Argonne NATIONAL LABORATORY

NOVEMBER 7, 2019

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Argonne National Laboratory Postdoctoral Research and Career Symposium

November 7th, 2019

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2019 Postdoctoral Research and Career Symposium
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2019 Postdoctoral Research and Career Symposium

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Agenda

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

MORNING SESSION

9:00 AM — Welcome Remarks from Kimberly Conroy Sawyer, Deputy Laboratory Director for Operations/Chief Operations Officer

9:15 AM — Keynote Address by Valerie Taylor, Argonne Distinguished Fellow, Director of the Mathematics and Computer Science Division, Argonne National Laboratory

10:00 AM — Poster Session A and Free Networking

NETWORKING LUNCH

11:30 AM — Organized Networking Lunch with Company Representatives and Career Mentors

AFTERNOON SESSION

1:30 PM — Poster Session B and Free Networking

3:00 PM — Career Panel Discussion–Alumni from diverse career paths

- Prasanna Balaprakash, Computer Scientist, Argonne National Laboratory
- Dolly Batra, RD&E Group Leader, Polymer Research, Nalco Water-an Ecolab Company
- Chad Husko, Founder and CEO, Iris Light Technologies, Inc.
- Casey Larsen, Assistant Professor of Chemistry, Benedictine University
- Jonnathan Medina Ramos, Staff Scientist, Flinn Scientific

4:30 PM — Presentation of Poster Awards and Closing Remarks from Stephen K. Streiffer Interim Deputy Laboratory Director for Science, Associate Laboratory Director, Photon Sciences, and Director of the APS

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2019 Keynote Address
Career Paths: Curves, Hills, and Turns

Dr. Valerie E. Taylor, Director of the Mathematics and Computer Science Division and Argonne Distinguished Fellow, Argonne National Laboratory

Dr. Taylor held multiple leadership roles at Texas A&M University, prior to joining Argonne. Most recently, she served as the senior associate dean of academic affairs in the College of Engineering, a Regents Professor and the Royce E. Wisenbaker Professor in the Department of Computer Science and Engineering. Prior to that, she served as head of Computer Science and Engineering from 2003 to 2011. Before she joined Texas A&M, Dr. Taylor was a faculty member in Northwestern University's Electrical Engineering and Computer Science Department for eleven years.

Dr. Taylor has authored or coauthored more than 100 papers on high performance computing. She has developed and used models to analyze and improve the performance of many parallel, scientific applications, including finite element applications, molecular dynamics, cosmology, earthquake simulations, ocean modeling, and magnetic fusion.

Dr. Taylor is a fellow of the Institute of Electrical and Electronics Engineers (IEEE) and of the Association for Computer Machinery (ACM). She has received numerous awards for distinguished research and leadership, including the 2001 IEEE Harriet B. Rigas Award for significant contributions in engineering education; the 2002 Outstanding Young Engineering Alumni Award from the University of California at Berkeley; the 2002 A. Nico Habermann Award for increasing diversity in computing; and the 2005 Tapia Achievement Award for Scientific Scholarship, Civic Science, and Diversifying Computing. Dr. Taylor is also the executive director of the Center for Minorities and People with Disabilities in Information Technology (CMD-IT).

Dr. Taylor earned her bachelor's degree in electrical and computer engineering and master's degree in computer engineering from Purdue University in 1985 and 1986, respectively. She received her PhD in electrical engineering and computer science from the University of California at Berkeley in 1991.

Welcome Remarks Speaker

Kimberly Conroy Sawyer, Deputy Laboratory Director for Operations/Chief Operations Officer at Argonne National Laboratory

Kim Sawyer is responsible for leading and driving the strategies and actions to achieve efficient, effective, and safe operations at Argonne. Leveraging her extensive experience within the national laboratories, the Department of Energy, and the private sector, Kim works with leaders across the laboratory to continuously improve the services that support Argonne's world-changing science, technology, and engineering.

Sawyer has more than 35 years of experience working with national laboratories, the private sector, government agencies, and their associated governing boards. She served as the Deputy Laboratory Director and Executive Vice President for Mission Support at Sandia National Laboratories for more than six years. In this role, she developed a strategy to focus the organization to achieve operational excellence, built an integrated team, and established the organizational structure and project management to deliver exceptional results and high employee morale. Prior to Sandia, Sawyer spent nearly 10 years in successive operations, engineering, and computing leadership roles at Lockheed Martin in a variety of divisions and locations.

Sawyer holds a master's degree in mathematics and computing from the University of Massachusetts Lowell and a bachelor's degree in business administration from Robert Morris University

Closing Remarks Speaker

Stephen K. Streiffer, Interim Deputy Laboratory Director for Science, Associate Laboratory Director, Photon Sciences, and Director of the Advanced Photon Source

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

The APS is the brightest source of high-energy X-rays in the Western Hemisphere and is used to study the structures of materials and processes at the atomic scale. It is also the largest scientific user facility in the North America, with more than 3,500 users visiting each year.

He has also served as interim director of Argonne's Center for Nanoscale Materials, a national user facility that provides capabilities explicitly tailored to the creation and characterization of new functional materials on the nanoscale. The center's portfolio includes research on electronic and magnetic

materials and devices, nanobio interfaces, nanofabrication, nanophotonics, theory and modeling, and X-ray microscopy.

Dr. Streiffer's scientific expertise is in nanostructured complex oxides and in structural characterization of materials particularly using transmission electron microscopy and X-ray scattering techniques.

Overarching themes in his research program include the development of novel concepts for integration of oxide heterostructures, establishing a fundamental understanding of polar interfaces, and exploring how these interfaces may be manipulated to influence electronic and chemical function.

His active research projects focus on utilizing in-situ synchrotron X-ray methods to probe chemical vapor deposition of complex oxides as well as phase transformations and nanoscale size effects in ferroic thin films. He is also currently involved in in-situ synchrotron X-ray studies of the synthesis of InGaN heterostructures as part of an effort to expand the basic understanding of materials for energy-efficient solid state lighting. He has authored or co-authored more than 150 scientific publications and holds one patent.

Career Panelists

Dr. Prasanna Balaprakash, Computer Scientist, Argonne National Laboratory

Prasanna Balaprakash is a computer scientist with a joint appointment in the Mathematics and Computer Science Division and the Leadership Computing Facility at Argonne National Laboratory. His research interests span the areas of artificial intelligence, machine learning, and high-performance computing. He is a recipient of the U.S. Department of Energy 2018 Early Career Award. He was a postdoc in the Mathematics and Computer Science Division from 2010 to 2013. Prior to Argonne, he worked as a Chief Technology Officer at Mentis Sprl, a machine learning startup in Brussels, Belgium. He received his PhD from CoDE-IRIDIA (AI Lab), Université Libre de Bruxelles, Brussels, Belgium, where he was a recipient of Marie Curie and F.R.S-FNRS Aspirant fellowships.

Dr. Dolly Batra, RD&E Group Leader, Polymer Research, Nalco Water – An Ecolab Company

Dr. Dolly Batra is a Group Leader in the Polymer Research group at Nalco Water, an Ecolab company. She is an organic and polymer chemist with extensive experience in the design and synthesis of polymeric materials, nanocomposites and small molecules. Dr. Batra joined Nalco in 2014 as a Staff Scientist. She currently leads the development of water-soluble polymers for applications in various industries, including Paper, Energy and Wastewater. Before joining Nalco, she held various research positions at Amcol International in Hoffman Estates, and at TIAX LLC, a nanotechnology company in Boston. She was a Distinguished Post-Doctoral Fellow at the Center for Nanoscale Materials (CNM) at Argonne National Lab until 2006. At the CNM, Dr. Batra synthesized and developed various biocompatible, nanostructured polymers. Dr. Batra completed her graduate work in organic and polymer chemistry under the direction of Prof. Ken Shea at the University of California, Irvine (UCI). She conducted research in the development of molecularly imprinted polymers (MIPs) for the selective recognition of biomolecules. She received her Bachelors of Science in Biochemistry from the University of Delaware. Dr. Batra is the author of several patents and publications in the field of organic and polymer chemistry and has presented at various conferences and meetings around the country.

Dr. Chad Husko, Founder and CEO, Iris Light Technologies

Chad is a scientist turned entrepreneur, and the Founder/CEO of Iris Light Technologies, Inc. The Iris mission is to solve 'the silicon laser problem' holding back the rapidly growing silicon photonics (light chip) industry. Iris's laser technology enables applications in optical communications in data centers, sensors, and biophotonics. Iris is supported by the Chain Reaction Innovations program based at Argonne National Lab.

At Iris, Chad incorporates international experience from a wide variety of environments and cultures ranging from universities, government labs, and industrial companies in the USA, Australia, and the Netherlands. While a Fulbright Scholar, he was a researcher in the industrial R&D lab of Thales in Paris, France. In these roles, Chad has successfully built teams, raised over $1M in funding, and managed programs resulting in 30+ publications, 4 patents, and presentations to diverse audiences ranging from business professionals to technical professionals to grade schools.

Chad actively promotes the optics and photonics industries through professional service and public outreach. His recent contributions include serving in the inaugural class of Optical Society (OSA) 'Ambassadors' in 2016, as chair of several OSA award committees, and the Traveling Lecturer program. In 2017, he was selected as an OSA Senior Member in recognition of his professional contributions.

Chad holds a Ph.D. and M.S. in Applied Physics from Columbia University (New York, USA), and B.S. degrees in Physics and Mathematics from Loyola University Chicago. Chad's love of languages led him to complete an M.A. and B.A. in Spanish from New York University and Loyola alongside his technical studies.

When he's not wearing the many hats of a start-up CEO, Chad can be found sailing Lake Michigan.

Dr. 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, when not playing with her 11 month old son Brody, Casey enjoys cooking and experimenting with food… which is really just doing chemistry in the kitchen!

Dr. Jonnathan Medina Ramos, Staff Scientist, Flinn Scientific

Jonnathan Medina Ramos, PhD, is a staff scientist at Flinn Scientific, developing content and educational products for K-12 and college level physical sciences. Prior to joining Flinn, Jonnathan was a postdoctoral researcher at Argonne National Laboratory, and a volunteer for Argonne's Education Outreach programs. Jonnathan holds a Bachelor of Science in chemistry (Universidad del Valle, Colombia), and a PhD in Chemistry from Virginia Commonwealth University (Richmond, VA). During his PhD and postdoctoral training (University of Delaware and Argonne National Laboratory), Jonnathan served as a teaching assistant and a mentor to several generations of students. As a researcher, Jonnathan has authored and co-authored scientific articles published in peer-reviewed journals, and became a co-inventor in two US Patents.

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Poster Abstracts – Session A

BIOLOGY

A-1

Information and Communication-Centric Molecular Communication in Biological Cells

Zhameeth Sakkaff[1], Christopher Henry[2], and Massimiliano Pierobon[1]

[1]Department of Computer Science and Engineering University of Nebraska - Lincoln, NE, USA
[2]Data Science and Learning Division, Argonne National Laboratory (ANL), Argonne, IL, USA

Biological cells have the ability to sense and communicate information with each other and the environment through the exchange of molecules and chemical reactions. Understanding the way this information propagates in single or multiple cells is important since their behavior has an impact on human health, our environment, food, and its engineered control would enable game-changing application. At the basis of these communications, the paradigm of Molecular Communication (MC) stands in the application of information and communication theory to model and analyze information exchange through chemical reactions and molecular transport. The Challenge stands in the application of MC to specific biochemical mechanisms at the basis of biological cells, where these mechanisms are only partially understood, and cell's models do not always address the complexity of molecular processes. A solution stems from the analysis of what is currently known about the major processes to regulate their behavior. The objectives of this presentation are to model and analyze cells' natural communications with unconventional tools, from computer communication theory, and understand the potential of these tools in future applications. First, information propagation in cell signal transduction pathways is modeled to quantify how cells modify their behavior based on the environment. To demonstrate a potential application, this model is used to understand how impairments in this capability can be at the basis of cancer. Second, the impact of the information propagation on cell's behavior is modeled and analyzed on cell metabolism for various input environmental conditions. An application of these research results is shown through the utilization of tools from coding theory to inform the efficient design of wet-lab experiments. For this, a computational tool named Run Flux Mutual Information Analysis (RFMIA) is developed to understand single or inter-species interactions. Last, the aforementioned concepts are extended to address the theoretical modeling of multi-scale integrated biological pathways, which encompass signal transduction, gene regulation, and metabolism, to provide an end-to-end perspective of MC through a biological cell. Overall, this research, which stems from results and technological developments in computer communications, explores novel realms, biology, where these concepts can be applied for innovative applications.

A-2

Interprotein Electron Transfer Biohybrid System for Photocatalytic H_2 Production

Udita Brahmachari, P. Raj Pokkuluri, David M. Tiede, Jens Niklas, Oleg G. Poluektov, Karen L. Mulfort, and Lisa M. Utschig

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

Worldwide there is a large research investment in developing solar fuel systems as clean and sustainable sources of energy. The fundamental mechanisms of natural photosynthesis can provide a source of inspiration for these studies. Photosynthetic reaction center (RC) proteins capture and convert light energy into chemical energy that is ultimately used to drive oxygenic water-splitting and carbon fixation. For the light energy to be used, the RC communicates with other donor/acceptor components via a sophisticated electron transfer scheme that includes electron transfer reactions between soluble and membrane bound proteins. Herein, we reengineer an inherent interprotein electron transfer pathway in a natural photosynthetic system to make it photocatalytic for aqueous H_2 production. The native electron shuttle protein ferredoxin (Fd) is used as a scaffold for binding of a ruthenium photosensitizer and H_2 catalytic function is imparted to its partner protein, ferredoxin $NADP^+$-reductase (FNR), by attachment of cobaloxime molecules. We find that this 2-protein biohybrid system produces H_2 in aqueous solutions via light-induced interprotein electron transfer reactions (TON >2500 H_2/FNR), providing insight about using native protein-protein interactions as a method for fuel generation.

A-3

Quantum Chemistry Informed Machine Learning to Predict Energies of Large Organic Molecules

Naveen Dandu, Logan Ward, Rajeev Assary and Larry Curtiss

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

Accurate prediction of thermochemical properties of large molecules is significantly limited to their size and computational cost. To overcome this limitation, one can make use of machine learning as it provides an opportunity of bypassing the tradeoff between accuracy and computational cost. In this work, we performed machine learning to predict energies of large molecules using delta learning models trained on small organic molecules. For this strategy, we first performed quantum chemistry calculations on a subset of 201 molecules with heteroatoms between 10 and 14, from Pedley dataset that are having reliable experimental enthalpies of formations with small uncertainties. Computed G4MP2 enthalpies of formations of those 201 molecules have an accuracy of 1.46 kcal/mol. Calculations at B3LYP and ω-B97XD levels were also performed to compare their efficiencies. Among these two functional, ω-B97XD shown to be performing better, with smaller deviations. As the next step in our strategy, we trained a subset containing 13,026 molecules (10% of 133k molecules of QM9 dataset), using FCHL delta and SCHNET delta models. With these trained models, we predicted atomization energies of those 201 molecules, whose number of heavy atoms is higher than any of the molecules in trained set, with accuracies to less than 1 kcal/mol. The trained models are published online and one can use these models to predict G4MP2 energies of much larger molecules by providing B3LYP optimized coordinates and B3LYP or ω-B97XD total energy.

A-4

Upcycling Waste Plastics into Value-Added Products

Robert M. Kennedy[1], Gokhan Celik[1], Ryan A. Hackler[1], Magali Ferrandon[1], Akalanka Tennakoon[2,3], Smita Patnaik[2,3], Anne M. LaPointe[4], Salai C. Ammal[5], Andreas Heyden[5], Frédéric A. Perras[2], Marek Pruski[2,3], Susannah L. Scott[6], Kenneth R. Poeppelmeier[7],Aaron D. Sadow[2,3], Massimiliano Delferro[1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, United States
[2]U.S. DOE Ames Laboratory, Ames, Iowa 50011, United States
[3]Department of Chemistry, Iowa State University, Ames, Iowa 50011, United States
[4]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14583, United States
[5]Department of Chemical Engineering, University of South Carolina, Columbia, South Carolina 29208, United States
[6]Department of Chemical Engineering, University of California, Santa Barbara, California 93106, United States
[7]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States

Synthetic polymers are ubiquitous and critical to the function of modern life. However, the ubiquity of polymers has resulted in an enormous and growing amount of polymer waste, which has a long lifetime in the environment and is inefficient to recycle. Polymer waste is both a threat to the environment and economy, and an untapped resource of energy-rich hydrocarbons. If the large macromolecules that make polymers could be chemically transformed or "upcycled" into value-added products, rather than disposed of as waste or downcycled into lower grade plastics, the energy and value put into the polymers could be reclaimed and turned into new applications. Here, we focus on developing efficient and innovative catalytic materials for converting waste polymers into more valuable products in a selective manner –catalytic upcycling. Novel approaches are being explored where the selective catalytic conversion of waste polymers is achieved by designing supported metal catalysts with spatially organized sites. These sites cleave hydrocarbon polymers into relatively uniform fragments through interactions of the polymer macromolecules with the metal catalysts. The production of uniform fragments, rather than a random distribution, is the first step to efficiently converting waste polymers into new high-value hydrocarbon feedstocks.

A-5

Ion-specific clustering of metal-amphiphile complexes in solvent extraction

Srikanth Nayak[1], Kaitlin Lovering[1], and Ahmet Uysal[1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, United States

The efficient separation of heavy elements, including lanthanides and actinides, is an important task for many technological applications. Solvent extraction (SX) is the most common technology used in refining and reprocessing of heavy elements. Understanding, and controlling the mass transport through interfaces is a key challenge in SX. Extractant molecules used in SX are typically amphiphilic, so they alter the interface between the aqueous and organic phases. The precise nature of these interfacial effects on SX, in terms of extraction capacity and selectivity, are not well understood. Generally, heavier lanthanides are extracted better than the lighter lanthanides, which has been attributed to increasing ligand binding as the cation's charge density increases due to the so called lanthanide contraction. However, in some extraction systems middle and lighter lanthanides are extracted better. A particularly interesting case is that of Aliquat 336, a quaternary ammonium extractant. While thiocyanate salt of Aliquat 336 extracts heavier lanthanides, the nitrate salt shows the reverse trend. The molecular-scale origins of this peculiar behavior is not understood. We present results from small angle X-ray scattering experiments on the organic phase obtained from extraction with trioctylmethylammonium (TOMA, a major component of Aliquat 336) nitrate and thiocyanate to understand the mesoscale origins of these trends. Our results show differences in clustering behavior of lanthanide-extractant complexes in nitrate and thiocyanate media. In the case of thiocyanate medium, number of lanthanide-extractant complexes per cluster appears to be

directly correlated with extraction efficiency while in the nitrate medium it varies non-monotonically across the lanthanide series, suggesting different mechanisms dominate in the presence of these two anions. We discuss the implications of these results to our understanding of extractant assisted ion and mass transport at the oil/aqueous interface with an emphasis on transient species that cannot be observed in static experiments.

A-6

Developing Strategies for Computational K-edge XANES Spectroscopy

Prajay Patel,[1] Cong Liu,[1] and Massimiliano Delferro[1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL60439

X-ray Absorption Near-Edge Structure (XANES) spectroscopy has been utilized to determine key features of the local chemical environment such as first and second shell coordination, electronic configuration, and oxidation state of the metal. Due to the high sensitivity of XANES to the oxidation state and local coordination of the metal, vanadium complexes, which exist in a redox equilibrium of three oxidation states and a variety of coordination environments, are of particular interest. Yet to properly interpret experimental XANES spectra, theoretical calculations are often required to portray specific electronic transitions. In this work, XANES spectra are modeled using time-dependent density functional theory (TDDFT) for approximately30 vanadium complexes and several vanadium-silica cages that mimic single-site heterogeneous catalysts. Orbital analysis was done to identify significant contributions to key transitions and to establish qualitative trends within the local chemical environment of vanadium. This analysis provides insight into the development of strategies for understanding the chemical behavior of catalysts.

A-7

Highly Fluorescent Benzothiadiazole Redoxmers and Emission Quenching vs. Electrolyte Salt

Lily A. Robertson[1,2,3],Yuyue Zhao[1,2],Garvit Agarwal[1,2], ZhouYu[1,2], Rajeev S. Assary[1,2], Lei Cheng[1,2], Ravindra B. Weerasooriya[4], Varun Singh[2,4], Ksenija D.Glusac[2,4], Ilya A. Shkrob[1,2], Lu Zhang[1,2], and Jeffrey S. Moore[1,3,5]

[1]Joint Center for Energy Storage Research, Argonne, IL 60439
[2]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439
[3]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801
[4]Department of Chemistry, University of Illinois at Chicago, Chicago, IL 60607
[5]Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL 61801

The success of redox-active organic molecules for flow battery technology depends on their stability, solubility, and cyclability in all states of charge. 2,1,3-Benzothiadiazole (BzNSN) is a highly negative anolyte (molecule capable of being reduced) with very good solubility as a neutral molecule.[1] However, its solubility drops precipitously as a radical anion. Thus, new BzNSN derivatives were synthesized designed to improve radical solubility by incorporating solvating groups. While some solvating groups had limited success due to increased instability to charging, their synthesis prompted other useful properties –strong fluorescence based on substituent position on the arene ring. Ultimately, a methylacetamide functionalized BzNSN1-CH3displayed strong fluorescence and long radical lifetime, ~130 hours, while the corresponding acetamide BzNSN 1 (i.e., no methyl group) decayed after 15 minutes. Further, H-cell cycling of 1-CH3was very stable in tetraethylammonium bis(trifluoromethane)sulfonamide supporting electrolyte and destabilized after ~20 cycles with the lithium bis(trifluoromethane)sulfonimide supporting electrolyte, but these data were very similar to H-cell cycling of the unsubstituted BzNSN. Spectroelectrochemical experiments to correlate fluorescence quenching vs. state of charge are underway to understand the effect of supporting electrolyte on aggregation.

[1]Duan et al., *ACS Energy Lett*. **2017**, *2*, 1156–1161.

A-8

Exploring Chemical Structure and Dynamics with Broadband Microwave Spectroscopy

Nathan A. Seifert[1], Wolfgang Jäger[2], Kirill Prozument[1]

[1]Chemical Sciences & Engineering, Argonne National Laboratory, Lemont, IL 60439
[2]Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

Though it has been an established spectroscopic technique since the 1940s, microwave spectroscopy has experienced a renaissance in research due to modern improvements and innovations in solid-state, digitization, and signal generation technologies. Now, through the use of chirped-pulse Fourier transform microwave and millimeter-wave (CP-FTMW/mmW) spectroscopy, microwave instrumentation can probe a wide range of chemical systems, ranging from highly excited diatomics and Rydberg molecules, to large hydrogen-bonded organic molecular complexes containing 20+ heavy atoms. Since microwaves probe the rotational degrees of freedom in molecules, CP-FTMW spectroscopy is a highly sensitive and structure-specific technique that allows state-and structurally-resolved spectroscopy of systems including vibrationally excited, isotopically substituted, and reactive molecules. This poster summarizes modern design and capabilities of CP-FTMW instrumentation, with emphasis on the key aspects of quality instrument design. This includes a description of the highly sensitive, low-frequency CP-FTMW molecular beam instrument designed at the University of Alberta for studying molecular complexes, and a high-frequency, millimeter-wave instrument built at Argonne for time-resolved dynamics of photolyzed molecules in a uniform gas flow. As an illustrative example of the power of CP-FTMW spectroscopy, we describe initial and exciting results regarding the spectroscopy and superfluid-like dynamics of pyridine embedded in ^{4}He van der Waals clusters.

A-9

Frhodo: An Interactive Chemical Kinetics Simulation Software For Experimentalists

Travis Sikes[1] and Robert Tranter [1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439

Comparing experimental observables to simulations in high-temperature chemical kinetics is an involved and time-consuming process. Frhodo is a program designed to alleviate some of the difficulties in modifying a chemical kinetics mechanism so that it accurately matches experimental observables, currently density gradients. To this end, Frhodo has been developed to seamlessly load experiments, run a simulation at the experimental conditions, and plot the result within milliseconds. It also has the option to modify a loaded chemical kinetics mechanism in memory to rapidly update the user on how the changes affect the simulation. The software also has an optimization routine that can minimize the SSE between the experimental and simulation results of batches of experiments by modifying set Arrhenius parameters within uncertainty bounds. In this way, thousands of permutations can be simulated within minutes resulting in a less biased answer for the researcher to investigate. Finally, a simulation explorer has been developed which allows the selection of many chemically important parameters to display in detailed, graphical format. Through the simulation explorer and the general design of this program, the idea has been to elevate the capabilities of the researcher through an assistive tool that can maximize efforts through decreasing repetitive procedures.

A-10

A diversified machine learning strategy for predicting and understanding molecular melting points

Ganesh Sivaraman[1], Nicholas Jackson[2,3], Benjamin Sanchez-Lengeling[4,5], Álvaro Vázquez-Mayagoitia[6], Alán Aspuru-Guzik[7,8,9], Venkatram Vishwanath[1], and Juan de Pablo[2,3]

[1]Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, IL 60439
[2]Center for Molecular Engineering and Materials Science Division, Argonne National Laboratory, Lemont, IL 60439
[3]Pritzker School of Molecular Engineering, University of Chicago, Chicago, Illinois 60637, United States
[4]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138, United States
[5]Google Research, Brain Team
[6]Computational Science Division, Argonne National Laboratory, Lemont, IL 60439
[7]Department of Chemistry and Department of Computer Science, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6, Canada
[8]Biologically-Inspired Solar Energy Program, Canadian Institute for Advanced Research (CIFAR), Toronto, Ontario M5S 1M1, Canada
[9]Vector Institute, Toronto, Ontario M5G 1M1, Canada

The ability to predict multi-molecule processes, using only knowledge of single molecule structure, stands as a grand challenge for molecular modeling. Methods capable of predicting melting points (MP) solely from chemical structure represent a canonical example, and highly desirable in many crucial industrial applications. We will present a diversified Machine learning (ML) approach to tackle this challenging problem.

ENERGY

A-11

Visualizing Heterogeneity in Lithium Ion Batteries Under Extreme Cycling Conditions

Harry Charalambous[1]*, Kamila M. Wiaderek[1], Uta Ruett[1], Olaf Borkeiwicz[1], Leighanne Gallington[1], Wenqian Xu[1], Andrey A. Yakovenko[1], Daniel P. Abraham[2], Alison R. Dunlop[2], Andrew N. Jansen[2], Bryant J. Polzin[2], Venkat Srinivasan[2], Yang Ren[1]*

[1] X-Ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2] Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439

Electric vehicles are currently limited by low driving range and long charge times due to limits of lithium ion batteries. Higher lithiation/delithiation potential in cathode (NMC) and anode (graphite) materials is necessary to increase driving range while the ability to charge quickly without degrading the battery is critical in order to eliminate the inconvenience of long charge times. In order to achieve these goals we must first understand the mechanisms of capacity fade under high voltage and high charging rate cycling and specifically, inhomogeneities in batteries exacerbated by extreme charging conditions. Use of high energy synchrotron x-rays allows a non-destructive, high throughput study of lithium ion batteries during operation. We present dynamic studies of pouch cells, determining the evolution of cycling behavior at select parts of the cell, as well as mapping the cell area, both anode and cathode, and correlating inhomogeneity in both components.

A-12

Towards Exascale Simulations In ICEs: A Particle-Laden Turbulent Jet Simulation Using Nek5000

Juan D. Colmenares F.[1], Muhsin M. Ameen[1], Saumil S. Patel[2]

[1]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
[2]Computational Science Division, Argonne National Laboratory, Argonne, IL 60439

Large-eddy simulation of a particle-laden turbulent jet is performed using the massively parallel, high-order code, Nek5000. Coupled with the Parallel Particle-In-Cell Library in Fortran (ppiclF), the dynamics of suspended particles are modeled using an Euler-Lagrange framework on thousands of MPI processes. Two-way coupling between the particles (Lagrangian field) and the gas phase (Eulerian field) is achieved using an interpolation/projection procedure. Results for mean velocity and turbulence intensities in the single-phase and two-phase jet simulations are presented and compared against experimental data. The results show the potential use of the current approach to model two-phase flows. Future work is discussed, which includes implementation of spray submodels to extend modeling capabilities of Nek5000 for complex geometries like internal combustion engines.

A-13

Materials Discovery via Quantum Chemistry-informed Active Learning

Hieu A. Doan, Garvit Agarwal, Rajeev S. Assary

Materials Science Division, Argonne National Laboratory, Lemont, IL 60439

The degradation of redox-active organic molecules (ROMs) is one of the major factors that limit the longevity of a flow battery. Hence, the capability to design ROMs with improved stability would have a critical impact on the advancement of this energy storage technology. One promising approach is to impart ROMs with mesolytic cleavage motifs that allow for programmable bond dissociation and regeneration from their dysfunctional oligomeric and polymeric counterparts. Given a candidate library of 2,300 mesolytic cleavage motifs based on homobenzylic ethers (HBEs), our goal is to screen for those with a suitable oxidation potential (E^{ox}) window. We first employed high-throughput Density Functional Theory to compute E^{ox} values for all 2,300 HBEs, and then used the generated data to train a Gaussian process regression model for E^{ox} prediction. Concomitantly, an active learning model based on Bayesian optimization was developed to achieve the same goal. We found the active learning model demonstrated not only significant efficiency improvement over the regression one but also robust capability in identifying more promising candidates in an additional dataset of 55,000 HBEs. Our findings highlight the efficacy of quantum chemistry-informed active learning as an enabling approach for materials discovery in the vast chemical space.

A-14

Numerical Modeling of Multiphase Internal-and Near-Nozzle Flows of Fuel Injectors

Hengjie Guo[1], Roberto Torelli[1], Lorenzo Nocivelli[1], and Sibendu Som[1]

[1]Energy Systems Division, Argonne National Laboratory, Lemont, IL 60439

Numerical modeling of the internal-and near-nozzle injection flows has attracted interest within both academic and industrial communities. The accurate reproduction of the multiphase physics such as flash boiling and cavitation can provide undoubtedly useful insights to better understand the performance of the injector. In the first part of this poster, simulations were carried out to investigate the in-nozzle flow of a single-hole diesel injector

which is designed to trigger flow separation. Realistic injector geometry and full needle motion obtained from x-ray measurements performed at Argonne's APS were employed. The results agreed well with experimental data of mass flow rate and discharge coefficient. The simulations also correctly captured the flow separation and gas layer thickness inside the orifice that were witnessed in the experiments. In the second part, simulations were performed to study the jets discharged from a straight flow channel to reveal the behaviors of under-expanded flash boiling jets. The expansion ratio (η_{exp}) and the injection pressure were identified as two key factors determining the characteristics of under-expanded flashing jets. When η_{exp} is high enough, the expansion is so strong that the flow becomes supersonic and Mach disks appear near the orifice exit.

A-15

Corrosion Monitoring and Control in Molten Chloride Based Concentrated Solar Power Systems

Jicheng Guo[1], Nathaniel C. Hoyt[1], Mark. A. Williamson[1]

[1]Chemical and Fuel Cycle Technology Division, Argonne National Laboratory, Lemont, IL 60439

Molten mixtures of $MgCl_2$-KCl-NaCl are promising heat transfer fluid (HTF) candidates for the next generation concentrated solar power systems (Gen3 CSP), because of their low cost, high decomposition temperature, and favorable heat transfer characteristics. However, if not properly controlled, molten chloride salts can cause the corrosion of high-temperature metal alloys, such as Inconel, in CSP systems. Here we demonstrate an automated corrosion monitoring and control system that can be used to maintain the health of the structural alloys over long durations. The monitoring system includes a multifunctional voltammetry sensor that is able to measure the redox potential of molten $MgCl_2$-KCl-NaCl mixtures as well as the presence of corrosion products. The sensor is capable of detecting corrosion products, such as Cr^{2+} and Fe^{2+}, quantitatively at low concentrations (less than100ppm) with less than 2% error. The corrosion control capability is facilitated by the in-situ electrolytic production of Mg metal that is automatically initiated when the sensor indicates salt conditions favorable to corrosion. The results show that the corrosion is effectively mitigated when the salt potential is maintained to be sufficiently cathodic.

A-16

High-Voltage Decomposition of Lithium-Ion Battery Electrolyte Indicated by Proton Generation

Toru Hatsukade[1], Milena Zorko[1], Dominik Haering[1], Nenad M. Markovic[1], Vojislav R. Stamenkovic[1], and Dusan Strmcnik[1]

[1]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439.

Knowledge of the degradation mechanism inside lithium-ion batteries (LIBs) is critical in designing robust next-generation materials. While significant efforts have led to advancement in characterization techniques and in our general understanding of the numerous decomposition reactions, the complex, multicomponent nature of batteries has hindered our progress towards developing a complete picture of these processes. In this work, we elucidate the decomposition of electrolyte at high potentials by monitoring the potential-dependent generation of protons—a proposed decomposition product—via a rotating ring-disk electrode (RRDE) setup. Using H2oxidation reaction (HOR) as a model reaction, we first determine that protons generated at the disk electrode can be detected at the ring electrode with a ring collection efficiency of ~20%in battery electrolytes. We then show that protons are indeed generated during electrochemical decomposition of battery electrolyte. Furthermore, we determine that approximately half of the decomposition current is going towards proton generation, which agrees with many mechanisms proposed in literature. Overall, our work demonstrates the use of RRDE as a facile method for determining potential-dependent electrolyte stability.

A-17

Tailoring Silicon Anode Surface for Chemical and Electrochemical Stability for Lithium-ion Battery

Sisi Jiang[1], Haihua Liu[2], Lu Zhang[1], Nathan R. Neale[3], and Zhengcheng Zhang[1],*

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439
[2]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[3]Chemistry and Nanoscale Sciences Center, National Renewable Energy Laboratory, Golden, CO 80401, US

Silicon has been considered as one of the most promising anode materials for next generation high-energy lithium-ion battery due to its extremely high theoretical capacity. However, Si undergoes a huge volume change and particle pulverization and more importantly forms a highly unstable solid electrolyte interphase (SEI) during lithiation and delithiation. Compared with bulk Si, nanostructured Si (<150 nm) largely resolved the pulverization issue. However, the intrinsic electrolyte reactivity with the lithiated Si particles still exists resulting in the gradual active lithium loss and capacity degradation. This poster present a novel approach attempting to stabilize the surface of the Si particles is reported. Plasma synthesized silicon nanocrystals with Si-H terminal groups were subject to hydrosilylation with various organic compounds containing an allyl group. Surface functionalization could stabilize the Si/electrolyte interface affording much improved Coulombic efficiency and cycling performance.

A-18

Tetragonal Tungsten Bronze Framework $V_4Nb_{18}O_{55}$ as an Intercalation Material for Mg Battery Cathodes

Ian D. Johnson[a,b,c‡],Gene Nolis[c,d‡],Kit McColl[a], Yimin A. Wu[c,e], Daisy Thornton[a], Linhua Hu[c,d], Hyun Deog Yoo[f], John W. Freeland[g], Furio Corà[a], Jeremy K. Cockcroft[a], Ivan P. Parkin[a], Robert Klie[e], Brian Ingram[b,c], Jordi Cabana[c,d*] and Jawwad A. Darr[a*]

[a]Department of Chemistry, University College London, 20 Gower Street, London, WC1H 0AJ, UK.
[b]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, USA.
[c]Joint Center for Energy Storage Research, Argonne National Laboratory, Lemont, IL 60439, USA.
[d]Department of Chemistry, University of Illinois at Chicago, Chicago, IL 60607, USA.
[e]Department of Physics, University of Illinois at Chicago, Chicago, IL 60607, USA
[f]Department of Chemistry and Chemical Institute for Functional Materials, Pusan National University, Busan 46241, Republic of Korea.
[g]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA.

[‡]The contributionof IDJ and GN to this work was equal.

There is considerable academic and industrial interest in Mg batteries, which could offer approximately double the energy density of Li-ion batteries if paired with a suitable cathode operating at high capacity and potential. However, there are currently very few oxide cathode materials which have demonstrated reversible and efficient Mg^{2+} insertion and extraction. Herein, the authors provide conclusive evidence of electrochemical insertion of Mg^{2+} into the tetragonal tungsten bronze $V_4Nb_{18}O_{55}$, with a maximum reversible electrochemical capacity of 75 mA h g^{-1}, which corresponds to a magnesiated composition of $Mg_4V_4Nb_{18}O_{55}$. Experimental electrochemical magnesiation/de-magnesiation revealed a large voltage hysteresis with charge/discharge (1.12 V vs Mg/Mg^{2+}); by limiting magnesiation to a composition of $Mg_2V_4Nb_{18}O_{55}$, this hysteresis can be reduced down to only 0.5 V. Hybrid-exchange Density Functional Theory (DFT) calculations suggest that some Mg sites are accessible via low-energy diffusion pathways, but that larger kinetic barriers need to be overcome to access the entire structure. The reversible Mg intercalation involved concurrent V and Nb redox activity and changes in crystal structure, confirmed by a mixture of X-ray diffraction, X-ray absorption spectroscopy, and energy-dispersive X-ray spectroscopy. Therefore, the tetragonal tungsten bronzes are of high interest as intercalation cathode materials in Mg batteries.

A-19

State-of-the-Art in Pre-Chamber Spark-Ignition Modeling

Joohan Kim, Riccardo Scarcelli, Sibendu Som, Ashish Shah, Munidhar Biruduganti, Douglas Longman

Energy Systems Division, Argonne National Laboratory, Lemont, IL 60439

Pre-chamber spark-ignition is now receiving great attention in the automotive industry due to its capability for providing a spatially distributed, volumetric ignition source and extending the lean operating limit. The performance of pre-chamber combustion highly relies on the geometry configuration such as the number of orifices, orifice diameter, orientation, as well as the fueling strategies inside the pre-chamber such as active and passive operation. However, the science base and fundamental understanding of pre-chamber combustion are still not fully explored and secured, which are considered the essential ingredients to accelerate the market penetration of pre-chamber technology with optimization. Furthermore, due to its complex physics of turbulent jet igniting the mixture of main-chamber, it is not clear which turbulent combustion model is appropriate to simulate and analyze the ignition and combustion processes of the pre-chamber application. In this study, two turbulent combustion models widely adopted in engine modeling community were evaluated and validated under RANS framework. A set of experimental data acquired from a medium-duty natural gas engine with a pre-chamber spark-ignition system were employed for the model assessment. The in-cylinder pressure, heat release rate, and a non-dimensional combustion index were used for analyzing the simulation results. The simulation revealed that there were turbulence-chemistry interactions and multi-regimes of turbulent combustion exhibited during the pre-chamber combustion, and those were challenging for models to match the experimental data.

A-20

Achieving High Li Transference Number and High Coulombic Efficiency via Single-ion Conducting Polymer Electrolyte for Li-ion Batteries

Kewei Liu, Sisi Jiang, Chen Liao*

Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States

Driven by the fast-growing demand for high energy density and safety of Li-ion batteries, a number of efforts have been applied on developing Li-ion conducting solid electrolyte. Polymer electrolyte with its unique flexibility and low-cost has been regarded as one of the promising candidates. However, the performance of the conventional lithium ion polymer electrolyte is greatly limited due to the low transference number of Li, which is the active species in battery cycling. Gradient concentration of Li^+ exists in a conventional Li-ion battery cell, resulting in polarization and impedance from concentration gradients. In this work, a single-ion conducting polymer electrolyte is prepared via an efficient thiol-ene reaction initiated by UV light. A high unity Li transference number of 0.93 is achieved by anchoring anions onto the polymer network. The polymer electrolyte exhibited an ionic conductivity of 10^{-4} S/cm at 35 ºC. Utilized in a Li//LFP cell set-up, the cells with single-ion conducting electrolyte delivered a promising averaged coulombic efficiency of 99.95% for 200 cycles.

A-21

The Role of Co and Mn Cations for High-Ni NMC Layered Cathode: A Revisiting

Xiang Liu, Gui-Liang Xu, and Khalil Amine

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

The Ni-nickel rich $Li(NiMnCo)O_2$ cathode with high energy density is one of promising material for next generation lithium ion batteries. Beside increase of the Ni content, decrease the Co content is preferred because of the limited globe resources of cobalt. However, the combination of high Ni and low Co may cause a severe capacity degradation, as well as rise the safety concern. We proposed here, by carefully tune the stoichiometric concentration of Co and Mn in Ni-rich cathode, we successfully synthesized the cathode materials of $Li(Ni_{0.83}Mn_{0.06}Co_{0.11})O_2$, $Li(Ni_{0.83}Mn_{0.085}Co_{0.085})O_2$ and $Li(Ni_{0.83}Mn_{0.11}Co_{0.06})O_2$. By comparison study of the cycling performance and phase transformation properties during in situ cycling/heating of the as-prepared 3 cathode materials, the role of Co and Mn can be clearly distinguished.

A-22

ActivO: A Novel ActiveOptimization Approach Using Ensemble Machine Learning

Opeoluwa Owoyele[1], Pinaki Pal[1]

[1]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439

A novel design optimization technique based on active learning using an ensemble of machine learning algorithms is developed. In this approach, a weak learner is used to identify promising regions within the design space to explore, while the strong learner is used to locate the exact location of the optimum within the promising region. For each design iteration, an aristocratic approach is used to select a set of nominees. Exploration is done by randomly selecting points within regions where the weak learner-predicted merit is higher. The global optimum as predicted by the strong learner is also evaluated to enable rapid convergence to the actual global optimum once the most promising region has been identified by the optimizer. Different optimization test cases with ActivO are demonstrated: (i) a two-dimensional multi-modal surface and (ii) a complex internal combustion (IC) engine optimization case with nine control parameters related to fuel injection, initial thermodynamic conditions, and in-cylinder flow. It is shown that ActivO is significantly faster and lowers the number of function evaluations that are needed to reach the optimum design configuration (by at least 80%), when compared to traditional optimization techniques, such as micro-genetic algorithm and particle swarm optimization.

A-23

Computational Diagnostics of Limit Phenomena and Non-ideal Combustion in Practical Propulsion Systems

Chao Xu, Prithwish Kundu, Pinaki Pal, and Sibendu Som

Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439

Limit phenomena such as ignition and extinction in practical propulsion systems are complex due to the strong interactions of various physical processes, especially between fuel chemistry and flow turbulence. Advanced computational flame diagnostics based on high-fidelity simulations, e.g., large-eddy simulations (LES), can identify critical flame features in these complex combustion systems. In this poster, a novel computational diagnostic is developed to quantify the roles of individual physical processes, such as chemistry and diffusion, by projecting the chemical and diffusion source terms into the chemical explosive mode. Using the new diagnostic,

different local combustion modes including auto-ignition, diffusion-assisted ignition, and extinction are uniquely identified. The new approach is then applied to turbulent spray flames at various thermodynamic conditions, to identify key physics that govern flame ignition and extinction in a range of practical propulsion systems including internal combustion engines and gas turbines. The developed computational diagnostic tool enables quantitative understanding of near-limit flame dynamics and non-ideal combustion, and thus has the potential to facilitate advanced fuel development and improved combustor designs.

A-24

Metal Perfluoroalkoxyaluminate as Electrolytes for Rechargeable Divalent Ion Batteries

Mengxi Yang[1,2], Ka-Cheong Lau[1,2], Trevor J. Seguin[1,3], Emily V. Carino[1], Justin G. Connell[1], Kristin A. Persson[1,3,4], and Chen Liao[1,2]

[1]Joint Center for Energy Storage Research, Lemont, IL 60439
[2]Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439
[3]Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
[4]Department of Materials Science and Engineering, University of California Berkeley, Berkeley, CA 94720

Multivalent cation batteries have gained significant research interests in recent years due to their potential in achieving high energy density systems. One challenge in the field is to develop both reductively and oxidatively stable electrolytes that efficiently support metal deposition and cation insertion. Previous work has highlighted the development of a weakly-coordinated perfluoroalkoxyaluminate anion as high-voltage electrolytes for magnesium-ion batteries. Through computational and experimental studies, the extended electrolyte stability window in triglyme was attributed to a balanced ion-association and anion-solvent interactions. In this presentation, we describe our efforts to apply the strategies of using weakly coordinated systems to other divalent metal-ions such as calcium and zinc.

A-25

Unexpected electrochemical behaviors of 2,1,3-benzothiadiazole in various electrolytes: a solvation study to probe the interaction between redoxmer and cations

Yuyue Zhao[1], Yu Zhou[2], Jingjing Zhang[1], Ilya A. Shkrob[1], Lei Cheng[2], Lu Zhang[1]*

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439
[2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439

Redoxmers or redox active materials often determine the performance of flow batteries. The solvation or the interaction between redoxmers and surrounding electrolytes is a crucial factor that can affect the properties of redoxmers, including redox behaviors. In this study, a systemical approach is adapted to probe such interaction between 2,1,3-benzothiadiazole (BzNSN)and electrolytes with different solvents and salts. BzNSN is a high-energy-dense anolyte molecule with a low redox potential. When cycled in flow batteries, the choice of salts significantly impact the redox potentials and cycling life. As shown in Figure 1, when measured in electrolytes containing Li-based salts, BzNSN delivers increased redox potentials, implying Li^+ involved interactions. Moreover, by changing cations of different sizes, such as Na^+, K^+ and NEt_4^+, the increased size of cations results in decreased redox potential of BzNSN, which shows a nearly 200 mV shifts from -1.65 V for Li^+ to -1.85 V for NEt_4^+. For an anolyte material, the lower redox potential usually leads to worse stability as it becomes thermal dynamically unstable. Surprisingly, this is not the case for BzNSN in electrolytes with different cations. Despites the lower redox potential, BzNSN radical cation delivers a much longer life time (t1/2 = 90 h) in 0.5 M KTFSI acetonitrile electrolyte than in LiTFSI acetonitrile electrolyte (t1/2 = 42 h). This is the first time that we observe an anolyte redoxmer can deliver a longer life time at a lower potential, which might be a ground-breaking approach

for designing high energy density flow batteries.

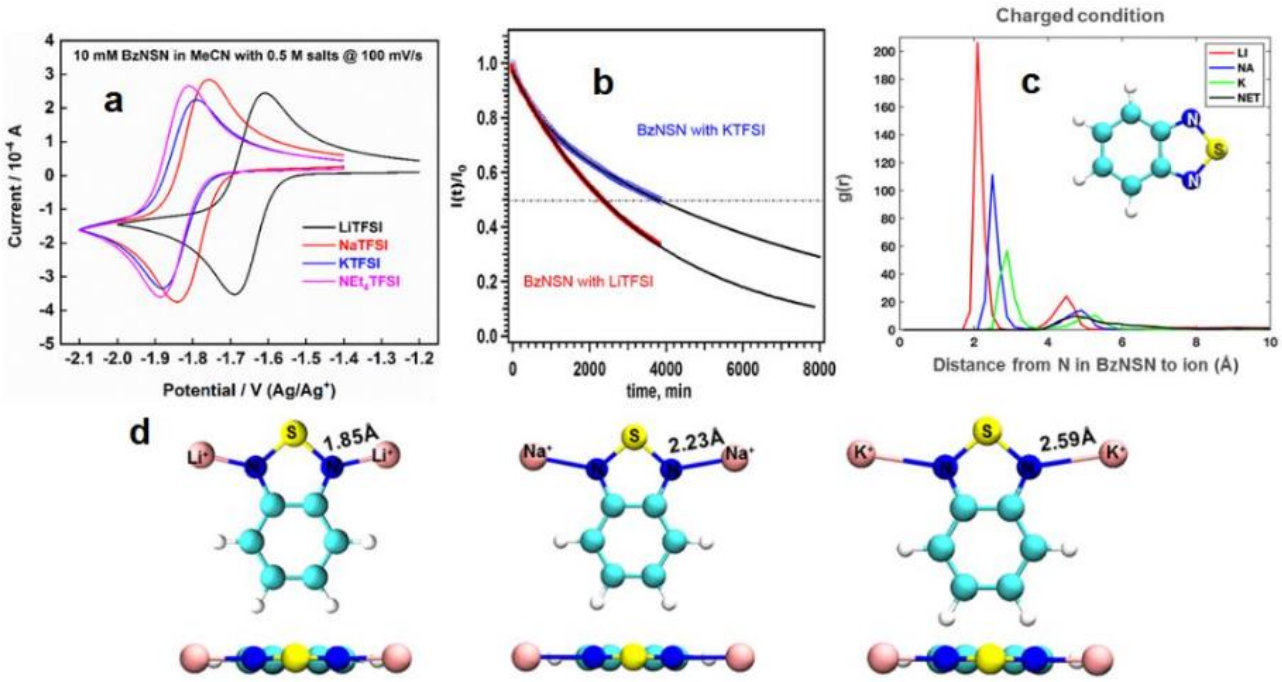

Figure 1.a) CV curves of BzNSN with different salts; b) EPR kinetics of charged BzNSN radical anion(20 mM) with different salts (0.5M in acetonitrile);c) Radial distribution function (RDF) between the nitrogen atom in BzNSN radical anionand the cations (e.g., Li^+, Na^+, K^+, and NEt_4^+).The coordinates of NEt_4^+ are represented by the center nitrogen atom. d) The charged BzNSN with two coordinated cations top and side view.

MATHEMATICS AND COMPUTER SCIENCE

A-26

Scalable Diffusion Convolution Recurrent Neural Network for Large-Scale Traffic Forecasting

Tanwi Mallick[1], Prasanna Balaprakash[1,2] and Eric Rask[3]

[1]Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439
[2]Argonne Leadership Computing Facility, Argonne National Laboratory, Argonne, IL 60439
[3]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439

Traffic forecasting approaches are critical to developing proactive and reactive strategies for mobility. More specifically, accurate forecasting of traffic conditions at a range of timescales is used for an ever-increasing number of decisions related to assessment and control of specific corridors as well as a range of routing and optimization solutions related to Intelligent Transportation Systems. Traffic forecasting is a challenging problem: The key traffic metrics such as flow and speed exhibit complex spatial and temporal correlations that are difficult to model with classical forecasting approaches such as autoregressive integrated moving average, Kalman filter, artificial neural networks, support vector regression, convolutional neural networks, and recurrent neural

networks. From the spatial perspective, locations that are close geographically in the Euclidean space (for example, two locations located in opposite directions of the same highway) may not exhibit a similar traffic pattern, whereas locations in the highway network that are far apart (for example, two locations separated by a mile in the same direction of the same highway) can show strong correlations. Many traditional predictive modeling approaches cannot handle such spatial correlation in non-Euclidean space. From the temporal perspective, because of different traffic conditions across different locations (e.g., diverse peak hour patterns, varying traffic flow and volume, highway capacity, incidents, and interdependencies), the time series data becomes nonlinear and non-stationary, rendering many statistical time series modeling approaches ineffective.

Recently, deep learning approaches have emerged as high-performing methods for traffic forecasting. In particular, Li et al. [1] developed a diffusion convolution recurrent neural network (DCRNN) that models complex spatial dependencies using a diffusion process on a graph and temporal dependencies using a sequence to sequence recurrent neural network. DCRNN have achieved state-of-the-art results in traffic forecasting by capturing the spatiotemporal dynamics of the traffic. Despite the promising results, adopting DCRNN for large highway networks still remains elusive because of computational time and memory bottlenecks. To overcome these problems, we propose an approach to apply DCRNN for a large highway network. We develop a graph-partitioning approach to decompose a large highway network into smaller networks and train them simultaneously on a moderately sized cluster with GPUs.

For the first time, we forecast the traffic of the entire California highway network with 11,160 traffic sensor locations simultaneously using one-year (2018) of data from the California Department of Transportation (CalTrans) Performance Measurement System (PeMS). With the entire dataset, DCRNN algorithm fail to train due to the out-of-memory issue. Therefore, we partition the graph into 4, 8, 16, 32, 64 and 128 partitions using a fast graph partitioning package, Metis and evaluate the impact of the number of partitions on the training time and accuracy. We find that 64 partitions give the best speed forecasting with 2.02 mph as the median of mean absolute error (MAE) of all 11,160 locations. Simultaneous training on 64 GPUs reduces the training time from 47 hours on 4 GPUs to 3 hours. To assess the impact of training data size, from the full 36 weeks of training data, we selected the last 1, 2, 4, 12, 20, and 36 weeks of data for the training. We find the best accuracy with 36 months of training data which implies that our approach leverages large training data to improve the accuracy. Since the best forecasting accuracy and speedup were obtained by using 64 partition, we used it as a default partition and further reduce the median of MAE to 1.98 mph (slight improvement of the median reflects large improvement of the forecasting accuracy in individual sensor level) by considering overlapping nodes approach to include spatially correlated nodes from different partitions. In addition, we tune the hyperparameters for 64 partition using scalable hyperparameter search package, DeepHyper and reduce the median of MAE to 1.91 mph. We adapt and train a single model to forecast multiple time series such as speed and flow simultaneously, using multi-task learning framework. The median of MAE,from speed only model, 2.02 got reduced to 1.98 and the median of MAE, from flow only model, 21.20 got reduced to 20.64 using multi-task learning.

The DCRNN model once trained can be run on traditional hardware such as CPUs for forecasting without the need for multiple GPUs and could be readily integrated into a traffic management center. Once integrated into a traffic management center, the model would likely lead to better decisions making given the capability to make large-scale and accurate forecasts regarding future traffic states.

[1] Li, Y., R. Yu, C. Shahabi, and Y. Liu, Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting. In International Conference on Learning Representations (ICLR ’18), 2018

A-27

Understanding Performance Variability in Standard and Pipelined Parallel Krylov Solvers

Hannah Morgan[1], Patrick Sanan[2], Matthew Knepley[3], and Richard Tran Mills[1]

[1]Mathematics and Computer Science Divison, Argonne National Laboratory, Argonne, IL 60439
[2]Institute of Geophysics, ETH Zurich, Zurich, Switzerland
[3]Computer Science and Engineering, University at Buffalo, Buffalo, NY 14260

In this work, we collect data from runs of Krylov and pipelined Krylov methods in an effort to understand and model the impact of machine noise and other sources of variability on performance. We find large intra-node variability for standard methods that is reduced in pipelined methods, directly supporting conjecture, as well as large variation between statistical distributions of runtimes across iterations. Based on these results, we improve upon a previously introduced nondeterministic performance model by allowing iterations to fluctuate over time. We present our data from runs of various Krylov algorithms across multiple platforms as well as our updated non-stationary model that provides good agreement with observations and suggest how it can be used as a predictive utility.

A-28

Boundary Integral Constrained Optimization for a Multiscatterer Helmholtz Problem

Oana Marin[1], Marieme Ngom[1], and Barry Smith[1]

[1]Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439

We seek to determine the optimal distribution of a collection of dielectrics such that the power stemming from waves scattered off the dielectric surfaces achieves its maximum in a target region. The physical problem is modeled using the Helmholtz equation, and whereas previous work focused on a finite differences discretization, we examine a corresponding boundary integral formulation. The change of simulation framework is justified by an increase in accuracy due to a more rigorous treatment of dielectric interfaces as well as the free-space boundary conditions via the Sommerfeld condition. Additionally the particular parametrization chosen induces a reduced state variables space, which facilitates a speed-up for the chosen optimization strategies. To ensure well-conditioning of the Helmholtz problem, we model the problem using the Combined Field Integral Equation (CFIE) formulation in the half-space plane. The derivatives are verified against finite differences evaluations of the gradient of the objective function. The optimization itself is performed using the Limited Memory Variable Metric (LMVM) algorithm as well as steepest descent methods, and two types of objective functions are considered.

A-29

REFINED (REpresentation of Features as Images with NEighborhood Dependencies): A Novel Feature Representation for Convolutional Neural Networks

Raziur Rahman[1], Ranadip Pal[2]

[1]Data Science and Learning Division, Argonne National Laboratory, Lemont, IL, 60439
[2]Electrical and Computer Engineering, Texas Tech University, Lubbock, TX, 79409

Deep learning with Convolutional Neural Networks has shown great promise in various areas of image-based classification and enhancement but is often unsuitable for predictive modeling involving non-image-based features or features without spatial correlations. We present a novel approach for representation of high dimensional feature vector in a compact image form, termed REFINED (REpresentation of Features as Images with NEighborhood Dependencies), that is conducible for convolutional neural network based deep learning. We consider the correlations between features to generate a compact representation of the features in the form of a two-dimensional image using minimization of pairwise distances similar to multi-dimensional scaling. We hypothesize that this approach enables embedded feature selection and integrated with Convolutional Neural Network based Deep Learning can produce more accurate predictions as compared to Artificial Neural Networks, Random Forests and Support Vector Regression. We illustrate the superior predictive performance of the proposed representation, as compared to existing approaches, using synthetic datasets, cell line efficacy prediction based on drug chemical descriptors for NCI60 dataset and drug sensitivity prediction based on transcriptomic data and chemical descriptors using GDSC dataset. Results illustrated on both synthetic and biological datasets shows the higher prediction accuracy of the proposed framework as compared to existing methodologies while maintaining desirable properties in terms of bias and feature extraction.

A-30

Bayesian Optimization of Expensive Oracles with Input-dependent, Correlated Noise

S. Ashwin Renganathan[1], Jeffrey M. Larson[1] and Stefan Wild[1]

[1]Mathematics and Computer Science Division, Argonne National Laboratory, Lemont IL 60439

Quantum computers hold promise to offer a paradigm shift in computational speed-ups over classical computers, that can benefit a large variety of scientific computing applications. However, near-term quantum computers are expected to be crippled by noise, even for modest size computations. One approach to enable quantum computers to produce *useful* results is seek operational parameters that minimize their error.

Our problem considers a parametrized quantum device (or simulation) whose control parameters can be perturbed, and observations can be made for a given computation with specified inputs. However, there is no knowledge of the system behavior and each observation is expensive to make. Furthermore, the observations are corrupted by input-dependent and temporally correlated noise. Our goal is to make optimal decisions over a finite time horizon with limited information from the past.

We propose a solution via Bayesian optimization (BO) where, a prior probability distribution is assigned to the unknown objective function and its *aposteriori* probability distribution conditioned on the available observation serves as a surrogate model of the objective function. This model is computationally cheap and hence can efficiently guide the search for optimum. As a first step, we demonstrate the methodology on canonical problems of varying characteristics.

A-31

Simulation and Bayesian Parameter Inversion for Earth's Mantle Flow with Plates

Johann Rudi[1], Georg Stadler[1], Omar Ghattas[1], Michael Gurnis[1]

[1]Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439

We target Earth's mantle convection with associated plate tectonics at a global scale. The computational methods that we have developed are capable of adaptively resolving small-scale features (about 1 km) and highly nonlinear physics at plate boundaries, which influence dynamics at continental scales (over 1000 km).

We present new advances on various levels of a nonlinear implicit solver for Earth's instantaneous mantle flow governed by nonlinear instantaneous Stokes PDEs: (i) heterogeneity-robust Schur complement preconditioning, (ii) hybrid spectral–geometric–algebraic multigrid, and (iii) nonlinear preconditioning of an inexact Newton–Krylov method. Our advanced numerical methods show (nearly) optimal computational performance with respect to degrees of freedom and the parallel algorithms demonstrate scalability to large numbers of compute cores.

Going beyond simulation of Earth's mantle flow, we are interested in the inversion of uncertain parameters in the mantle's model given velocities at the surface as observational data. We present computational methods for large-scale inverse problems posed in a Bayesian statistical framework by introducing a Gaussian prior distribution for the uncertain parameters. The maximum a posteriori (MAP) estimate and an approximation of parameter uncertainties at this MAP point is obtained from the solution of an optimization problem governed by the model PDE and second-order derivatives (Hessians), respectively. Newton's method is used for solving the optimization problem, which requires first- and second-order derivatives of the parameter-to-observable map. These operations are performed in an efficient and scalable fashion using adjoint methods.

A-32

Performance Evaluation and Analysis of Bayesian Neural Network at Scale

Himanshu Sharma[1], Elise Jennings[1]

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

Deep neural networks (DNN) are accelerating the pace of research in many scientific domains such as medical science, biological and materials science, weather prediction, computer vision and chemistry. However, the major limitation of these feed forward networks is the lack of robust uncertainty quantification for the predictions. Bayesian neural networks (BNN) can address these limitations with some additional computational overhead. Understanding how these networks perform and any potential bottlenecks are crucial in obtaining results at scale. In this work we present a performance and scalability comparison of the VGG-16 convolutional network, with and without Bayesian layers, using the distributed training framework Horovod on the Cray-X40 system, Theta, at Argonne Leadership Computing Facility. The study will provide guidelines for training a Bayesian neural network at scale and will aid in understanding the limitations and benefits over a conventional neural network.

A-33

Accelerated Reliability Test of Power Electronics Devices and Components

Moinuddin Ahmed[1], Christopher Stankus[1], Angel Yanguas-Gil[1], John Hryn[1]

[1]Applied Materials Division, Argonne National Laboratory, Argonne, IL 60439

Argonne power Electronics group is involved in reliability study of high power (600 V-1700 V) electronics. We have developed methodology to stress device at high temperature and high radiation environment at an accelerated rate to measure life-time. We also perform statistical data analysis, ML based degradation model and understand physics-of-device failure.

Poster Abstracts – Session B

ENGINEERING

B-1

High fidelity simulation of Spark-Ignition engines in the framework of spectral element methods

Tanmoy Chatterjee[1], Saumil S.Patel[2], and Muhsin M. Ameen[1]

[1]Energy Systems Division, Argonne National Laboratory, Lemont, IL 60439
[2]Computational Science Division, Argonne National Laboratory, Lemont, IL 60439

High-fidelity numerical simulations of spark ignition (SI) engines provide a reliable way to understand the flow, ignition, combustion and emission processes inside the cylinder and thus help design cleaner and more efficient engines. In such advanced computational fluid dynamic methods, the design of the mesh is critical towards generating physically consistent, high fidelity data especially in regions of complex boundaries inside the cylinder, e.g., near the spark plugs. This is primarily due to the mesh deformation caused by the motion of the valve near the plug and also finer mesh sizes in the spark plug region. In the current work, we demonstrate the use of an overlapping grid (overset) methodology to design the mesh in the spark-plug region in a 2D SI engine-like geometry for a high-order simulation, based on the spectral element method (SEM). The data in the overlapping region is exchanged between the spark-plug geometry and the geometry containing rest of the objects like the piston, head, valve etc., using a high order spectral interpolation technique. This methodology is further extended for simulations of 3D TCCIII engine geometry in the framework of filter-based large eddy simulation. The designed simulations were tested to be scalable with 70% efficiency for 16,000 MPI processes in Argonne leadership computing facility machine, Theta. Different intake boundary conditions based on the continuity of piston fluxes as well as time varying 0D simulations (GTPower) have been tested which elucidate our understanding of the large scale structures generated from the intake stroke jet and interacting with the spark plug. This study serves as a stepping stone towards designing high-fidelity, massively parallelized engine simulations which are essential not only for the fundamental understanding of turbulence but also designing reduced order models for predictive simulations.

B-2

CFD Modeling of Flame Spray Pyrolysis for Large-scale Manufacturing Applications

Debolina Dasgupta[1], Pinaki Pal[1], Roberto Torelli[1], Sibendu Som[1], Noah Paulson[2], Joseph Libera[2], and Marius Stan[2]

[1]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
[2]Advanced Manufacturing Division, Argonne National Laboratory, Argonne, IL 60439

Flame spray pyrolysis (FSP) is a versatile, cost effective, scalable, and easy-to-handle method for large-scale production of oxide nanoparticles (e.g., SiO_2, TiO_2) from relatively cheap precursors. The process allows for strict control of the particle size and distribution and can continuously produce highly pure and thermally stable particles. It is well known that the particle size and morphology are strong functions of flame temperature, residence time of the particles in the flame, precursor concentration, and the flow field within the reactor. However, the nature of interactions between the complex fluid dynamics, chemistry and mechanism of nanoparticle formation is not well understood. This necessitates an extensive study of FSP-related phenomena, which can be further utilized to develop strategies for achieving desired product quality and scaling up the overall yield. The current work focuses on CFD modeling of such complex systems. A test setup is created and validated against literature, demonstrating the capability of the model to capture the complex FSP physics. The FSP burner at manufacturing engineering research facility (MERF) is then simulated to provide insights for flame anchoring, stabilization and particle formation. In addition, the data is used for reduced-order modeling (ROM) to relate the input and output parameters of the system.

B-3

CFD Modeling of Unmanned Aerial Systems

I-Han Liu, Roberto Torelli

Energy Systems Division, Argonne National Laboratory, Lemont, IL,60439 USA

Unmanned Aerial Systems (UASs) find application in both commercial and defense fields by carrying out numerous operational tasks. A UAS' configuration is designed based on the mission that the system will perform, such as flying speed, altitude, endurance, maneuvers, etc. During the design process of a UAS, aerodynamics play a major role as the aircraft's performance depend on them. Therefore, when designing aircrafts, the accurate knowledge of the UAS' aerodynamic coefficients is a key factor in the definition of the aircraft's dynamic model. In this work, a computational fluid dynamics (CFD) methodology is proposed to perform large-scale 3-D simulations of selected NACA airfoils and a UAV, the Pioneer RQ-2A. An incompressible, transient, Reynolds-Averaged Navier-Stokes formulation closed by the RNG k-ε turbulence model was used to perform simulations at Reynolds numbers range from 5×10^4 to 1×10^6. The model was validated against wind-tunnel and CFD data available from the literature. The results were in good agreement and the model was able to predict the stall conditions. The goal of this project is to map the aerodynamic coefficients across the whole operating range of a UAS and feed this information to a system simulation tool for aircraft dynamic control system design.

B-4

Improved Catalyst Selectivity and Longevity Using Atomic Layer Deposition

Zheng Lu[1], Arrelaine Dameron[2], RyonTracy[2], Christopher P. Nicholas[3], Leigh M. Abrams[3], Paul T. Barger[3], Tao Li[4,5], Christopher L. Marshall[1]

[1]Chemical Sciences and Engineering, Argonne National Laboratory, Lemont, IL60439
[2]Forge Nano, Louisville, CO 80027
[3]Honeywell UOP Catalysis Research, Des Plaines, IL 60016
[4]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439
[5]Department of Chemistry, Northern Illinois University, DeKalb, IL 60115

Many important industrial scale chemical reactions rely on catalysts and require high temperatures to achieve commercially viable product yields.[1] However, catalysts deactivate over time and lose surface area due to thermal degradation (sintering), fouling, and poisoning. Decreased catalytic activity results in lower selectivity and higher yields of unwanted byproducts. In many cases, the remedy for sintering of metals is to raise the reactor temperature and thus increase energy consumption, or to remove and replace the spent catalyst, which is expensive and leads to loss in productivity.

This project is overcoming catalyst degradation issues via an ALD overcoating technology that deposits protective layers around the active metal, preserving catalyst integrity under reaction conditions.[2,3] The ALD overcoating technique applies one or more protective layers to the catalyst to inhibit metal sintering. Channels introduced into the ALD layers provide reactants with access to the catalyst's active metal and improve reaction selectivity. This project is applying the overcoating technology to extruded platinum-based catalysts used in the propane dehydrogenation (PDH) to propylene. The effect of these overcoated layers on PDH rate, selectivity, and catalyst deactivation will be reported.

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B-5

Accelerating Reynolds-Averaged Navier-Stokes Turbulence Modeling With Machine Learning

Romit Maulik[1], Himanshu Sharma[1], Saumil Patel[2], Bethany Lusch[1], Elise Jennings[1]

[1]Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont IL 60439, USA
[2]Computational Science Division, Argonne National Laboratory, Lemont IL 60439, USA

Multiple disciplines rely on computationally intensive simulations for scientific and engineering insight into complicated problems. One such example is that of the computational fluid dynamics (CFD) of turbulent flows for which extremely large scale simulations are the norm. Reynolds-averaged Navier-Stokes governing equations (RANS), the workhorse of practical CFD, rely on the use of cost-intensive compute kernels for the calculation of turbulence quantities. In this study we accelerate RANS with an artificial neural network that maps from initial conditions to steady-state turbulent eddy-viscosities without the solution of an additional set of coupled partial differential equations. We achieve accurate steady-state results with significant reduction in time-to-solution when compared to cases which actually include the turbulent eddy-viscosity equations. Our results indicate that the proposed framework represents an excellent opportunity for rapid parameter space exploration.

B-6

Numerical Simulation of the Injection of Super-Heated Fuel for Gasoline Direct Injection Applications

Lorenzo Nocivelli, Sibendu Som

Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439

The injection characteristics of gasoline surrogates are studied under different ambient pressure and temperature conditions. Injection under flash-boiling conditions can enhance liquid atomization and evaporation, providing the possibility of improvement in the fuel/air mixing. These super-heated conditions often introduce phenomena that are not taken into account in the standard modeling of sprays for engine applications. The present work proposes a numerical investigation of the behavior of Engine Combustion Network's 8-hole spray-G injector, starting at the subcooled nominal condition and reducing the ambient pressure at constant low temperature to reach the flare flash-boiling condition. To initialize the properties of the injected fuel, the flow in the nozzle is simulated with an Eulerian approach, handling the two phases with a mixture model and the phase change, due to cavitation and flash boiling, with the Homogenous Relaxation Model. A map of the mixture kinematic and thermal behavior is obtained at the interface between the injector and the chamber to initialize the Lagrangian parcels simulations. A literature-based vaporization model is implemented to obtain the proper description of the characteristic features of a multi-hole spray under super-heated conditions, like plume-plume interaction. The numerical representation of the spray is validated in terms of penetration and radial spreading on DBI images, reproducing the light attenuation profiles caused by the presence of the liquid spray.

B-7

Development of Teststand Digitizer Emulator Module for Gamma Ray Energy Tracking Array (GRETA)

Shefali Saxena[1],John T. Anderson[2], and Michael B. Oberling[2]

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

GRETA is a realization of a full 4π γ-ray tracking detector, capable of reconstructing the energy and three-dimensional position of γ-ray interactions within a compact sphere of high-purity germanium crystals. The main

electronics components of digital data acquisition system for GRETA are digitizers, filter boards and trigger and timing systems. In this work, a teststand digitizer emulator module is developed for the testing of trigger and timing system. The teststand module consists of a Xilinx Virtex-6 ML605 evaluation board, Silicon Labs evaluation board and an SFP interface daughter card. The ML605 FPGA board is developed to provide the necessary trigger primitives and status information to the trigger system to allow the formation of triggers and for the overall monitoring of the health of the GRETA system. The serial link SFP interface module connects the timing and trigger module to digitizer emulator module using the National Semiconductor DS92LV18 Serializer/Deserializer (SerDes). The firmware is configured using Xilinx ISE in VHDL. The teststand module sends fast leading-edge discriminator signals at the rate of 4 Gbps using 8b/10b encoded data stream to trigger and timing module and receives system timestamps from the trigger and timing module at the rate of 1 Gbps.

B-8

Full-field high-resolution ultrasonic imaging using noncontact ultrasonic scanning measurements and machine learning

Homin Song[1] and Yongchao Yang[1,2]

[1]Decision and Infrastructure Sciences Division, Argonne National Laboratory, Lemont, IL 60439
[2]Currently at Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, Houghton, MI 49331

Here we present full-field high-resolution ultrasonic imaging approaches using noncontact ultrasonic scanning measurements and machine learning techniques. Two different ultrasonic imaging approaches are presented: (1) wavefield filtering-based near-field imaging approach and (2) machine learning-based far-field imaging approach. For near-field imaging, a frequency-wavenumber domain filtering technique is presented to extract the energy of non-propagating oscillatory fields and thus to detect and locate zones of distributed cracking. In a separate effort for far-field imaging, a data-driven machine learning approach is presented to bypass the diffraction limit, which limits the spatial resolution of existing far-field imaging methods, and hence to achieve high-resolution imaging results. The presented approaches are evaluated using numerical simulation and experimental data collected from various specimens (e.g. concrete and aluminum). The results demonstrate that high-resolution damage visualization can be achieved using the near-field imaging approach and that the machine learning-based far-field imaging approach enables the recovery of fine morphological features of small damage.

B-9

High-fidelity Geometry Generation from CT Data using Convolutional Neural Networks

Aniket Tekawade[1], Brandon A. Sforzo[1], Katarzyna E. Matusik[1], Alan L. Kastengren[1], Christopher F. Powell[1]

[1]Energy Systems Division, Argonne National Laboratory, 9700 South Cass Avenue, Lemont, IL, 60439

The X-ray Fuel Spray research at Argonne National Laboratory is aimed at utilizing synchrotron X-ray diagnostics for providing insights into automotive fuel injection. One important task is to generate high-fidelity geometries or iso-surfaces of steel fuel injector nozzles from X-ray Computed Tomography measurements, to be used as inputs to realistic CFD simulations of fuel injector flow. These fuel nozzles contain 3D features between 5 -500 micron and are imaged at a pixel resolution of 1 micron. The main bottleneck to automated generation of an STL geometry from X-ray CT data is the segmentation or surface determination process –conversion of the CT volume into a binary map that classifies each voxel as belonging to either injector metal or flow domain, accurately locating the metal surface at the transitions between these domains. Here, we describe our recent success in automating the segmentation process itself, which is challenging because various artifacts that arise from X-ray imaging and CT reconstruction confound the identification of threshold values needed for traditional segmentation algorithms. A

convolutional neural network (CNN)coupled with a tailored loss function is implemented to achieve state-of-the-art accuracy in surface localization with limited manual intervention. Through data augmentation, the model can be trained on less than 30% of the slices drawn from two CT scans of different automotive injectors that were manually segmented and is tested on a third. Our architecture achieves state-of-the-art accuracy at lower computation time and GPU memory requirement compared to U-net, one of the most popular architectures for image segmentation.

B-10

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

Lauren Valentino[1], Yupo Lin[1]

[1]Applied Materials Division, Argonne National Laboratory, Argonne, IL 60439

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

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

B-11

CFD Evaluation of Gasoline Compression Ignition at Cold Conditions in a Heavy-Duty Diesel Engine

Le Zhao[1], Muhsin Ameen[1], Yuanjiang Pei[2], Yu Zhang[2], Praveen Kumar[2], Tom Tzanetakis[2], and Michael Traver[2]

[1]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
[2]Aramco Services Company: Aramco Research Center –Detroit, MI 48377

Achieving robust ignitability for compression ignition of diesel engines at cold conditions is traditionally challenging due to insufficient fuel vaporization, heavy wall impingement, and thick wall films. Gasoline compression ignition (GCI) has shown good potential to offer enhanced NOx-soot tradeoff with diesel-like fuel efficiency, but it is unknown how the volatility and reactivity of the fuel will affect ignition under very cold conditions. Therefore, it is important to investigate the impact of fuel physical and chemical properties on ignition under pressures and temperatures relevant to practical engine operating conditions during cold weather.

0-D simulations were performed to evaluate the ignitability of different gasoline-like fuels and the impact of initial pressure and temperature on the autoignition behavior over a range of equivalence ratios. A Lagrangian-Eulerian modeling approach with Reynolds-Averaged Navier-Stokes (RANS) formulation was used for 3-D CFD combustion simulations. The comparisons with the measured engine in-cylinder pressure, heat release rate, and

emissions at all operating conditions showed that CFD model results were in good agreement with experiments. Experimentally validated CFD simulations were further used to gain insight into spray, ignition and combustion processes for GCI under the cold operations by investigating the sensitivity towards thermal boundary conditions and spray model constants.

ENVIRONMENTAL SCIENCE

B-12

A Scalable Multiphysics Modeling Package For Critical Networked Infrastructures Using PETSc DMNetwork

Getnet Betrie[1], Barry Smith[2], and Hong Zhang[2]

[1]Environmental Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Mathematics and Computer Science Division, Science Division, Argonne National Laboratory, Lemont, IL 60439

Critical infrastructures involve multiphysics, are cross-disciplinary, and have multiple interdependencies. Simulation of an individual infrastructure without accounting for such interdependencies is insufficient to support decision-making. However, existing tools are deficient in that they either lack coupling or are rigidly coupled, can simulate only steady-state solutions, and/or lack scalability. Thus, they are not suitable to understand the impact of one system failure on the other systems, simulate transient nature of the systems, or be applied for real-time problems at large spatial and temporal scales. To address these limitations, we are developing a scalable-multiphysics-modeling package using PETSc DMNetwork. The package allows simulating networked multiphysics systems that are represented by linear and nonlinear equations, as well as differential algebraic equations, on extreme-scale computers. This poster presents the key features of DMNetwork, currently developed models for power and water networks in the package, and their applications to simulate power grid and river systems at scale of the continental U.S., and future work for gas and transportation systems.

B-13

Implementation of Machine learning to Predict Northern Circumpolar SOC Stock

Sagar Gautam[1] and Umakant Mishra[1]

[1]Environmental Science Division, Argonne National Laboratory, Lemont, IL 60439

Soil organic carbon (SOC) changes in circumpolar region could result in significant impacts on atmospheric carbon concentration. The exact mapping of the SOC over large spatial scale is challenging due to spatial and temporal variability. In this study we compared multiple machine learning technique to map the spatial distribution of SOC over the northern circumpolar region. The method includes generalized linear model (GLM), gradient boosting model (GMB), support vector machine (SVM), random forest (RF), decision tree (DT), Multinarrative Adaptive Regression Splines (MARS)and gradient boosting machine (GRB). Machine learning algorithm is trained and tested using the observed top soil SOC data for more than 2000 points across circumpolar region. Eight different predictor variables including; land use, bed rock geology, precipitation, temperature, slope, aspect and sediment transport index is used to predict the SOC. The simulation is conducted at resolution of the 250 m grid, by resampling all the data into similar resolution. The comparison among the model are made based on the root mean square error of the prediction, coefficient of the variation and final spatial map of soil organic carbon. The prediction maps depicted spatial variation in SOC content over northern circumpolar region. The accuracy ranking of the compared methods in decreasing order include RF, GBM, MARS, GLM, DT and SVM.

B-14

Differential Roles of Mn and Co in Ni-Rich Layered Oxide Cathodes

Shankar Aryal, Jessica L. Durham, Albert L. Lipson, Ozgenur Kahvecioglu

Applied Materials Division, Energy and Global Security, Argonne National Laboratory, Lemont, IL 60439

Layered oxides, composed of nickel, manganese, and cobalt (NMC), are sought after as cathode materials which provide improved energy density, cycle life, and safety in commercial lithium ion batteries (LIBs). Ni-rich layered oxides ($LiNi_{1-x-y}Mn_xCo_yO_2$) can provide practical discharge capacities >200 mAh/g and ~4 V discharge potential vs Li/Li^+, making them a promising cathode for next generation LIBs. However, rapid capacity fade during cycling and heat-related safety concerns are delaying their successful transition to industry. In Ni-rich NMC cathodes, Ni is the redox active cation while Co and Mn are generally believed to provide structural strength and to enhance thermal stability during cycling. Therefore, Ni-rich compositions with optimized Mn and/or Co content are being studied to further boost the performance of LIBs.

We report systematic performance optimization of $LiNiO_2$, $LiNi_{0.9}Mn_{0.1}O_2$, and $LiNi_{0.9}Co_{0.1}O_2$ Ni-rich cathodes synthesized by utilizing a Taylor Vortex Reactor. Synchrotron based X-ray diffraction (SXRD), X-ray absorption spectroscopy (XAS) and focused ion beam (FIB) imaging of pristine and cycled cathodes after 100 cycles were used to provide important information on degradation mechanisms. Additionally, the role of Mn and Co on electrochemical performance stabilization was elucidated using the crystallographic information from XRD refinement and electronic state analysis from XAS providing valuable information to design future Ni-rich layered oxide cathodes.

B-15

Rheological Characterization of Polyelectrolyte Complexes

Jelena Dinic[1,2], Matthew V. Tirrell[1,2]

[1]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637

Polyelectrolyte complexation is an entropically-driven process that occurs when oppositely charged polyelectrolytes are mixed together in aqueous media. Electrostatic attraction between oppositely charged polyelectrolytes drives phase separation into a polymer-rich complex phase and a polymer-depleted supernatant phase. The present study focuses on understanding how the intermolecular interactions dictate the rheological response of polyelectrolyte complexes formed by mixing weak oppositely charged polyelectrolytes. We find that the complexes formed between weak polyelectrolytes can form solid precipitates that exhibit solid-like viscoelastic response in the oscillatory shear measurements. We contrast the rheological response with behavior previously observed for complexes formed between strong polyelectrolytes, and explore how varying pH and ionic strength influence the structure and rheology of polyelectrolyte complexes.

B-16

Fermi Surface Topology and Evidence of Non-trivial Berry Phase in the Flat-band Semimetal Pd_3Pb

Mojammel A. Khan[1], Nirmal Ghimire[1], Terry Sullivan[1], Anand Bhattacharya[1], J.S. Jiang[1], Po-Hao Chang[2], John Singleton[3], and John Mitchell[1]

[1]Materials Science Division, Argonne National Laboratory, Argonne IL 60439
[2]Department of Computational and Data Sciences, George Mason University, Fairfax, Virginia 22030
[3]National High Magnetic Field Laboratory, Los Alamos National Laboratory Los Alamos, New Mexico 87545

Crystalline solids have emerged as testbeds in the search for exotic fundamental particles for example, three-dimensional topological semimetals offer a chance to explore new topological phases beyond those predicted in high-energy physics. Along this journey, many new phases have been discovered, including skyrmions, Weyl fermions, and Majorana fermions. Here, a study of the Fermi surface of the putative topological semimetal Pd_3Pb has been carried out using Shubnikov-de Haas oscillations measured in fields of up to 60 T. A multi-sheet Fermi surface has been reconstructed from the oscillation data. A Berry-phase analysis yields a non-trivial phase for two bands along high symmetry directions, confirming the topological nature of Pd_3Pb.This study helps access the fundamental physics of exotic particles but also strongly suggest the application of such exotic states to future technologies such as spin-based electronics and quantum computation.

B-17

Microfluidic Reactors for Applications in Controlled Synthesis of Nanoparticles and in Biology

Abhiteja Konda,[a] Ryan Dohn,[b] Rebecca Back,[b] P V Krishna Nittala,[a,c] Ralu Divan,[a] Tijana Rajh,[a] Supratik Guha,[a,c] and Anindita Basu[a,b]

[a]Center for Nanoscale Materials, Argonne National Laboratory Lemont, IL 60439, USA.
[b]Department of Medicine, University of Chicago, Chicago, IL 60637.
[c]Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637.

Single-cell genomics research has gained significant and rapidly growing interest due to its ability to characterize a population of cells at epigenomic, transcriptomic, or proteomic level with a single-cell resolution that is critical to understanding the genomic heterogeneity between individual cells comprising a population. The transcriptional heterogeneity in microbes exists as a response to the ever-changing complex environment, and understanding this heterogeneity in these unicellular organisms is critical to addressing some of the challenges in industry and medicine. The current single-cell techniques that predominantly focus on multicellular organisms cannot be readily transferred to unicellular organisms due to the differences in their size (~1 μm), composition (concomitantly small amount of RNA),and a tough, adaptive cell wall that permits their survival in harsh environments (extreme pH or temperatures, anti-microbials, etc.). In the present work, a droplet-based approach is used to transcriptionally profile each microbial species at single-cell resolution and high throughput. A suite of different techniques (both physical and chemical) including the use of microelectromechanical systems [MEMS], plasmon resonance (using anisotropic gold nanoparticles), laser ablation, acoustic waves, either used independently or in combination are studied for the lysis of the cell wall—a key challenge to overcome for the success of the project. The single-cell lysates are then used as input for high-throughput single-cell RNA-Seq. This work will significantly enhance the current technologies and will enable generalized, cost-effective single-cell RNA sequencing in microbes at high throughput and therefore will be vital to advancing science from different fronts for applications in synthetic biology, environmental engineering, energy, and medicine.

B-18

Atomic Layer Deposition of ZnO Cluster Arrays: Controlling ZnO Nucleation Through Hydrogen Plasma-induced Chemical Activation of Sic-supported Epitaxial Graphene

David J. Mandia;[1,2] Leighton O. Jones;[2,3] Nathan P. Guisinger;[4] Matthew S. Rahn;[5] Mark C. Hersam;[2,5] George C. Schatz;[2,3] Alex B.F. Martinson[1,2]

[1]Materials Science Division (MSD), Argonne National Laboratory; Lemont, IL, USA
[2]Center for Light Energy Activated Redox Processes (LEAP), Northwestern University, Evanston, IL, USA
[3]Departmentof Chemistry, Northwestern University, Evanston, IL, USA
[4]Center for Nanoscale Materials (CNM), Argonne National Laboratory, Lemont, IL, USA
[5]Department of Materials Science & Engineering, Northwestern University, Evanston, IL, USA

Solar fuels catalysis is vital to developing new technologies for creating value-added products from alternative feedstocks, such as carbon dioxide and water. Inhomogeneities in typical "state-of-the-art" synthesis techniques for heterogeneous catalysts severely limit the accuracy of determining the chemical composition of active sites and elucidating mechanistic details for catalysis. In the present work, we synthesize discrete, few-atom metal oxide cluster arrays to gain insight into the relationship between cluster size/shape and catalytic activity/efficiency. Clusters are synthesized with exquisite synthetic control via atomic layer deposition (ALD) on chemically modified epitaxial graphene (EG) on SiC. Metal oxide/nitride/sulfide ALD thin film growth is strongly inhibited on graphene. Understanding the factors contributing to unintentional and intentional nucleation and growth on EG will benefit from the use of an accurate, precise imaging technique such as AFM and STM. Furthermore, we employ an in-situ plasma treatment (H_2, N_2, O_2) of EG to create attachment points for intentional cluster nucleation via ALD. DFT calculations predict energetically favorable surface terminations of graphene after H_2 plasma treatment with H-terminated surface sites becoming the chemical handles for controlled ZnO nucleation. Discrete ZnO clusters will be synthesized and cluster size, morphology, distribution, and density of clusters will be determined via XPS and AFM, with nucleation monitored by in-situ spectroscopic ellipsometry. Control over the nucleation and distribution of these clusters has implications for enhanced catalytic activity of the ZnO clusters by tuning the cluster size based on either the number of ALD cycles or by tuning the plasma pre-treatment time.

B-19

Ion-Specific Effects of Divalent Ions on the Structure of Polyelectrolyte Brushes

Dean J. Mastropietro[1,2], Xin Xu[3], Marina Ruths[4], Matthew V. Tirrell[1,2], and Jing Yu[3]

[1]Center for Molecular Engineering, Argonne National Laboratory, Argonne, IL 60439
[2]Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637
[3]School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798
[4]Department of Chemistry, University of Massachusetts Lowell, Lowell, Massachusetts 01854

Polyelectrolytes are macromolecules consisting of charged repeat units (monomers). Anchoring many polyelectrolytes to a surface at high grafting densities forms a polyelectrolyte brush. Polyelectrolyte brushes create a highly repulsive interface that resists friction forces and fouling in the presence of aqueous environments, however, these properties are highly susceptible to multivalent ions. This work uses surface forces apparatus (SFA) measurements, atomic force microscopy (AFM) imaging, and isothermal titration calorimetry (ITC) to investigate the effect of $Mg(NO_3)_2$, $Ca(NO_3)_2$, and $Ba(NO_3)_2$ on brush height (SFA/AFM), topology (AFM), and thermodynamics (ITC) of polystyrene sulfonate (PSS) brushes. We demonstrate that Mg^{2+} and Ca^{2+} decrease brush height by a lesser degree than Ba^{2+}. Additionally, AFM images show that PSS brushes form micelle-like features in the Ba^{2+}, which are absent in the presence of Mg^{2+} and Ca^{2+}. Finally, ITC results show that these ion-specific effects result from lower binding enthalpies between PSS and Ba^{2+} than between PSS and Mg^{2+}/Ca^{2+}.

B-20

Electronic Structure and Lattice Dynamics of Strongly Correlated Materials: DFT+DMFT Approach

Vijay Singh, Benny Wah, and Hyowon Park

Department of Physics, University of Illinois at Chicago, Chicago, Illinois, 60607, USA

Computational materials design of strongly correlated materials (SCM) has been challenging in modern condensed matter physics since it requires the development of more accurate methodologies beyond density functional theory (DFT). In the poster, I will present our recent development of an efficient computational method so called DMFTwDFT to treat dynamical correlations in SCM. I use dynamical mean-field theory (DMFT) in combination with DFT to compute the electronic structure and lattice-dynamics of strongly correlated f-and d-electron systems, specifically, rare-earth metals and $LaNiO_3$. The main point of the debate in f-electron system is related to the understanding of the role played by f electrons —they are localized or itinerant, or more exactly how many f electrons are localized or itinerant. For this reason, the theoretical and experimental investigations of the electronic structure of rare-earth metals have always occupied an important position in rare-earth research. In $LaNiO_3$, the electronic structure and its relation to lattice dynamics are still under debate. Here, I use the DMFT+DFT method implemented using the maximally localized Wannier function as the local basis set and combining various DFT codes to study electronic and structural properties of these materials. Our results will be also compared to other DMFT+DFT codes employing different local basis sets and DFT implementations

B-21

Machine learning based framework for phase diagrams and discovery of new phases

Srilok Srinivasan[1], Troy Loeffler[1], Henry Chan[1], Mathew Cherukara[1], Pierre Darancet[1], Subramanian Sankaranarayanan[1,2]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL, USA
[2]Department of Mechanical and Industrial Engineering, The University of Illinois at Chicago, Chicago, IL, USA

We have developed a machine learning based framework to identify new metastable phases of matter, determine and validate phase diagrams in chemical systems without any recourse to experimental information. Specifically, we demonstrate our machine learning approach on carbon. We use evolutionary algorithms to sample design space with chemically informed geometric constrains to identify candidate metastable phases. Using our framework, we compute the Gibbs free energy of the candidate metastable phases to generate the metastable phase diagram. Such metastable phase diagrams will shed light on the possible reaction pathway and the intermediate metastable phases during phase transformation (eg: graphite to diamond). Furthermore, within the graphite family of structures, a single graphene layer has exotic electronic properties ranging from exceptional transport properties to topological structures exhibiting quantum hall effect, owing to its two-dimensional nature. We employ our high throughput framework to further explore topological geometries of quasi-1D graphene nanoribbons satisfying mirror and/or inversion symmetries. We show that by discretizing the nanoribbons into smaller motifs, the topological class of the nanoribbon can be understood in terms of the band inversion induced by the change in coupling between the motifs when they are laterally shifted. We have identified, using our framework, 224071 topologically non-trivial graphene nanoribbons phases. We train a deep neural network (DNN) on the adjacency matrix to identify relevant geometrical features of the topological structures in the latent space.

B-22

Novel Solid Lubricants for Use in Multifarious Environments at High Load and Sliding Speeds

Aditya V. Ayyagari, Kalyan Mutyala, and Anirudha V. Sumant*

Center for Nanoscale Materials, Argonne National Laboratory, 9700 S Cass Ave, Lemont IL 60439, United States

Existing solid lubricants such as MoS_2 and Graphite lack the adaptability to dynamically changing atmospheres. This study presents the results of a novel 2D materials based solid lubricant developed at Argonne National Laboratory that has overcome this drawback and shown exceptional performance in multifarious environments namely, ambient (humid) atmosphere, dry nitrogen and in vacuum. Solution processed 2D-Molybdenum disulfide and Graphene-oxide were *sonixed* and deposited on to stainless steel substrate using a simple spray-coating technique. The tribological performance of the coatings showed very low friction and wear, at 0.03 (in dry nitrogen); 0.05 (in vacuum) and 0.08 (in ambient air) in comparison to steel-on-steel tribopair (at 0.78). Raman spectroscopy of the tribolayers showed increased MoS_2 peak intensity with increasing normal load and sliding velocity. This in conjunction with absence of MoOx peaks indicates a strong resistance to intercalation with moisture and oxygen. Transmission electron microscopy revealed that highly aligned MoS_2 packets were sandwiched between graphene-oxide layers which may have helped in preventing oxidation of MoS_2 and thus leading to the excellent tribological performance in all environments.

B-23

Molecular assembly of amino acids on Cu(111)

Constance Pfeiffer[1] and Nathan Guisinger[1]

[1]Nanoscience and Technology Division, Argonne National Laboratory, Argonne, IL 60439

Amino acids are the building blocks of proteins. Using a scanning tunnel microscope to study how they assemble on surfaces, useful information can be obtained for controlling material symmetry and thus the development of atomically manufactured molecular networks. Furthermore, it can lead to generating artificial condense matter testbeds and inducing unusual behaviors. There are twenty simple amino acids and except for glycine, all present either D-or L-chirality. Proteins, however, selectively use only the L-configuration of amino acids. In attempt to understand this selectively as well as obtain an understand of the molecular assemblies of amino acids on surfaces, we have studied several amino acids on a Cu(111) surface. The amino acids investigated, tryptophan and threonine, form basic building blocks that exhibit a distinct chirality depending on which configuration is adsorbed.

B-24

Protein Analogous Micelles for Intracellular Delivery of Peptide Therapeutics

Yu Tian[1,2], Mathew R. Schnorenberg[2,3], James L. LaBelle[3] and Matthew V. Tirrell[1,2]

[1]Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637
[2]Center for Molecular Engineering, Argonne National Laboratory, Lemont, IL 60439
[3]Departmentof Pediatrics, Section of Hematology/Oncology, University of Chicago, Chicago, IL 60637

In cancer treatment, drugs can be categorized into two types, small molecules and full-size biologicals (anti-body). Therefore, it leaves a gap in the size of the druggable therapeutic targets, including a variety of protein-protein interactions regulate the apoptosis/cell survival balance. While peptides fall in this size gap can potentially be developed into new drugs to treat cancer. However, preclinical peptide therapeutics generally have low in vivo efficacy due to the poor cell permeability and the high proteolysis sensitivity. By attaching hydrophobic moieties to the therapeutic peptides, the conjugated amphiphilic drug compounds can self-assemble into micelles with some chemical properties analogous to proteins. Because of the high chemical versatility of the peptides, such a design of protein analogous micelle system can be highly modular to achieve the cell permeability, longevity, targeting, and combined delivery of therapeutics. In this work, therapeutic peptides targeting intracellular p53 pathway and BCL-2 family proteins are chemical modified as peptide amphiphiles to formulate into micellar nanoparticles. In vitro cell culture experiments have demonstrated the high potency against wild type p53 DLBCL cell lines.

PHYSICS AND HIGH ENERGY PHYSICS

B-25

Search for Dijet Resonances in Events with an Isolated Lepton Using $\sqrt{s}$ = 13 TeV Proton-Proton Collision Data Collected by the ATLAS Detector at the Large Hadron Collider

S. Chekanov, J. Love, J. Proudfoot, S. Darmora

High Energy Physics Division, Argonne National Laboratory, Argonne, IL 60439

A search for new physics in particle collisions is performed at a center of mass energy of $\sqrt{s}$ = 13 tera electron Volts (TeV) with an integrated luminosity of $79.8 fb^{-1}$ recorded by the ATLAS detector at the Large Hadron Collider. This search was performed using invariant mass of two jets (m_{jj}), distributions ranging from 0.22-6.3 TeV in events with at least one isolated lepton (e or μ) are searched for excesses above background expectations. Selecting events based on the presence of a lepton can probe lower m_{jj} than traditional inclusive dijet searches and targets a large range of new physics models with a final-state lepton. Signatures of such processes include associated production of a W or Z boson. No statistically significant deviation from the background hypothesis is found. In the absence of signals indicating the presence of new physics, limits are calculated based on generic Gaussian signals with a width ranging from that determined by the detector resolution to 15% of the resonance mass. Contributions from a signal with effective cross-section ranging from 50 fb to 0.1 fb are excluded in the mass range between 0.25 TeV and 6 TeV. As a next step, a neural network technique is planned to be used to improve sensitivity to investigate a wide range of theories beyond the Standard Model.

B-26

Engineering nonlinear dissipation across two superconducting cavity modes

Juliang Li[1], Jeffrey Gertler[2], Chen Wang[2]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2]Physics Department, University of Massachusetts Amherst, Amherst MA 01003

Dissipation engineering has emerged in recently years as a promising way to allow efficient control of complex quantum systems. The key ingredient for such dissipative quantum control is to synthesize non-trivial dissipation operators (jump operators), such as linear superposition of photon loss in two oscillators or (nonlinear) two-photon loss in one oscillator. In this talk we present experiments towards synthesizing various nonlinear jump operators across two oscillator modes. Our system employs a 3D cQED device architecture that has two quantum memory modes and one reservoir mode (potentially two) that are coupled via transom qubit(s). The system has shown the capability to couple two highly-coherent oscillator modes to a reservoir (readout) mode and to implement four-wave mixing. We leverage these coherent multi-body interactions to engineer cross-cavity two-photon driven dissipation, with further extension to arbitrary 2nd order polynomial of creation/annihilation operators of two cavities.

B-27

Search for Novel Physics using Deep Underground Neutrino Experiment

Aleena Rafique and Zelimir Djurcic

High Energy Physics Division, Argonne National Laboratory, Lemont, IL 60439

The Deep Underground Neutrino Experiment (DUNE) is a leading-edge experiment for neutrino science and proton decay studies. The single-phase liquid argon prototype detector (PortoDUNE) at CERN is a crucial milestone for the DUNE that will inform the construction and operation of the far detector modules. In this poster, I will present the current status of reconstructing Michel electrons from cosmic-ray muons in the ProtoDUNE detector. These Michel electrons are distributed uniformly inside the detector and serve as a natural and powerful sample to study the detector's response for low-energy (tens of MeV) interactions as a function of position. We have developed a selection tool to identify such Michel electrons which could benefit any LArTPC experiment generically.

B-28

Single-particle structure of ^{207}Hg and the creation of heavy elements

T. L. Tang[1], B. P. Kay[1], C. R. Hoffman[1], D. K. Sharp[2], J. P. Schiffer[1], L. P. Gaffney[3], M. R. Mumpower[4], E. F. Baader[3], P. A. Butler[4], W. N. Catford[5], G. de Angelis[6], F.Flavigny[7], S. J. Freeman[2], E. T. Gregor[6], M. D. Gott[1], J. Konki[3], M. Labiche[9], I. Lazurus[9], P. T. MacGregor[2], I. Martel[4], R. D. Page[5], Zs. Podolyák[6], O. Poleshchuck[10], R. Raabe[10], A. Arokiaraj[10], F. Recchia[11,12], J. F. Smith[13,14], S. V. Szwec[15], and J. Yang[10]

[1]Argonne National Laboratory, Lemont, IL 60439, U.S.A.
[2]University of Manchester, Manchester, U.K.,
[3]CERN, Genève, Switzerland,
[4]Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, U.S.A.
[5]University of Liverpool, Liverpool, U.K.
[6]University of Surrey, Guildford, U.K.
[7]Laboratori Nazionali di Legnaro, Legnaro, Italy
[8]Institut de Physique Nucléaire, Université Paris-Saclay, 91406 Orsay, France
[9]STFC Daresbury Laboratory, Warrington, U.K.
[10]KU Leuven, Belgium
[11]Universitàdegli Studi di Padova, Padova, Italy
[12]INFN Padova, Padova, Italy
[13]University of the West of Scotland, Paisley, U.K.
[14]SUPA, Scottish Universities Physics Alliance, Glasgow, U.K.
[15]University of Jyvaskyla, Finland.

The single-particle structure of the N=127 isotones below ^{209}Pb along is terra incognita. Using a ^{206}Hg beam produced at the CERN's ISOLDE facility at an energy of 7.4 MeV/u, the single-neutron excitations in ^{207}Hg have been measured via the ^{206}Hg(d,p) reaction in inverse kinematics. The energy and position of protons emitted at backwards angles were measured using the new ISOLDE Solenoidal Spectrometer (ISS) at a magnetic field strength of 2.5 T. The $1g_{9/2}$, $2d_{5/2}$, $3s_{1/2}$, $2d_{3/2}$ and $1g_{7/2}$ orbitals were observed in ^{207}Hg.

With the single particle energies of the ^{209}Pb and those of ^{207}Hg, now known for the first time, a Woods-Saxon (WS) potential was fitted on a common footing; the rms variation of the WS levels with respect to the experimental levels was~ 200 keV. The extrapolation the neutron excitations at N=127 to the neutron threshold shows that the neutron dripline for N=127 is around gadolinium with Z = 64. It is around this Z that the r-process starts to create heavy elements with N>127, and eventually actinides.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Contract Number DE-AC02-06CH11357.

SYNCHROTRON RESEARCH

B-29

Radiation Heating Mitigation on the SuperConducting Arbitrary-Polarized Emitter (SCAPE) Undulator

Laura Boon[1] and Yury Ivanyushenkov[1]

[1]Accelerator Systems Division, Argonne National Laboratory, Argonne, IL 60439

The SuperConducting Arbitrary-Polarized Emitter (SCAPE) is a new type of superconducting undulator design proposed for Advanced Photon Source-Upgrade which will provide circular and linear polarization to beamline 4. SCAPE consists of two 1.5m long undulator magnets in a single cryostat. with a 3mm-raduis beam chamber.

Recent analysis of the dipole radiation heating on the beam chamber suggests 160W of heating. This is much greater than the 20W of power on the Helical Superconducting Undulator. Unless the power can be reduced there will have to be a re-design of SCAPE for it to operate in the ring. This work presents what is being done to mitigate the synchrotron radiation heating on the beam chamber, analyzing possible solutions and discussing the pros and cons of each.

B-30

Solving the Solvation Structure of Ions: X-ray Absorption Studies on Multivalent Ions in Solution

Darren M. Driscoll[1,2], Nathan Hahn[2,3], and Mahalingam Balasubramanian[1, 2]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439
[2]Joint Center for Energy Storage Research, Argonne National Laboratory, Lemont, IL 60439
[3]Material, Physical and Chemical Sciences Center, Sandia National Laboratories, Albuquerque, NM 87158

X-ray absorption fine structure (XAFS) studies of liquid electrolytes have been performed to identify the elemental and geometric coordination around multivalent cations. Progress has been made in the characterization of first- and second-coordination shells around multivalent cations such as Ca^{2+} and Zn^{2+} in a multitude of organic and aqueous systems. Specially, the coordination environment of Ca^{2+} in a solution of tetrahydrofuran (THF) and BH_4^- [1] anions was found to exhibit characteristics of both Ca-O interactions as well as Ca-BH_4 interactions through the analysis of the XAFS data. Through careful fitting, using optimized coordination geometries and photoelectron scattering pathways, we have elucidated the local structure of calcium cations. We can calculate the coordination numbers and distances of both solvent molecules and anions around the cationic molecule. Multi-anion experiments including tetrakis(hexafluoroisopropoxy)borate (BHFIP), a weakly coordination anion and a variety of different halogens (Br^-, Cl^-) were found to induce contact-ion pairs in solutions, exhibited by pronounced changes in the extended fine X-ray structure (EXAFS) of the liquid electrolyte. These studies suggest the contact-ion pairing in certain cation-anion systems may impact the overall viability of certain cation-anion-solvent compilations in electrochemical systems.

B-31

Hard X-ray Fluorescence Measurements with Transition Edge Sensors at the Advanced Photon Source

Tejas Guruswamy[1], Lisa M. Gades[1], Antonino Miceli[1], Umeshkumar M. Patel[1], John T. Weizeorick[1], and Orlando Quaranta[1]

[1]X-ray Science Division, Argonne National Laboratory, Lemont IL 60439

X-ray Fluorescence (XRF) and X-ray Emission Spectroscopy (XES) are well-known, powerful techniques for elemental and chemical analysis, where improvements in detector technology directly lead to improved science outcomes. At the Advanced Photon Source (APS), we are developing a new detector array based on superconducting Transition Edge Sensors (TESs) for hard X-ray energies (2 to 20 keV). TESs provide an order-of-magnitude improvement in energy resolution compared to the best semiconductor-based energy-dispersive spectrometers, while still allowing for a high count rate and spatial resolution unlike wavelength-dispersive spectrometers. Here, we present a series of recent XRF measurements, involving combinations of transition metals with closely spaced emission lines (e.g. Co/Ni/Cu), undertaken with our prototype TESs. We make quantitative comparisons with the silicon-drift detectors available to beamline users at the APS, and outline our progress towards enabling new X-ray science.

B-32

Robust method to decipher atomistic structure of molecule in solution using high-energy solution X-ray scattering

Tae Wu Kim and David M. Tiede

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

Structural characterization of newly synthesized molecule is essential for understanding its function related with the molecular structure. In this regard, high-energy solution X-ray solution scattering (HESXS) can be an alternative way for obtaining the structural information of target molecule in liquid phase as a complementary method with X-ray absorption spectroscopy (XAS). However, the analysis method to extract the structural information from the HESXS signal has not been established yet. Here, we describe the new analysis method using chemical knowledge from quantum mechanical calculation and molecular dynamics simulation. As an exemplary work, the method was employed to determine molecular structure of Ru-based photocatalyst in solution. It showed that the photocatalyst has the slight different conformation in solution relative to in crystalline phase and forms the inter-molecular network between solute and surrounding polar solvents.

B-33

Algorithm to automate trajectory tuning for the APS-U undulators

M. Qian[1], Y. Pia[1], I. Vasserman[1], and J. Xu[1]

[1]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, USA

The Advanced Photon Source (APS) is having a major upgrade to its storage ring. The APS upgrade (APS-U) project plans to build forty new Hybrid Permanent Magnet Undulators (HPMUs), and modify and reuse twenty existing HPMUs. In order to meet the APS-U undulator radiation requirements, the quality of the undulator magnetic field needs to be fine-tuned to the specifications. The traditional method of tuning depends on tuning specialist's personal experience and is usually time consuming. Therefore is not desirable for mass production of undulators. We developed algorithm that automatically optimizes the undulator trajectory and phase tuning based on the Differential Evolution scheme. Testing of the algorithm on various existing undulator measurement data shows that it is efficient and precise. A detailed description of the algorithms and performance is reported.

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Argonne National Laboratory launched in May its first startup incubator. Chain Reactions Innovations (CRI) is the Midwest's first energy and science technology incubator that embeds entrepreneurs from industry and academia into a national laboratory. This new two-year program provides a few unique opportunities for the postdoc community. You can join as a member of a startup and get two years at Argonne to grow your startup before

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Acknowledgments

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Kathy Eggers of the Argonne Leadership Institute
Argonne Visitors Center and Security Staff
Ali Tucker, Catering

All the wonderful volunteers who served as poster judges

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