the local flow field and fuel-air mixing. Large-eddy Simulations (LES) is a computational fluid dynamics framework that has been shown to accurately capture flow CCVs arising out of random turbulent fluctuations. For direct-injection (DI) engines where the fuel is injected at high pressure directly into the combustion chamber, the injection process of the high-momentum fuel has a significant effect on the cylinder flow and mixing. The injection process is also subject to shot-to-shot variations that introduce flow CCVs, and there has been much less simulation work to characterize this source of variability. This work simulates flow and spray variability in an optically accessible, direct-injection spark-ignition (DISI) engine as well as their interactions to better understand spray variability and its ultimate effect on engine cyclic variability.

A-31
Digital Modulation of Nickel Valence in Cuprate-Nickelate Heterostructures

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Past years have seen sophisticated approaches to design novel materials aiming to engineer their properties.[1] Charge doping is a key tuning parameter. Typically, the dopant cannot be confined to one atomic layer due to diffusion of dopant in growth direction.[2] Thus, effects of charge and disorder cannot be separated. We suggest doping through insertion of a positively charged layer, LaO^+, which allows for a digital modulation of the nickel valence in cuprate-nickelate heterostructures.

We use atomic layer-by-layer, ozone assisted molecular beam epitaxy to grow structures with the chemical formula $[(La_2CuO_4)_nLaO(LaNiO_3)_m]_l$. X-ray absorption measurements and DFT simulations confirm that the charge provided by the LaO^+ layer is exclusively accommodated in the nickelate layers, leaving the cuprate layers as inert separating layers. The electrons reside mostly in the out-of-plane, z^2-orbitals and the valence state of nickel is modulated within the nickelate stack.

The insertion of LaO^+ layers shows a way of charge doping without introducing disorder and if one LaO^+ layer at the bottom of a nickelate stack is replaced by SrO, the diffusion in growth direction will be blocked because the nickelate layers cannot be hole-doped in these growth conditions. Hence, confinement of the dopant could be feasible.

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A-32
Tailoring Magnetic Skyrmions by Geometric Confinement of Magnetic Structures

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Nanoscale magnetic skyrmions have interesting static and transport properties that make them candidates for future spintronic devices. Control and manipulation of the size and behavior of skyrmions is thus of crucial importance. Using a Ginzburg-Landau approach, we show theoretically that skyrmions and skyrmion lattices can be stabilized by a spatial modulation of the uniaxial magnetic anisotropy in a thin film of centro-symmetric ferromagnet. Remarkably, the skyrmion size is determined by the ratio of the exchange length and the period of the spatial modulation of the anisotropy, at variance with conventional skyrmions stabilized by dipolar and Dzyaloshinskii--Moriya interactions (DMIs).

A-33
Performance optimization of WEST and Qbox on Intel Knights Landing

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We will present performance optimization of two electronic structure codes, Qbox and WEST, on Theta, a 2nd generation Intel-Xeon-Phi based supercomputer at the Argonne Leadership Computing Facility. Qbox is an ab-initio molecular dynamics code based on plane wave density functional theory (DFT) and WEST is a post-DFT code for excited state calculations within many-body perturbation theory. We focus on improving the strong scaling of both codes to support full-machine calculations on leadership computational resources. In WEST, an additional layer of parallelization was implemented – band parallelization over electrons, which directly improves the scalability by a factor proportional to the number of electrons. In Qbox, we implemented a data remap method – on-the-fly redistribution of data into optimal ScaLAPACK contexts to reduce the communication costs for tall-skinny and small-symmetric matrix operations, which improved the scalability of hybrid functional DFT calculations. The optimization of these two codes on the KNL platform enables efficient computation of optoelectronic properties of large nanostructured systems for use in solar and thermal energy conversion device.

Key words: High Performance Supercomputing, Electronic Structure, Nanostructured Materials

B-1
Effect Of Redshift Uncertainties On Galaxy Clustering And Baryonic Acoustic Oscillations

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In the upcoming era of high-precision galaxy surveys, it becomes necessary to understand the impact of noisy redshift estimators on cosmological observables. Here we explore the effect of redshift errors on galaxy clustering and baryonic acoustic oscillations (BAO). We derive analytic expressions for their impact which we contrast with the results from hundreds of N-body simulations. We find that on scales not dominated by shot noise, redshift errors increase the signal-to-noise of the power spectrum and the BAO contrast with respect to the case where redshift errors are negligible. Furthermore, we find that redshift errors induce a scale dependence on the information encoded in the BAO scale, and that the dependence of this information on the Hubble parameter decreases with their magnitude. Finally, we present a quick theoretical method to forecast the expected precision with which the Hubble parameter and the angular diameter distance can be measured in galaxy surveys based on the redshift error, number density, and large-scale bias of the analyzed sample.

B-2
Microphone Array Signal Processing Algorithms to Locate and Quantify Building Leakages

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This poster will demonstrate the abilities of microphone array signal processing methods such as acoustic beamforming and nearfield acoustic holography (NAH) to detect and quantify leakages in building envelopes. A loudspeaker was placed inside a building and a tonal sound was played. Microphone array measurements were obtained from the outside of the building. Acoustic beamforming was efficient in localizing the major leakages in the building. The NAH results provided more accurate sound pressure levels. However, a large measurement area is required to obtain acceptable reconstructions using NAH. A single microphone was used to measure the sound pressure level inside the building model which was used as a reference for quantification calculations. The difference between the inner and outer sound pressure levels was related to the area of the leakage.

B-3
Implementing mathematical expressiveness in a DSL

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My work describes the implementation of the mathematical expressiveness in the Diderot programming language. Diderot is a domain-specific language for scientific visualization and image analysis. The datasets are produced by digital imaging technologies that sample physical objects at discrete points. Algorithms in this domain are used to visually explore the data and compute features and properties. Diderot is designed to enable the translation of visualization ideas into code by providing a mathematically familiar syntax and high-level language. My work enables a high-level of programmability by, designing and implementing our intermediate representation and addressing the technical challenges that arise. I evaluate the correctness of our implementation with two complimenting parts; formalizing the properties in our rewrite system and automated testing of our implementation. Lastly, I take the first step to extend the language to another domain, the finite element community. As a result, the Diderot user can write intuitive code, compile programs with complicated tensor math, and believe in the correctness of the compiler. It is important and challenging work to improve the expressivity of the language.

B-4
Incorporation of Acoustic Levitation in Nanomaterials Synthesis and Dynamic Characterization

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The ongoing development of acoustic levitation is providing a high degree of control in introducing increasingly smaller samples (droplets) and container-less manipulation of various samples including nanoparticles, bio-molecules, fuels, and photo-catalytic compounds. Integration of levitated droplets into small angle X-ray scattering (SAXS) experiment at Advanced Photon Source (APS) offers a unique ability of time-resolved characterization of materials. As a proof of concept, a solution of gold nanoparticles has been dispensed and trapped into acoustic levitator for a pump-probe experiment. Results showed a very good reproducibility (s <1%) and a time independent cumulative damage mechanism, most probably due to the photonic removal of ligand of the gold nanoparticles. In another development, an automated method has been employed to load the levitator using micro-dispensers. By utilizing this dispensing technique, two different solutions, a gold precursor (HAuCl4) and a reducing agent ($NaBH_4$), have been mixed into a single droplet to synthesize gold nanoparticles, and acquired data for real-time characterization of the particles. Preliminary results of this experiment showed successful synthesis of gold nanoparticles in the acoustically levitated droplets. This novel method has the potential for *in-situ* synthesis and dynamic characterization of a wide variety of materials.

B-5
Nanoporous Metals and Nanomaterials Synthesis in Acoustically Produced Microgravity Field

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Although nature is rich in porous materials, nanoporous metals are an exception and their fabrication process is challenging due to the surface energy constraints. The finite-size effect and metallic nature of the nanoporous metals place them at the forefront as potential platforms for many technological applications such as sensing, catalysis, environmental remediation, biotechnology, filtration, protective coatings, energy related devices, energy storage, accelerator components, and next-generation X-ray optics etc.[1-5] Herein, we present a well-established strategy for the preparation of multifunctional nanostructured 3D porous metals based on the combination of inorganic-chemistry and electrochemistry. The fabrication of 3D bicontinuous nanoporous metal structures still represents a real challenge.

An acoustic levitator has been successfully integrated at the Advanced Photon Source for in situ high-energy x-ray induced nanoparticles synthesis and diffraction measurements. In this work, we emphasize innovative containerless (zero-contact) nanoparticles synthesis methods in which extrinsic heterogeneous nucleation issues have been completely omitted through the use of an acoustically produced microgravity field. Application of the developed technique allows very high purity or “phase-pure” nanoparticles to be made.

Acknowledgments
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B-6

Understanding Phosphorous-Based Additives. Density Functional Theory Studies of Additive Interaction at NMC Cathode Surfaces

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Nickel-rich layered oxide cathode materials have seen widespread deployment due to their high gravimetric capacity and high average discharge voltage. However, achieving this high capacity requires charging voltages above the potential at which the electrolytes decompose at the cathode surface (>4.5 V vs. Li/Li+), which leads to impedance rise and capacity loss. One strategy to stabilize this interface is using electrolyte additives that, in small amounts, can change chemical interactions at the interface and affect stability. We present recent Density Functional Theory (DFT) efforts aimed at elucidating the mechanism of reaction of electrolyte molecules on $Li(Ni_{1-x-y}Mn_xCo_y)O_2$ (NMC) surfaces. We determined the first oxidation steps of select alkyl carbonate electrolyte species. We also used Ab Initio Molecular Dynamics (AIMD) to explore possible adsorption configurations of several phosphite and phosphate molecules on the most reactive NMC surfaces; and computed the relative stability of different additives and their derivatives on NMC surfaces. At high states of charge, we found different reactive pathways depending on additive characteristics such as the size of the functional groups in the phosphite molecule and the degree of decomposition of such species. These studies provide some insights into the mechanism of phosphite additive oxidation on the cathode.

B-7

Thermodynamic Properties of HfO_2 Utilizing Reactive Force Fields

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High-k dielectric materials for complementary metal-oxide-semiconductor (CMOS), are of particular importance for creating Dynamic Memory Allocation (DRAM) devices. Many CMOS properties strongly depend on material defects such as vacancies, interstitials, defect clusters that occur during synthesis, and thermal treatment. However, the relentless miniaturization or scaling of the MOS transistor and associated infrastructure on chip create the demand for ever thinner gate oxides than SiO_2. Any SiO_2 replacement must satisfy stringent requirements that include thermodynamic stability in contact with Si, high dielectric constant, *k*, band offsets for electrons and holes > 1 eV, and stability throughout a high-temperature CMOS manufacturing process. Hafnia, HfO_2, satisfies most of the requirements. As such this work focuses on structural properties of different phases of hafnia utilizing recently developed EAM+QEQ (Streitz-Mintmire) potentials. Here we use a combination of molecular dynamics simulations, high-energy x-ray diffraction and neutron diffraction to benchmark the atomic interactions in the high temperature stable liquid and low-density amorphous solid states of hafnia. The diffraction results reveal an average Hf-O coordination number of ~7 exists in both the liquid and amorphous nanoparticle forms studied. The results indicated that density has a strong effect on the polyhedral connectivity.

B-8
Transient Mid-Infrared Spectroscopy Revealing Slow Thermal Equilibration in Hybrid Organic- Inorganic Perovskites

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Hybrid organic-inorganic perovskites (HOIPs) are emerging semiconductors for photovoltaics, solid-state lighting and information processing. In contrast to inorganic semiconductors, HOIPs consist of organic and inorganic sub-lattices (OSL and ISL) presenting disparate atomic masses and bond strengths. The intimate, nanoscopic interpenetration of these components with a lack of strong electronic and vibrational coupling presents challenges to the understanding of charge and heat transport. Here we investigate phonon equilibration processes in HOIPs by transiently probing the mid-infrared vibrational modes of the OSL following above-bandgap excitation. The strong temperature sensitivity of the vibrational modes of the OSL permit direct access to lattice thermalization with tens-of-femtosecond time resolution. We observe inter-sub-lattice thermal equilibration on timescales as slow as hundreds of picoseconds attributable to the sequential phonon populations of the ISL and OSL, respectively. The long-lasting non-equilibrium in HOIPs may appreciably alter the electronic configuration and contribute to a low thermal conductivity.

B-9
Compositional Effect on Al_2O_3 Coatings of Lithium-ion Cathodes

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Surface Al_2O_3 coating has been proved to be an effective and commercial friendly approach to improve the cyclability of cathode materials in Li-ion batteries by preventing chemical and structural evolutions during battery operations. However, there is still a lack of systematic investigations of the cathode compositional effects on the surface alumina coatings. In this work, we used a wet-chemical method to synthesize a series of Al_2O_3-coated $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ (NMC532), $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622), and $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811). Using nuclear magnetic resonance, electron microscopy and high-resolution X-ray diffraction techniques, we have shown that the morphology and chemistry of the coating layers are highly dependent on annealing temperatures and cathode compositions. On all tested NMC particles, higher annealing temperature leads to more homogeneous and more closely attached coating on cathode materials with the formation of $LiAlO_2$ phase. Meanwhile, from NMC532 to 622 and 811, the decreasing Mn content facilitates the diffusion of surface aluminum into the bulk after high-temperature annealing, leading to a transfer from surface coating to bulk dopant, which is confirmed by local Al chemical environment evolution, local lattice distortion and surface morphology change. The initial surface Co segregation observed in pristine NMC particles is also found to have obvious influence to the chemical environment of the diffused aluminum. Density functional theory calculations indicate that the incompatibility between Mn and Al could be the reason of the composition dependence of surface Al intercalation. Finally, we demonstrate that the diffusion of Al into the bulk leads to poor cyclability in electrochemical tests, indicating the importance of the coating-cathode compatibility to the electrochemical performance of coated cathode materials. These results are important in developing a better coating method for the next generation cathode materials of lithium ion batteries.

B-10
A Hybrid Silicon-phosphorene Nanolaser

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Generating and amplifying light in silicon (Si) continues to attract significant attention due to the possibility of integrating optical and electronic components in a single material platform. Unfortunately, silicon is an indirect band gap material and therefore an inefficient emitter of light. With the rise of integrated photonics, the search for a silicon laser has evolved from a scientific quest to a major technological bottleneck for scalable, CMOS-compatible, light sources. Recently, emerging two-dimensional (2D) materials have opened the prospect of tailoring material properties based on atomic layer number. Few-layer phosphorene, which is isolated through exfoliation from black phosphorus (BP), is a great candidate to partner with silicon due to its layer-tunable direct band gap in the infrared where silicon is transparent. Here we demonstrate a hybrid silicon nanolaser composed of a few-layer phosphorene film coupled to a silicon photonic crystal (PhC) cavity resonator. The few nanometer BP emitter layer allows this hybrid system to behave as a single material as seen by the optical field. We obtain single-mode lasing in the main telecommunications band of 1.55 μm (Eg = 0.8 eV) under continuous wave (CW) optical excitation at room temperature. The solution-processed BP film, comprised of many BP flakes, enables the demonstration of lasing across a broad range of emission wavelengths. Our work highlights the versatility of the Si-BP material platform for creating novel, optically-active devices in integrated silicon chips.

B-11
Analyzing Large Radar Datasets Using Python

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Global climate model (GCM) developers looking to improve parameterizations in climate models need large observational data from instruments such as radars, wind profilers, and aircraft. Observations from a large variety of cases in a wide variety of meteorological conditions provides the best dataset for developing climatologies to guide GCM parameterization. In this study, the use of Python to analyze many terabytes of radar data on Argonne National Laboratory's Bebop and U.S. Department of Energy (DOE) Atmospheric Radiation Measurement (ARM)'s Stratus supercomputer is demonstrated. In particular, the Python ARM Radar Toolkit, Python software useful for the gridding, processing, and plotting of radar files, is adapted to process thousands of scans in parallel using various distributed computing frameworks. Various distributed computing frameworks such as Dask, IPython clusters, PySpark, and joblib are explored with the advantage and disadvantages of each shown. In particular, the performance of standard radar data analysis techniques such as phase processing, gridding, deriving quasi-vertical profiles, plotting, and calculating statistical coverage across the differing distributed computing frameworks for different radar systems will be shown. Early results indicate that multiple months of radar data can be processed on a small scale (1000+ cores) cluster in order of 10 minutes.

B-12
In Situ Coherent X-ray Scattering Studies during thin film growth of GaN

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High-energy x-rays provide a powerful tool for in-situ time-resolved studies of materials processes such as epitaxial film growth. Their penetrating nature allows observations inside growth chambers under actual process conditions, and their short wavelength provides sensitivity to atomic-scale structure. With the continued increase in coherent flux to be delivered by advanced synchrotron radiation facilities, coherent x-ray techniques promise to provide new insight into materials synthesis. The fluctuations observed by x-ray photo correlation spectroscopy (XPCS) can elucidate atomic dynamics in these systems more clearly than average quantities obtained from scattering with incoherent beams. These methods can reveal the atomic rearrangements underlying crystal growth mechanisms such as step motion, island nucleation, step-edge barriers, and surface transport.

We have developed a new instrument [1] that exploits this ongoing revolution in synchrotron sources, optics, and detectors to enable in situ studies of Organometallic Vapor Phase Epitaxy (OMVPE) growth of III-nitride materials using coherent x-ray methods. The system includes: high resolution positioning of the sample and detector; an x-ray transparent chamber wall for incident and diffracted beam access over a wide angular range; and a sample mount with minimal thermal motion, giving the sub-micron positional stability and reproducibility needed for coherent x-ray studies. To provide fundamental understanding of OMVPE processes, the instrument enables surface x-ray photon correlation spectroscopy, microbeam diffraction, and coherent diffraction imaging of atomic-scale surface and film structure and dynamics during growth.

We present examples from our initial studies of surface coherent x-ray scattering during OMVPE of GaN. We will show simulations and initial measurements of speckle dynamics in coherent scattering during layer-by-layer growth. We observe that the arrangement of the islands that nucleate and coalesce to form each crystal layer shows a strong correlation from layer to layer.
Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering.

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B-13
Modeling the Fast Orbit Feedback Control System for APS Upgrade

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The expected beam sizes for APS Upgrade are in the order of 4 microns for both planes. Orbit stabilization to 10% of the beam size with such small cross-sections requires pushing the state of the art in fast orbit feedback control, both in the spatial domain and in dynamical performance; the latter being the subject of this paper. In this paper, we begin to study possible performance benefits of moving beyond the classic PID regulator to more sophisticated methods in control theory that take advantage of a-priori knowledge of orbit motion spectra and system non-linearities. A reliable model is required for this process. Before developing a predictive model for the APS Upgrade, the system identification methodology is tested and validated against the present APS storage ring. This paper presents the system identification process, measurement results, and discusses model validation.

B-14
Improving Turbulent Combustion Simulations Using Artificial Neural Networks

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Tabulation of chemistry has shown to drastically reduce computational costs of high fidelity simulations and are being used to design reciprocating and jet engines. Multidimensional chemistry manifolds in CFD are however limited in dimensionality due to memory and computational speed constraints. This is also known as the “curse of dimensionality”. This work demonstrates development of Artificial Neural Networks for advancing the state-of-art in turbulent combustion modeling. This generic approach is shown to significantly reduce the memory footprint of the CFD code and push towards higher dimensional manifolds with significantly lower memory usage. The approach is validated against constant volume spray experiments as well as engine simulations with detailed chemistry mechanisms. These approaches now enable the use of detailed chemistry mechanisms with 3000+ species in the simulation and development of future low temperature combustion engines. The work shows the overall efficacy and capabilities of machine learning algorithms to reduce multidimensional data sets without losing accuracy.

B-15
Intergranular Cracking as a Major Cause of Long-Term Capacity Fading of Layered Cathodes

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Layered lithium transition metal oxides are promising high-capacity cathode materials for Li-ion batteries. However, capacity fading has restricted the practical capacity to less than 70% of the theoretical capacity. Higher initial capacity can be achieved by charging to a higher voltage, yet this initial gain in capacity is quickly offset by the rapid fade in capacity. Understanding the capacity fading mechanism will help develop strategies to mitigate this problem. We used operando X-ray powder diffraction to follow the reactions of the layered $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ over extended charge-discharge cycles at a slow current rate. The operando result shows that the capacity loss can be explained by the heterogeneity developed in the electrode after extended charge-discharge cycles.

B-16
Modeling the Influence of Nozzle-Generated Turbulence on Diesel Sprays

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The central aim of this work is to improve the physical representation of spray breakup physics within today's engine simulation packages. A new experimental methodology, called the scattering absorption measurement ratio technique, was developed and applied in a high-pressure spray chamber to characterize the average size of droplets formed from the spray breakup process. Comparison between predicted and measured drop size distributions revealed for the first time that a spray atomization model, premised on aerodynamic wave growth theory, could capture the experimentally measured spray structure under conventional diesel engine conditions. However, under environments relevant for advanced timing strategies, it was found that turbulence generated inside the nozzle likely enhances the primary breakup process. Although several turbulence-induced breakup models have been proposed in the literature, the assumed integral scaling was found to be inconsistent with the experimental droplet sizing measurements. However, empirical correlations describing droplets formed from eddies within the inertial sub-range of the turbulence spectrum were better able to capture the measured sensitivities in droplet size to changes in ambient and injection conditions. These findings informed recommendations for an improved hybrid spray breakup model, capable of representing both aerodynamic and

turbulent breakup mechanisms in the atomization of non-cavitating diesel sprays.

B-17
De novo synthesis of phosphorylated tri-block copolymers with pathogen virulence suppressing properties that prevent infection-related mortality

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Phosphate is a key and universal "cue" in response to which bacteria either enhance their virulence when local phosphate is scarce, or downregulate it when phosphate is adundant. Phosphate becomes depleted in the mammalian gut following physiologic stress and serves as a major trigger for colonizing bacteria to express virulence. In the present study, we describe *de novo* synthesis of phosphorylated polyethylene glycol compounds with three defined ABA (hydrophilic/-phobic/-philic) structures ABA-PEG20k-Pi20 and linear polymer PEG20k-Pi20 absent of hydrophobic block. 20k demonstrate the molecular weight of Poly (ethylene glycol) block, while Pi20 represent the repeating units of phosphate. Polymers were tested for their efficacy against *Pseudomonas aeruginosa* virulence *in vitro* and *in vivo*. Results indicate that all phosphorylated polymers suppressed phosphate sensing, virulence expression and lethality in *P. aeruginosa.* Among all the phosphorylated polymers, ABA-PEG20k-Pi20 displayed the greatest degree of protection against *P. aeruginosa*. From the results of PEG20k-Pi20 in which the hydrophobic core is absent, it's verified that the hypdrophoic core of ABA-PEG20k-Pi20 is a key structure in its protective effect against *P. aeruingosa*, in part, due to its ability to coat the surface of bacteria. Taken together, synthesis of novel polymers with defined structures and levels of phosphorylation may elucidate their anti-virulence action against clinically important and lethal pathogens such as *P. aeruginosa*.

B-18
Age Dating of Sr-90 Source Material

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While the consequences of an attack utilizing a radiation dispersal device (RDD) would not be nearly as severe as those associated with an Improvised Nuclear Device (IND), the likelihood of an RDD attack by a terrorist organization is much higher. Because of this, there has been an effort to develop methods for age-dating radiological sealed sources in recent years. The work presented includes the investigation of a new separation scheme that utilizes a less costly extraction chromatographic resin than what has been used previously and results in the isolation of Sr-90's stable granddaughter, Zr-90. This allows the strontium quantification to be done radiometrically while the zirconium quantification can be done on any conventional ICP-MS. Using a combination of radiometric and conventional analyses allows for the parallel analysis of samples, increasing throughput in an emergency.

B-19
From Nanodisk to the Universe

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The idea of nanotechnology was introduced more than half of a century ago. Since then, it has been changing people's lives daily, from medicine products to electronic devices. Same for scientific research, with advancing nanofabrication and characterization techniques, researchers are now able to access, analysis and manipulate

objects that were inaccessible before. In this work, three projects with different fabrication techniques implemented will be discussed. Firstly, the investigation of static and dynamic properties of magnetic nanodisks[1] and nanowires[2] prepared by Electron-beam lithography (EBL) will be discussed. Thanks for the highest pattern resolution provided by EBL, new magnetic phenomenon were observed due to the nanoscale geometry effects. Secondly, the fabrication process based on deep ultraviolet (DUV) lithography technique will be discussed.[3] DUV lithography provides opportunities to prepare nanostructures over a relatively large area with a faster processing speed compared to the EBL process. Last but not least, we will discuss the fabrication process and performance of large array of superconducting transition edge sensor detectors, which are fabricated for the latest generation cosmic microwave background experiment on the South Pole Telescope (SPT-3G).[4] These detector arrays were deployed to the South Pole at the end of 2016.

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B-20
A Novel Combustion Modeling Approach to Predict Engine Knock

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In the present work, a numerical approach was developed based on multidimensional computational fluid dynamics (CFD) to predict knocking combustion. The G-equation model was employed to track the propagation of the turbulent flame front and a multi- zone model based on temperature and equivalence ratio was used to capture auto-ignition in the end-gas ahead of the flame front. Moreover, a novel methodology was developed wherein a lookup table generated from a chemical kinetic mechanism could be employed to provide laminar flame speed as an input to the G-equation model, instead of using empirical correlations. To incorporate fuel chemistry effects accurately and lower the computational cost, a compact 165-species skeletal mechanism for four-component gasoline surrogates was developed. The engine CFD model was employed to perform numerical simulations under RON and MON conditions for different PRFs in a CFR engine. The skeletal mechanism was used to generate the lookup tables for laminar flame speed as a function of pressure, temperature and equivalence ratio. Parametric tests were conducted at different compression ratios and the predicted values of compression ratio at knock onset, delineating the boundary between “no knock” and “knock”, were found to be in good agreement with the available experimental data.

B-21
Combining Computer Simulations and Machine Learning for Accelerating Materials Design

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Machine learning tools have been progressively adopted by the materials science community to accelerate design of materials with targeted properties. However, in the search for new materials exhibiting properties and performance beyond that previously achieved, machine learning approaches are frequently limited by two major shortcomings. First, they are intrinsically interpolative. They are therefore better suited to the optimization of properties within the known range of accessible behavior than to the discovery of new materials with extremal behavior. Second, they require the availability of large datasets, which in some fields are not available and would be prohibitively expensive to produce. Here we describe a new strategy for combining genetic algorithms, neural

networks and other machine learning tools, and computer simulation to discover materials with extremal properties in the absence of pre-existing data. Predictions from progressively constructed machine learning tools are employed to bias the evolution of a genetic algorithm, with fitness evaluations performed via direct molecular dynamics simulation. We survey several materials design problems ranging from polymers to 2D inorganic materials with this framework.

B-22
A Shock Tube Study on the Thermal Decomposition of Organic Nitrites and Their Use as Radical Precursors

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Combustion accounts for over 80% of the world's energy supply, and therefore, understanding combustion systems is key in the pursuit to meet the world's energy demand and efficiency needs. Radical chemistry largely determines the reactivity and combustion properties of these systems. The study presented here focuses on the thermal decomposition of organic nitrites (R-ONO) as a class of molecules that can serve as convenient sources of radicals in combustion experiments because of the relative weakness of the RO-NO bond. The experimental investigations reported here were performed in a diaphragmless shock tube using laser schlieren densitometry in the temperature range of approximately 700-1000 K at pressures between 60-260 Torr. Each of the nitrites dissociates to form an alkoxy radical (RO) and NO, and the alkoxy radicals then rapidly dissociate to form an alkyl radical and formaldehyde. Throughout the modeling effort, particular attention was given to reactions involving alkyl radicals, which are ubiquitous in combustion systems, such as dissociation, combination, and disproportionation reactions. Nitrites may be used as a source of alkyl radicals to study crucial $R+O_2$ chemistry in temperature and pressure regimes where experimental data is currently lacking.

B-23
Unique Anion Hydration Is Coupled To Unexpected Anion Adsorption Behavior At A Soft Charged Interface

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The molecular-scale behavior of ions at aqueous charged interfaces is coupled with their hydration, and is fundamentally important to many macroscopic phenomena including: protein solvation, the movement of soil contaminants, electrochemical energy storage, and chemical separations. These phenomena are often driven by specific-ion-effects – the distinct behavior of ions at an interface. Here, we study the adsorption of $PtCl_6^{2-}$ at a positively charged Langmuir monolayer. Surface-sensitive x-ray techniques show that $PtCl_6^{2-}$ adsorbs in a diffuse layer at low bulk concentrations, and in the Stern layer at higher bulk concentrations. This is surprising because ions with a strong surface affinity, like $PtCl_6^{2-}$, are expected to adsorb in the Stern layer until the surface is passivated, then adsorb in the diffuse layer. Sum frequency generation – a surface-sensitive vibrational spectroscopy – shows that $PtCl_6^{2-}$ partially retains its hydration sphere after adsorption in the Stern layer. The unique interfacial hydration of $PtCl_6^{2-}$ is likely responsible for its unexpected adsorption behavior. This study provides important clues to solving the mystery of specific ion effects, and gaining a molecular-level understanding of solvent extractions.

B-24
Computer Vision for Image Matching in Electron Microscopy

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The knowledge of atomistic structure is paramount for understanding a variety of chemical and physical processes. Recent improvements in image acquisition and detection hardware have contributed to more reliable imaging at the atomic level, however, with imperfections such as vacancies or dislocations present in real materials systems, the contrast and resolution of the information available through direct imaging is often degraded or obscured. Image simulation is used to facilitate a better understanding of the image in these instances, but the standard workflow is typically manual and requires considerable expert discretion when identifying and interpreting the individual features. We have developed a framework, inspired by techniques from Computer Vision (CV), that uses a flexible representation for atomic resolution microscopy images to (1) partition the images into regions sharing similar column intensities and neighboring distances, as well as to (2) assess similarity between images in the presence of various geometric transformations, structural defects, and imaging noise. With this framework, automation can be used to not only to improve existing structure optimization techniques, but also to facilitate an accurate comparison between images obtained across different experimental and computational studies.

B-25
Large-eddy Simulations of Airflow Dynamics and Physics over the Island of Graciosa

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Three-dimensional numerical experiments are performed to explore the mechanical and thermal impacts of Graciosa Island on the sampling of oceanic airflow and cloud evolution. Ideal and real configurations of flow and terrain are planned using high-resolution, large-eddy resolving (e.g., $\Delta < 100$ meter) simulations. Ideal configurations include model initializations with ideal temperature and wind profiles to capture flow features over an island-like topography. Real configurations will use observations from different climatological background states over the Eastern Northern Atlantic, Atmospheric Radiation Measurement (ENA-ARM) site on Graciosa Island. Initial small-domain large-eddy simulations of dry airflow produce cold-pool formation upstream and von Kármán like vortices propagation downstream. Although the peak height of Graciosa is less than half kilometer, the Azores island chain has a mountain over 2 km, which may be leading to more complex flow patterns. Preliminary idealized moist simulations indicate that the cloud field is impacted due to the presence of the island. Further numerical experiments are planned to extend moist simulations to include realistic atmospheric profiles and observations of surface fluxes coupled with radiative effects. This work is intended to produce a useful simulation framework coupled with instruments to guide airborne and ground sampling strategies during the ACE-ENA campaign.

B-26
Three-dimensional Numerical Flow Modeling for Estimation of Local Scour

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Scour is the erosion of a stream-bed due to hydrodynamic forces. Local scour occurs around objects placed in the path of flow, such as bridge piers and abutments. In order to predict local scour, a three-dimensional stream-bed scour modeling methodology is being developed using commercial Computational Fluid Dynamics (CFD) software to compute sediment transport and an in-house morphodynamics code to compute displacements of the

bed and sand slides.

A multiphase Eulerian hydrodynamic model solves the flow field using Reynolds Averaged Navier-Stokes (RANS) equations with the high Reynolds number k– epsilon turbulence model using the commercial CFD software STAR-CCM+. The hydrodynamic model also solves for sediment transport (bed load and suspended sediment transport) and computes sediment entrainment and deposition rates. The morphodynamics Python script computes bed displacements from the entrainment and deposition rate distribution and morphs the bed. A sand slide model for non-cohesive sediment is also included in morphodynamics Python script to keep scour holes from becoming too steep. Simulations were performed for different flow conditions and for mean sediment diameters (0.25 mm to 4mm). The model agrees reasonably well with limited experimental data for equilibrium scour shape and size.

B-27
Anatomy of Low Voltage Switching in Cationic Filamentary Devices

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To date various combination of material stacks have been used to demonstrate resistive switching phenomenon in Metal-Insulator-Metal structures by formation of nanometer scale cationic filaments. We present a predictive framework based on materials parameters that establishes a comprehensive criterion for electrode metal selection useful for conductive-bridge resistive switching devices. Based on this criterion, we demonstrate experimentally, for the first time, threshold switching and memory switching using all C-MOS compatible materials with $Sn|HfO_2|Pt$ cross bar arrays. Sn, being isovalent with Si, offers greater advantage of designing a Si C-MOS compatible memory or selector switch for 3D crosspoint memory applications. Furthermore, we explain the conductive-bridge formation using various anode metals (Cu, Ag and Sn) by studying the time evolution of the cationic filament formation experimentally, based on time domain measurements (I vs. t) carried out under constant voltage stress and theoretically, by molecular dynamics simulations. The framework we developed for electrode metal selection and the methods demonstrated to understand the time evolution of filament formation here can easily be extended to variety of anode metals and will enable researchers in the field in designing low power electronic switches and neuromorphic systems using filamentary devices.

B-28
Nonthermal hot electron generation and relaxation in plasmonic metasurfaces

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Upon photoexcitation in plasmonic metallic nanostructures, surface plasmons rapidly decay to produce hot electrons near the metal's surface. These charge carriers can initially possess a nonthermal energy distribution that subsequently thermalizes through electron-electron scattering. Using a metasurface of substrate-coupled silver nanocubes in a nanopatch antenna geometry, we demonstrate the enhanced generation of nonthermal hot

electrons through both modeling and experiment. Due to the optical field hot spots within the gap of the antennas and their low plasmon resonance frequencies, nonthermal electrons with energies up to the photon energy are created through quantum optical transitions with non-conservation of linear momentum. Using ultrafast transient absorption spectroscopy, we then resolve the spectral and temporal response of nonthermal carriers on the femtosecond timescale. Due to the perturbation of multiple plasmonic modes and interband transitions within the metasurface, we are able to probe the optical response over 1000 nm from the ultraviolet to near-infrared. We find evidence for three distinct subpopulations of nonthermal carriers with distinct spectral and kinetic signatures. We propose these arise from anisotropic electron-electron scattering within the band structure of the metal.

B-29

Numerical Evaluation Of Shot-To-Shot Variability In A Heavy-Duty Diesel Injector Using Real Nozzle Geometry

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Cyclic variability in internal combustion engines arises from multiple concurrent sources, of which many are still to be fully understood and controlled. This variability can, in turn, affect the behavior of the engine resulting in undesirable deviations from the expected operating conditions and performance. Shot-to-shot variation during the fuel injection process may be a source of cyclic variability. This study focuses on shot-to-shot variability of the motion of the injector needle and its influence on the internal nozzle flow behavior using diesel fuel. Previous numerical studies from our group have shown that the in-nozzle flow is sensitive to fuel properties as well as to the needle lift and off-axis motion. This was shown to result in systematic orifice-to-orifice variability. X-ray imaging techniques have been used to extract high-resolution injector geometry images that include the sac, orifices, and needle tip, and the true dynamics of the needle in motion. These measurements showed high repeatability in the needle lift profile across multiple injection events, while the radial displacement was characterized by a much higher degree of randomness. A robust and previously validated computational setup has been adapted for the current 8-hole heavy duty common-rail diesel injector. The simulation results obtained using the x-ray scanned geometry have been validated against the available experimental data. The average off-axis motion has been perturbed (based on the variability found in the experimental measurements) to generate three new cases that present different amplitude and phasing of the radial displacement with respect to the baseline average motion. This revealed the effects of off-axis motion on shot-to-shot and orifice- to-orifice variations.

B-30

DES & Planck survey: Galaxy group-tSZ cross correlation

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Stacking Sunyaev-Zeldovich map of groups and clusters is a powerful tool to find average distribution of hot gas in these systems. The goals of this work are to estimate the redshift evolution of SZ signal and average bias weighted electron pressure of the universe. We stack SZ signal from Planck at all the detected redmapper groups from year 1 Dark Energy Survey data. We use groups at different redshift and mass to find the average pressure profile of these systems. We show that the detected signal can be modeled by a halo model using Battaglia pressure profile.

B-31
Direct Injection Spark Ignition (DISI) Engine Simulation for knock prediction

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Further improvement in thermal efficiency of SI engine is limited by engine knock. A predictive model is required to better understand knock phenomenon and co-optimize fuel properties and engine design to extend Knock-Limit-Spark-Advance (KLSA) and improve engine efficiency. In this work, a DISI engine is modeled using CFD software, Converge. A level-set approach is used to capture the turbulent flame front propagation and a well-stirred-reactor approach is applied to predict end-gas heat release and auto-ignition. The model is validated extensively with experimental data under knock-free conditions. Knocking case can be captured with advanced spark timing in simulation, by examining amplitude in pressure oscillation using a small Mach Courant-Friedrichs-Lewy (CFL) number. Alternatively, a knocking case can also be determined by examining the amount of end-gas heat release, which is less computational expensive and is able to achieve faster turnaround time.

B-32
Reduced Electron Exposure for Microscopy and Spectroscopy using Dynamic Sampling and Machine Learning

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Analytical electron microscopy and spectroscopy of biological specimens, polymers, and other beam sensitive materials has been a challenging area due to irradiation damage. There is a pressing need to develop novel imaging and spectroscopic imaging methods that will minimize such sample damage as well as reduce the data acquisition time. The latter is useful for high-throughput analysis of materials structure and chemistry. In this work, we present a novel machine learning based method for dynamic sparse sampling of EDS data using a scanning electron microscope. Our method, based on the supervised learning approach for dynamic sampling algorithm and neural networks based classification of EDS data, allows a dramatic reduction in the total sampling of up to 90%, while maintaining the fidelity of the reconstructed elemental maps and spectroscopic data. We believe this approach will enable imaging and elemental mapping of materials that would otherwise be inaccessible to these analysis techniques.

B-33
Reaction Heterogeneity in $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ Induced by Surface Layer

Antonin Grenier[1], Hao Liu[1], Kamila M. Wiaderek[1], Zachary W. Lebens-Higgins[2], Olaf J. Borkiewicz[1], Louis F. J. Piper[2], Peter J. Chupas[3], Karena W. Chapman[1]

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Using in-situ synchrotron X-ray diffraction (XRD) measurements, we show that commercially relevant $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) cathode intrinsically behaves as a solid solution upon lithium (de)insertion.[1] The occurrence of a so-called "two-phase" behavior, previously reported in the literature,[2] is not intrinsic to the material but is due to increased amounts of surface species. Analyses of the surface by X-ray photoelectron and diffuse reflectance infrared Fourier transform spectroscopies show that the layer is mainly composed of Li_2CO_3. The presence of such surface species is not only deleterious to the electrochemical performance of the battery, but it also induces a bi-modal phase distribution of NCA particles that may be misinterpreted as a two-phase

behavior.

References:
(1) Grenier, A.; Liu, H.; Wiaderek, K. M.; Lebens-Higgins, Z. W.; Borkiewicz, O. J.; Piper, L. F. J.; Chupas, P. J.; Chapman, K. W. Reaction Heterogeneity in $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ Induced by Surface Layer. *Chem. Mater.* **2017**, *29*, 7345–7352.
(2) Robert, R.; Bunzli, C.; Berg, E. J.; Novák, P. Activation Mechanism of $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$: Surface and Bulk Operando Electrochemical, Differential Electrochemical Mass Spectrometry, and X-Ray Diffraction Analyses. *Chem. Mater.* **2015**, *27*, 526–536.

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