



Annual Postdoctoral Research and Career Symposium

NOVEMBER 4TH & 5TH, 2020

ORGANIZED BY THE POSTDOCTORAL SOCIETY OF ARGONNE

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**2020 POSTDOCTORAL
RESEARCH AND CAREER
SYMPOSIUM**

Leadership Institute at Argonne National Laboratory

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Argonne National Laboratory Postdoctoral Research and Career Symposium

November 4th & 5th, 2020

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2020 Postdoctoral Research and Career Symposium
November 4th & 5th, 2020

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2020 Postdoctoral Research and Career Symposium
November 4th & 5th, 2020

Agenda

Note: All times are Central Standard Time

Day 1 – Wednesday, November 4, 2020

- 9:00 AM Welcome Remarks by Director Paul Kearns
- 9:15 AM Keynote by Professor Todd Allen
- 10:00 AM Technical Sessions 1
- 12:00 PM Lunch Break
- 1:00 PM Networking with Companies 1
- 3:00 PM Career Panel – Industry Track 1
- 4:00 PM Close of Day 1 Sessions
- 7:30 PM Trivia Night

Day 2 – Thursday, November 5, 2020

- 9:00 AM Career Panel – Academia/National Lab Track 1
- 10:00 AM Technical Sessions 2
- 12:00 PM Lunch Break
- 1:00 PM Networking with Companies 2
- 3:00 PM Career Panel – Industry Track 2
- 4:00 PM Award Presentations and Closing Remarks

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2020 Keynote Address



Dr. Todd Allen, Professor, University of Michigan

Dr. Todd Allen is a Professor at the University of Michigan and a Senior Fellow at Third Way, a DC-based Think Tank, supporting their Clean Energy Portfolio. He was the Deputy Director for Science and Technology at the Idaho National Laboratory from January 2013 through January 2016. Prior to INL, he was a Professor in the Engineering Physics Department at the University of Wisconsin, a position held September 2003–December 2012 and again from January 2016–December 2018. From March 2008 to December 2012, he was concurrently the Scientific Director of the Advanced Test Reactor National Scientific User Facility at INL. Prior to joining the University of Wisconsin, he was a Nuclear Engineer at Argonne National Laboratory-West in Idaho Falls. His Doctoral Degree is in Nuclear Engineering from the University of Michigan (1997), and his Bachelor's

Degree is in Nuclear Engineering from Northwestern University (1984). Prior to graduate work, he was an officer in the United States Navy Nuclear Power Program.

Welcome Remarks Speaker

Paul Kearns, Laboratory Director, Argonne National Laboratory



Paul K. Kearns has served as Director of the U.S. Department of Energy (DOE) Argonne National Laboratory since 2017. A biologist and accomplished steward of diverse scientific resources, Kearns has managed complex research and development enterprises for over 30 years, enabling them to achieve ambitious goals in energy, environment, and national security. As Argonne laboratory director, Kearns oversees multiple projects critical to Argonne's mission of accelerating science and technology to drive U.S. prosperity and security. Working to upgrade the Advanced Photon Source and launch the first exascale computer in the U.S. at the Argonne Leadership Computing Facility are critical to maintain U.S. leadership in science and technology. Argonne's leadership of the Joint Center for Energy Storage Research reflects the laboratory's long history of battery science expertise and collaboration.

As Argonne Chief Operations Officer from 2010 to 2017, Kearns directed over 900 staff providing mission support services in financial management, human resources, safety performance, business systems, technology commercialization, and facilities management. Kearns was an executive with Battelle Global Laboratory Operations for five years prior to joining Argonne. Kearns is a fellow of the American Association for the Advancement of Science. He serves on the Executive Committee of the DOE National Laboratory Directors' Council and the U.S. Council on Competitiveness' National Commission on Innovation and Competitiveness Frontiers.

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. Leonardo Bautista-Gomez, Barcelona Supercomputing Center



Dr. Leonardo Bautista-Gomez is a Senior Researcher at the Barcelona Supercomputing Center where he leads several projects on HPC resilience, deep learning, and blockchain technology. He was awarded a European Marie Curie Fellowship. In 2016, he was awarded the IEEE TCSC Award for Excellence in Scalable Computing (Early Career Researcher). Before moving to BSC he was a postdoctoral appointee at Argonne National Laboratory, where he investigated data corruption and error propagation. He did his Ph.D. in reliability for supercomputers at the Tokyo Institute of Technology in Japan.

Dr. Julie Bessac, Assistant Computational Statistician, Argonne National Laboratory

Dr. Julie Bessac received a B.Sc. degree in fundamental mathematics and an M.S. degree in probability and statistics, in 2008 and 2011, respectively, from the University of Rennes 1 in France. She received her Ph.D. in 2014 in applied mathematics from the University of Rennes 1 in France. Between November 2014 and July 2017, she was a postdoctoral appointee in the Mathematics and Computer Science Division at Argonne National Laboratory. Since July 2017, she has been an Assistant Computational Statistician at Argonne National Laboratory. Her research focuses on the statistical modeling, forecasting, and uncertainty quantification for diverse applications such as geophysical processes.



Dr. Ilias Bilonis, Associate Professor of Mechanical Engineering at Purdue University



Prof. Ilias Bilonis obtained his diploma in applied mathematics and physical sciences from the National Technical University of Athens in 2008. In 2013, he obtained his Ph.D. in applied mathematics from Cornell University. After graduation, he spent a year working as a postdoctoral appointee at the Mathematics and Computer Science Division of Argonne National Laboratory. In August 2014, he became faculty of Mechanical Engineering at Purdue University, where he established the Predictive Science Laboratory (PSL). The mission of Bilonis' is group is to create AI technologies that accelerate the pace of engineering innovation with particular emphasis on probabilistic approaches (thought of as an extension of logic under uncertainty) with an additional layer of causality (expressed through physical laws and graphical models). The

current applications of PSL span the range between technical (e.g., electric machines, high-performance materials) and sociotechnical systems (e.g., smart buildings, extra-terrestrial habitats). Bilonis' is currently the leader of the Awareness Thrust of the NASA-funded Resilient Extraterrestrial Habitats Institute, and he is responsible for the design and implementation of the health management of the habitat system. Other research support has been provided by NSF, DARPA, Ford, Purdue University, and the University of Illinois. Bilonis' has published more than 40 journal papers, two book chapters, and several conference papers. He has been very active advising Master and Ph.D. students, and in 2019 he was presented with the "Outstanding Faculty Mentor of Mechanical Engineering Graduate Students" award. Furthermore, he enjoys teaching and he has received the "Outstanding Engineering Teacher Recognition" three times.

Dr. Zina Jarrahi Cinker, Director General of Advanced Material Pandemic & Future Preparedness Taskforce

Dr. Zina Jarrahi Cinker serves as the Director General of Advanced Material Pandemic & Future Preparedness Taskforce (AMPT)-- an international, public interest organization with 15 country chapters focusing on use of advanced materials to solve some of humanity's most immediate challenges. As a globally recognized graphene expert, industrial business strategist, she has been focused on facilitating the commercialization of graphene and other advanced materials from breakthrough to industrialization and bridging the gap between academia and industry. She previously served as the executive director of the U.S. National Graphene Association. Dr. Jarrahi-Cinker received her PhD in the field of ultrafast spectroscopy from Vanderbilt University.



Chris Claxton, Principal, Volta Energy Technologies



Chris Claxton has over 15 years of experience in early-stage technology commercialization. He has been on the founding team of several technology start-up companies and has worked as a commercialization consultant to various government agencies including the NIH, NASA, and the U.S. Department of Energy. Before joining the Volta team in early 2020, Chris spent seven years as a Sr. Business Development Executive for Argonne National Laboratory, leading business development and technology licensing for the Lab's advanced electrochemical energy storage R&D program. While at Argonne, he worked alongside the Lab's scientists, engineers, and attorneys to successfully lead and close deals with companies across the energy storage value chain, including raw material suppliers, battery material manufacturers, cell and pack

manufacturers, system integrators, and automotive OEMs in North America, Europe, and Asia. Chris is currently a Principal at Volta Energy Technologies where he manages the firm's pipeline of energy storage venture deals. He holds a B.S. degree in Finance and Business from Indiana University.

Dr. Marvin Cummings, Program Manager, New York Academy of Sciences

Dr. Marvin Cummings is currently a Physical Science & Engineering program manager at the non-profit – New York Academy of Sciences, the oldest scientific organization in the United States. Prior to joining the Academy, he worked as a postdoctoral researcher within Argonne National Laboratory's X-ray Science Division (XSD) at the Advanced Photon Source. Marvin Cummings also received a 1-year appointment at the Getty Conservation Institute as a National Science Foundation postdoctoral fellow, where he studied Attic red-figure and black-figure pottery produced during the 6th to 4th centuries B.C.



Dr. Greg Halder, Business Development Executive, Argonne National Laboratory



Dr. Greg Halder is a Business Development Executive in the Technology Commercialization & Partnerships Division, where he supports industry partnerships and technology commercialization for Argonne's energy storage R&D programs, including as part of the Argonne Collaborative Center for Energy Storage Science (ACCESS) team. Greg is a former APS scientist, having led the *in situ* powder diffraction user program from 2010–2015. He returned to Argonne in 2017 to join the Technology Commercialization and Partnerships Division after spending two years in Austin, Texas, where he completed his MBA and worked in science and technology consulting for multiple customers, ranging from a water filtration startup to a Fortune 500 oil and gas company. Greg's scientific

background includes a Ph.D. in physical chemistry from the University of Sydney in Australia (2004) and a B.S. from the University of Otago in New Zealand (2000). He was the recipient of a 2007 Arthur Holly Compton ("Named") Postdoctoral Fellowship within Argonne's Materials Science Division, where he developed X-ray scattering techniques for studying the functional properties of molecular materials for energy storage and carbon capture technologies.

Dr. Erin Iski, Associate Professor, Department of Chemistry and Biochemistry, The University of Tulsa

Dr. Erin Iski is an Associate Professor of Chemistry at the University of Tulsa. She received her B.S. degree in chemistry from the University of Tulsa in 2005 and a Ph.D. from Tufts University in 2011 under the direction of Prof. Charles Sykes. While at Tufts, her research focused on the surface chemistry of large molecules on metal surfaces using scanning tunneling microscopy (STM). Utilizing the STM in the Sykes Lab, which was capable of low temperature scanning and ultra-high vacuum conditions, Dr. Iski successfully published over 15 peer-reviewed publications. After working as a Postdoctoral Fellow at Argonne National Lab with Dr. Nathan Guisinger in the Center for Nanoscale Materials, Dr. Iski joined the University of Tulsa in 2013. At TU, the Iski Group focuses



on the use of electrochemical STM (EC-STM) to study thermally stable nano-alloys of Ag on Au(111) and the assembly and interaction of amino acids on metal surfaces. In addition to research, Dr. Iski is committed to educational outreach within the Tulsa community and was recognized in 2016 with the Women of Distinction Award from the Tulsa Business & Legal News. She is a member of ACS, serving as the local ACS secretary for two years, the Executive Committee of the Surface Science Division of AVS, and the AAUW (American Association of University Women).

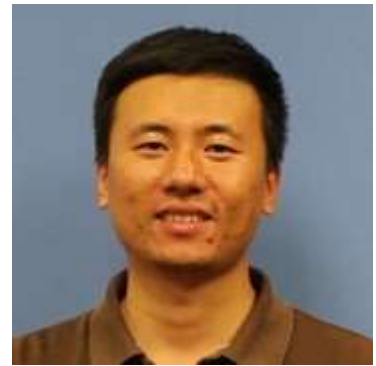
Dr. Steve Letourneau, ASM International



Steve received his Ph.D. in material science from Boise State University. Afterwards he accepted a postdoctoral appointment from Argonne where he collaborated closely with industry and academic partners on the development of novel atomic layer deposition recipes, including the scale of thin film processes up to 200 mm products. He currently works at ASM as a process engineer.

Dr. Fu Lin, Staff Research Engineer, Raytheon Technologies

Dr. Fu Lin is a Staff Research Engineer in Autonomous & Intelligent Systems, Raytheon Technologies Research Center. His research work focuses on control, optimization, and machine learning, with applications sponsored by several government agencies, including energy-efficient buildings (ARPR-E), fault detection for air revitalization systems (NASA), bio-threat detection and response in indoor environments (DHS), and cyber security for grid-interactive buildings (DOE). Dr. Lin has published 50+ peer-reviewed journal and conference papers with ~1600 citations. He has two design patents.



Dr. Youssef Nashed, Lead Computer Vision Scientist at Stats Perform



Dr. Youssef Nashed's research career spans more than 12 years, 5 countries, and a wide range of computer vision applications. He is currently the lead Computer Vision scientist at Stats Perform, the world's largest provider of sports data analytics. Before moving to industry, he held positions at Argonne National Laboratory and Northwestern University (2013–2020) as an Assistant Computer Scientist and a Research Assistant Professor, where he pioneered solutions for large scale x-ray image inversion problems at the Advanced Photon Source on the world's fastest supercomputers. He obtained his M.Sc. (2008) and Ph.D. (2013) degrees from the University of Hull (UK) and the University of Parma (Italy), respectively. His Ph.D. research focused on real-time detection and classification of patterns in images and videos for body pose estimation, histological structure localization, autonomous vehicles, and gesture recognition. He is (co)author of several publications in journals and conference proceedings, with topics ranging from image processing and computer vision, scaling AI algorithms on HPC platforms, to algorithm configuration using GPU-based metaheuristics. He is also the author of various open source software toolkits for virtual anthropology, image reconstruction, derivative-free optimization, and data management and visualization. In his current role, he leads a team of computer vision scientists in developing and deploying Deep Learning models for player detection, tracking, and activity recognition.

Dr. Giovanni Ramirez, Sales Manager US-West and Mexico and Applications Scientist, Bruker Nano Surfaces and Metrology Division

Dr. Giovanni Ramirez is a materials scientist and engineer specialized in surface engineering, coatings/thin films, tribology, and materials characterization. He received his B.S. degree in mechanical engineering (2006) and his M.Sc. degree in materials engineering from National University in Colombia (2008), and his Ph.D. from National Autonomous University of Mexico (2012). After receiving his Ph.D., He spent one year as a visiting scholar at Argonne National Laboratory, and after that he stayed for 3.5 more years as a Postdoctoral Researcher. After finishing his time at Argonne, he went to work for Bruker in 2017 as a Sr Applications Scientist, serving as a subject matter expert in different characterization techniques such as tribometry, surface metrology, and nanoindentation.



Dr. Ramirez has been involved in numerous research projects dealing with development and characterization of thin films/coatings for different applications. These include participation in research activities that were both basic and applied in nature and directed toward understanding of the underlying fundamental mechanisms involved in the behavior of many types of coatings and materials. He contributed to large project reports, key scientific publications (including one in *Nature*), and three U.S. patents.

In 2019 Dr. Ramirez was promoted to the position of Western US Sales Manager for Bruker Nano Surfaces and Metrology Division. His expanded role now combines his technical expertise with acquired skills in business development and with it carries responsibility for selling several million dollars of equipment every year. In this position, Dr. Ramirez serves as a customer consultant, where he strives to fully understand technical challenges for customers in academia, government, and industry, and then matches those requirements to solutions derived from a large portfolio of advanced offerings within the Bruker organization.

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BIOSCIENCES & BIOENGINEERING

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AI Guided Discovery of Self-assembly Peptide Sequences using Monte Carlo Tree Search and Coarse-Grained Simulations

Rohit Batra¹, Troy David Loeffler¹, Henry Chan¹, Srilok Srinivasan¹, Christopher H. Fry¹, and Subramanian KRS Sankaranarayanan¹

¹Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439

Peptide materials have a wide array of functions from tissue engineering, surface coatings, catalysis, and sensing. This class of biopolymer is composed of a sequence of 20 naturally occurring amino acids. As the peptide sequence increases, so does the searchable sequence space (trimer = 20^3 or 8,000 peptides and a pentamer = 20^5 or 3.2 M). Empirically, peptide design is guided by the use of structural propensity tables, hydrophobicity scales, or other desired properties and typically yields <10 peptides per study, barely scraping the surface of the search space. Here, we combine machine learning techniques, such as Monte Carlo tree search and random forest, with coarse-grained molecular dynamics (MD) simulations to develop a fully autonomous computational search engine to discover peptide sequences with high self-assembly propensity. We employed this strategy to efficiently search large spaces of trimer, pentamer and octamer peptides. Subsequent experiments on the identified sequences support our findings and demonstrate the ability of this approach for peptide design.

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Machine Learning Assisted Design of Secure Biosystems

Carla M. Mann¹, Rebecca Weinberg², Marie Gros², Peter Larsen², Gyorgy Babnigg², Sara Forrester³, Sarah Owens², Philippe Noirot², and Arvind Ramanathan¹

¹Data Science and Learning Division, Argonne National Laboratory, Lemont, IL 60439

²Biosciences Division, Argonne National Laboratory, Lemont, IL 60439

³Strategic Security Sciences Division, Argonne National Laboratory, Lemont, IL 60439

The design of secure biosystems is of crucial importance, particularly as modification of model organisms for studying biological processes becomes more extensive and more frequent due to increasing availability of cost-effective gene-editing technologies. Escape of such organisms from laboratories poses hazards to researchers, the environment, the general public, and public trust in the scientific community.

We propose leveraging CRISPR/Cas systems as the basis of molecular “self-destruct” systems by engineering model prokaryotes with a Cas9 gene and a self-targeting gRNA which induces double strand breaks (and therefore, cell death) in the bacterial genome with low efficiency under laboratory conditions, but with high efficiency upon evasion.

In order to identify gRNAs satisfying these parameters, we created a machine learning model, CRISPRAct, which uses sequence and genomic context features to train a state-of-the-art genomic transformer model in conjunction with a conventional neural network to predict log₂ fold change as a metric of activity for SpCas9 gRNAs in *E. coli*. CRISPRAct achieves a Mean Absolute Error of 0.62 and Spearman Correlation Coefficient of 46.8% on a set of 71,228 gRNAs and notably is able to correctly predict differential condition in the stationary and exponential phases of *E. coli* cell growth.

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Generalized Framework for Bacterial Infection Diagnostics from Human Gene Expression Data

Raziur Rahman¹ and James J. Davis^{1,2}

¹Data Science and Learning Division, Argonne National Laboratory, Lemont, IL 60439

²University of Chicago Consortium for Advanced Science and Engineering, University of Chicago, Chicago, IL 60637

According to the Centers for Disease Control and Prevention (CDC) report, in 2019 alone more than 50,000 people have died from Bacterial infection in USA which could have been reduced by proper diagnosis of the pathogens and antibiotic treatments. With the advent of high throughput next generation sequencing technology such as RNA-seq, diagnostic capacity for different pathogens has increased rapidly. RNA-seq data offers a robust technical analysis of cellular conditions using gene expression, but it requires a profound knowledge of computational tools that may need to be adjusted depending on the disease under study. Our research on more than 5000 bacteria-infected-human samples suggests that machine learning (ML) approaches can solve this problem by analyzing host gene expression data where cell response to pathogens is captured. Thus, we have built a generalized ML-based framework for identifying pathogens from cellular stress response data and providing information regarding the effect of the infection on cells. Our ML modeling result has shown ~90% accuracy in classifying bacteria species. In addition, we have located human genes which are especially responsive towards individual bacteria, which could be a breakthrough for drug discovery.

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Machine Learning-Based Feature Extraction to Characterize the Behavior of Organisms *in Vitro*

Zahmeeth Sakkaff¹, Pamela Weisenhorn², Christopher S. Henry¹, and James J. Davis¹

¹Data Science and Learning Division

²Biosciences Division, Argonne National Laboratory, Lemont, IL 60439

In natural environments, microorganisms may exist in their single/isolate-celled form or as mixed colonies of cells that may interact readily with one another and perform complex interactions and communication mediated by the exchange of chemical substrates. The culture conditions that were used to isolate and differentiate bacterial cells are potentially useful sources of information for predicting foe organisms and phenotypes. To aid in this overall effort, we have curated genome sequence data that are paired with nutritional requirements that measured using the Biolog system. In this work we are applying machine learning models to predict bacterial growth conditions, and to identify genes involved in various metabolisms. Random Forest (RF), Logistic Regression (LR), and classification and regression trees (CART) were used for making the predictions. Overall, F1 scores for predicting growth on each substrate range from 0.60 to 0.95. We report the performance of LR is significant compared to RF and CART. As a future work we are planning on performing drop-out experiments to see if certain genomes are artificially increasing or decreasing the accuracy.

Cas9-Induced Killing is an Effective Component of a Biocontainment System

Rebecca Weinberg¹, Carla Mann², Marie-Francoise Gros¹, Sara Forrester³, Peter Larsen¹, Gyorgy Babnigg¹, Dionysios Antonopoulos¹, Arvind Ramanathan², and Philippe Noirot²

¹Biosciences Division, Argonne National Laboratory, Lemont IL 60439

²Data Science and Learning Division, Argonne National Laboratory, Lemont IL 60439

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Genetically engineered microbes are increasingly widely applied to agriculture, industry, and environmental protection. However, unleashing these organisms into ecosystems requires awareness of risk and attention to possible unforeseen consequences. Therefore, development of biosecure containment systems will greatly improve confidence in using these organisms to their fullest capacity.

Components for killing bacteria include a CRISPR Cas9 enzyme paired with chromosome targeting guide RNA (gRNA). We have tested bacterial killing across three physiological conditions in targeted assays and library screens. We find that cells are very sensitive to Cas9 killing in rich media growing exponentially, and membrane damage is pronounced. Additionally, Cas9 dramatically diminishes cell viability for stationary or defined media conditions. However, the cell membrane is relatively protected. Our screens revealed dramatic disparities in gRNA efficacy including gRNAs with condition-specific function. This facilitated development of our Machine Learning (ML) models. Since our models are sensitive to physiological conditions, they will foster optimal selection of gRNAs for function across different environments.

These data reveal CRISPR to be a robust killing system across physiological conditions. Thus, we have created key biological components of a biocontainment system, and additionally developed an iterative process for biological testing and ML that will foster the development of increasingly efficacious biocontainment systems.

CHEMICAL SCIENCES

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Manipulation of Graphene-Polymer Interfaces for Improved Graphene Transfer

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Advanced optoelectronic device development requires a combination of outstanding mechanical and electronic properties. Graphene-polymer laminar composites provide one promising route, as graphene lends its impressive conduction and limited resistance to flexible, durable polymer films. This combination can yield the transparent electronic materials necessary for device developments, including smart contact lenses that detect blood sugar levels in real time, sensitive electronic windshields in driverless cars, neural probes to correct tremors in Parkinson patients, and rollable laptops and cell phones. In all of these instances, large, uniform graphene films must adhere to large polymer sheets reliably to produce laminar composite systems.

Currently, chemical vapor deposition growth of graphene on precursor metal foils is the most promising route to commercial, large-scale graphene production. This process yields graphene-metal stacks where graphene must be

transferred to a polymer film of interest. Successful transfer requires the graphene-polymer adhesion strength to be greater than the graphene-metal adhesion strength. Otherwise, graphene will remain adhered to its native foil. Thus, manipulation and control of interfacial graphene-polymer interactions is desirable. To this end, we probe the interfacial interactions within graphene-polymer laminar composite using infrared reflection absorption spectroscopy. We observe, for the first time, polymer chain rearrangement as induced by graphene.

We then connect these detected molecular movements to overall film adhesion using a spatially resolved optical transmission technique built on an in-house laser system. This method quantifies graphene coverage as a function of film area. We find that polymer chain composition and conformation strongly affect interfacial adhesion, and laminate interactions can be fine-tuned to enhance film stack adhesion. Data analysis are expanded to provide statistically relevant information about graphene spatial distribution as well.

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Cathode Materials as Catalyst Supports: A New Approach for Tuning Catalyst Reactivity

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The heterogenization of organometallic catalysts onto inorganic supports is a powerful strategy for developing heterogeneous, single-site, *homogeneous-in-function* catalysts. While the support is often chosen for its physical properties, its chemical properties are seldom employed to modulate the activity of the system. The treatment of supports as chemically dynamic ligands, akin to redox non-innocent ligands, represents a new frontier in the design and investigation of heterogenized catalysts. The electronic properties of redox non-innocent ligands allow them to participate in catalysis by storing and transferring electrons to the active site during key steps throughout the catalytic cycle. Thus, the utilization of lessons learned from homogeneous catalysis toward supports can produce catalysts with unprecedented reactivity. Cathode materials such as lithium manganese oxide (Li_xMnO_2) are attractive candidates for redox active supports due to the gamut of accessible charge states available as a function of their lithium content; resulting with a consistent active site geometry at a broad range of surface potentials. Herein we report a series of manganese oxide grafted nickel materials capable of catalyzing the hydrogenation of cyclohexene. Reactivity studies, structural characterization, and theory calculations will show that the activity of these materials is directly proportional to the charge state of the support.

1

Getting the Circular Economy Rolling: Catalytic Upcycling of Plastic Waste

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Inexpensive plastics from petroleum drove innovation and growth through the 20th century, while at the same time resulting in an enormous and exponentially increasing amount of plastic waste. Of human-made waste, plastic waste is especially concerning; it does not easily decompose on its own, nor do we have cheap or robust methods for recycling it. If the large polymer macromolecules in plastics could be chemically transformed or “upcycled” into value-added materials, 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. We take polyolefins (polyethylene, polypropylene), the most common polymers produced today, and convert them via metal-catalyzed hydrogenolysis to shorter alkanes. Importantly, the products of these reactions have narrow molecular weight distributions, making them suitable for applications in lubricants or waxes. With additional functionalization, the uniform hydrocarbons produced by catalytic hydrogenolysis could be converted to surfactants, repolymerized, or adapted to other applications.

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Amphiphile-Anion Interaction at Aqueous Interfaces: Sum Frequency Generation Spectroscopy and Synchrotron X-ray Scattering Studies

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The use of amphiphilic extractants for the selective transport of metal ions from an aqueous phase into an organic phase, known as liquid-liquid extraction, is one of the most common chemical separation processes used for heavy metal separations, such as rare earths and actinides. Depending on the nature of amphiphile, the background anions have a significant impact on the extraction process. The study of amphiphile-anion interaction is thus important to understand the interfacial phenomena for the selective and efficient extraction of critical rare earth elements. Here, we use surface sensitive techniques such as vibrational sum frequency generation spectroscopy (VSFG), X-ray reflectivity (XR), and X-ray fluorescence near total reflection (XFNTR) techniques to investigate the interfacial structure of selenocyanate (SeCN⁻) ions at a positively charged 1,2-dipalmitoyl-3-trimethylammonium-

propane (DPTAP) monolayer. It is observed that the presence of SeCN ions changes the water structure significantly near the interface and disturbs the ordering of monolayer. This fundamental investigation of the interfacial behavior of SeCN ions provides the molecular level information regarding the role of anions in rare earth metal separations.

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An Investigation on Feasibility of Atomic Layer Deposition Overcoating on Industrial Catalysts

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Currently, propylene is produced primarily through either steam or fluidized catalytic cracking. However, these two commercial approaches do not meet the current or future global demands for propylene. With the price of propane at historic lows due to the availability of propane from shale gas, propane dehydrogenation processes such as Oleflex™ from UOP which utilizes a highly active and selective supported platinum catalyst have become economically attractive. At the high temperatures of PDH, the stability of platinum catalysts can be limited by sintering of the platinum nanoparticles. Pt sintering results in lower propane activity and selectivity.

The goal of this project is to overcome catalyst (industrial catalyst, provided by company UOP) degradation via atomic layer deposition overcoating technology, which deposits protective layers over and around the active platinum metal, preserving catalyst integrity under reaction conditions. The scale-up of the catalyst production was performed. The resulting improvements in both the efficiency and selectivity will reduce the overall process energy.

3

Understanding the Photochemistry of Iron Complexes using Time-Resolved X-ray Spectroscopy

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Being a first-row transition metal, iron is an earth abundant element found in numerous natural and synthetic chemical processes making it an archetype for exploring and understanding new areas of chemistry. Iron has also been shown to be a viable substitute as a far less expensive and toxic alternative to ruthenium and osmium metal complexes, but with the risk of altering the chemical reaction dynamics. Therefore, it is paramount to understand and characterize the reaction dynamics and possible intermediate species for iron complex reactions. In this work we explore the photochemistry of $[\text{Fe}(\text{CN})_6]^{4-}$ in water, whereby upon optical excitation a CN^- ligand is removed and replaced by a solvent water molecule leading to the formation of $[\text{Fe}(\text{CN})_5(\text{H}_2\text{O})]^{3-}$ on the 20 ps timescale. To investigate the mechanism for this reaction we use X-ray emission spectroscopy as a means to follow and characterize the intermediate species ($[\text{Fe}(\text{CN})_5]^{3-}$) before solvent coordination. The element specific emission spectroscopy technique is a powerful way to track the spin-state of evolving intermediate species, but it can also yield insight into the covalency and ligand environment of intermediates.

Computational K-edge XANES for Single-Site Heterogeneous Vanadium Catalysts**Prajay Patel¹, Jeremy Kropf¹, David A. Kaphan¹, Massimiliano Delferro¹, and Cong Liu¹**¹Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439

Single-site heterogeneous catalysts (SSHCs) have received increasing attention due to their unique catalytic properties and well-defined active sites, effectively combining desirable attributes of both homogeneous and heterogeneous catalysis. To characterize the active site of SSHCs responsible for catalytic turnover, 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 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 vanadium complexes and SSHCs characterized at the Advanced Photon Source (APS) at Argonne National Laboratory. Significant contributions to key transitions are identified 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.

Ultrafast Relaxation Dynamics in Bimetallic Transition Metal Complexes Revealed by Transient Optical Absorption Spectroscopy**Brian T. Phelan¹, Pyosang Kim², Karen L. Mulfort¹, and Lin X. Chen^{1,2}**¹Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439²Department of Chemistry, Northwestern University, Evanston, IL 60208

Transition metal complexes (TMC) are attractive candidates for use in catalysis, optoelectronics, and quantum information science due to the synthetic tunability of the coordinating ligands which offers detailed control over structure, reactivity, light absorption, and spin properties. Since light activation is a key interest within these fields, understanding the excited-state relaxation dynamics following light absorption is critical. While bimetallic tetrapyridophenazine-bridged TMCs (M1tpphz-M2) were previously identified as interesting model structures demonstrating directional energy and electron transfer reactions relevant to light harvesting, these complexes exhibit convoluted excited-state potential-energy surfaces (PES) comprised of numerous closely-spaced excited states. Given the influence of structure and vibrations on excited-state dynamics, much effort has been directed at investigating the key vibrational modes that may couple the various excited states and drive excited-state relaxation through the PES. Here, ultrafast optical spectroscopy experiments reveal complicated sub-ps excited-state evolution superimposed with vibrational wavepacket signals comprised of low frequency modes which likely correspond to structural rearrangement occurring around both metal centers.

Harnessing Supramolecular Interactions to Promote Photoinduced Electron Transfer from Copper Phenanthroline Chromophores

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The process of converting solar energy into storable, transportable fuels requires a chemically and photochemically stable chromophore that efficiently absorbs visible light and remains in the excited state long enough for electron transfer to occur. Ruthenium trisbipyridine ($[\text{Ru}(\text{bpy})_3]^{2+}$) possesses favorable photophysical properties that have earned it a reputation as the benchmark molecular chromophore for this purpose. However, it is desirable to substitute less costly, more abundant first row transition metal-based alternatives. Copper bisphenanthrolines show promise in this regard because of their broad visible absorption arising from a metal-to-ligand charge transfer band reminiscent of that of $[\text{Ru}(\text{bpy})_3]^{2+}$. Unfortunately, many of these copper complexes have relatively short excited state lifetimes that compromise the efficiency of electron transfer to a catalyst or other electron acceptor. We have exploited the tendency of negatively charged copper phenanthrolines to organize into supramolecular assemblies with the dicationic electron acceptor methyl viologen to circumvent this issue and facilitate photoinduced electron transfer from chromophores with short-lived excited states.

Pore-scale Investigation of Oil Displacement by Smart Water Flooding Using Synchrotron X-ray Microtomography

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Recently, smart waterflooding has been regarded as an economical and effective technique to enhance petroleum oil recovery by controlling the salinity and ionic composition of injection water. However, the impact of ion types and concentrations on the oil displacement is still unclear, especially the flow dynamics at pore-scale. The goal of this research is to investigate the porescale oil displacement by smart waterflooding in an oil-wet carbonate reservoir rock at early stage of smart waterflooding.

The carbonate rocks containing formation brine and crude oil were flooded with synthetic seawater and other smart water solutions with different sulfate concentrations. The flooding processes were visualized with synchrotron X-ray microtomography at Advanced Photon Source at Argonne National Laboratory. The images were processed using Python and software Avizo.

The results from flooding tests showed that the smart water with lower sulfate concentration and seawater did not change the wettability of the pore surfaces. Higher sulfate ion concentrations in the smart water, in contrast, altered the wettability of carbonate pore surfaces from oil-wet to neutral-wet within the first few minutes of waterflooding.

Formic Acid Catalyzed Isomerization and Adduct Formation of an Isoprene-Derived Criegee Intermediate: Experiment and Theory

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Isoprene is the most abundant non-methane hydrocarbon emitted into Earth's atmosphere. Ozonolysis is an atmospheric sink for unsaturated hydrocarbons and generates reactive carbonyl oxide zwitterions ($R_1R_2C=O^+O^-$) known as Criegee intermediates (CIs). Isoprene ozonolysis leads to the formation of methyl vinyl ketone oxide (MVK-oxide), a four-carbon unsaturated CI. Recent work has demonstrated that the reaction of MVK-oxide with formic acid (FA) is a potentially significant sink for tropospheric FA. We present experimental and theoretical work that identifies and characterizes two reaction pathways in the reaction of MVK-oxide and FA. Direct experimental studies using multiplexed photoionization mass spectrometry (298 K, 10 Torr) demonstrate the formation of a highly oxygenated functionalized hydroperoxide product, resulting from the effectively barrierless insertion of MVK-oxide into formic acid. In addition, isotopically labeled experiments reveal a conformer-specific pathway where FA catalyzes the isomerization of *syn*-MVK-oxide to a vinyl hydroperoxide (2-hydroperoxybuta-1,3-diene, HPBD). High-level theoretical calculations demonstrate that this FA catalyzed pathway proceeds by a double hydrogen-bonded interaction followed by a concerted H-atom transfer via submerged barriers to regenerate FA and yield HPBD. The rates, mechanisms and branching of these reaction pathways will be discussed.

This material is based upon work supported by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences (BES), US Department of Energy (USDOE) under contract to University of Pennsylvania (DE-FG02-87ER13792) Argonne National Laboratory (DE-AC02-06CH11357) and Sandia National Laboratories). Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the USDOE's National Nuclear Security Administration under contract DE-NA0003525.

New Chromophores for Photochemical Water Oxidation at Low pH

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A strong demand for sustainable production of clean energy has been existed for decades. Consequently, solar-to-chemical energy conversion is the ultimate goal for scientists in the field of energy generation. A potentially controlled technology for this process is artificial photosynthesis (APS). Artificial photosynthetic reactions are determined primarily by three reaction processes: light-harvesting processes; charge generation and separation processes; and catalytic reaction processes. In the light-harvesting processes, chromophore, should efficiently absorb and convert the incoming solar energy into an excited state that can transfer an electron to an acceptor for the creation of a charge-separated state, thus generating the required thermodynamic driving force for the desired chemical reactions. One of the most commonly used chromophores are the ruthenium(II) polypyridyl, $[Ru(bpy)_3]^{2+}$ -type complexes. Due to their low redox potential, which is insufficient to activate a majority of the

developed water oxidation catalyst (WOC), most of the water oxidation processes in using $[\text{Ru}(\text{bpy})_3]^{2+}$ -type chromophores are carried out at intermediate or high pH. $[\text{Ru}(\text{bpy})_3]^{2+}$ -type chromophores, however, is rapidly decomposed at $\text{pH} > 4$, in a reaction that results in only minor formation of O_2 . Electron transfer from the WOC must therefore compete with decomposition of $[\text{Ru}(\text{bpy})_3]^{3+}$ to allow for efficient H_2O oxidation. Here we report different $[\text{Ru}(\text{bpy})_3]^{2+}$ -type derivatives which retain the distinct absorption ~ 460 nm but changing the oxidation potential from 1.26 V to 1.6 V vs NHE at pH 1. Based on the higher KIE of phosphonic acid-modified chromophores showed, a PECT mechanism was proposed.

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Building a Cu(I) HETPHEN Anthraquinone Supramolecular Assembly for Investigating Key Charge Accumulation Pathways in Solar Energy Conversion

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Developing molecular photocatalysts that can accumulate redox equivalents as a response to photoexcitation is of great interest in order to efficiently facilitate photon-driven reactions that require multiple electrons, such as water splitting and CO_2 reduction. Revealing and understanding fundamental excited state charge accumulation pathways in chromophore-catalyst supramolecular assemblies is key to achieve and control charge accumulation in these systems. A Cu(I) HETPHEN Anthraquinone triad supramolecular assembly was synthesized as a model complex to probe the charge accumulation pathways under illumination. The assembly was designed and consists of two Cu(I) HETPHEN motifs, acting as light absorbers and electron donors, and an anthraquinone central moiety, functioning as an electron acceptor and charge accumulation site. The structural characterization was achieved by NMR and X-ray crystallography and the steady state optical and electrochemical properties were investigated by UV/vis and cyclic voltammetry. The photon-to-charge conversion dynamics will be investigated by various methods, including spectroelectrochemical techniques, optical transient absorption, X-ray transient absorption and time-resolved infrared spectroscopy. The exact picture of the charge accumulation mechanism of this model complex will be concluded with the assistance of DFT calculation and implications for promoting long-lived charge accumulation in molecular systems will be proposed.

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Highly Selective Atomically Dispersed Copper Electrocatalyst for CO_2 Reduction to Ethanol

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Single-atom catalysts (SACs) are recently emerging as a new frontier in heterogeneous catalysis, and direct electrochemical conversion of CO_2 to ethanol offers a promising strategy to lower CO_2 emissions while storing energy from renewable electricity. However, current electrocatalysts offer only limited selectivity toward ethanol. Here we report a carbon-supported copper (Cu) single atom catalysts, synthesized by an amalgamated Cu-Li method, that achieves a single-product Faradaic efficiency (FE) of 91% at -0.7 V (vs the reversible hydrogen electrode, RHE) and onset potential as low as -0.4 V (RHE) for electrocatalytic CO_2 -to-ethanol conversion. The FE to ethanol was highly sensitive to the initial dispersion of Cu atoms and decreased significantly when CuO and large Cu clusters become predominant species. Operando X-ray absorption spectroscopy identified a reversible transformation from atomically dispersed Cu atoms to Cu_n clusters ($n = 3$ and 4) on application of electrochemical

conditions. First-principles calculations further elucidate the possible catalytic mechanism of CO₂ reduction over Cu_n.

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ENERGY

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Modelling Combustion in a Gasoline Compression Ignition Engine

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Gasoline compression ignition (GCI) is a partially premixed combustion concept which derives its superiority from higher volatility and longer ignition delay of gasoline-like fuels. The present work focuses on modelling combustion in a heavy-duty compression ignition engine using computational Fluid Dynamics (CFD). Simulations were carried out on a single cylinder of a multi-cylinder GCI engine that has a compression ratio of 17. The analysis has been carried out using different late fuel injection strategies and the results are compared with the experiments. RNG k- ϵ model is used to describe in-cylinder turbulence and KH RT model is used to simulate the fuel spray breakup. The simulation results are used to estimate the engine performance for different fuel injection strategies.

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Inverse Design of Self-Reporting Molecules for Redox Flow Batteries using Active Learning

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Redox flow batteries (RFBs) are a promising technology for stationary energy storage applications due to their flexible design, easy scalability and low cost. In RFBs, energy is carried in flowable redox-active materials (anolyte and catholyte redoxmers) which are stored externally and pumped to the cell during operation. Further improvement in the energy density of RFBs requires design of redoxmers with optimal properties i.e., wider redox potential window, higher solubility, and stability. Additionally, designing redoxmers with fluorescence enabled self-reporting functionality allows monitoring of the state-of-health of RFBs. Here, we employ high-throughput DFT calculations to generate database of reduction potentials, solvation free energies and absorption wavelengths of 1400 anolytes. Using simulated data, we develop machine learning models to predict the properties from text-based representation (SMILES) of molecular materials. We compare the efficiency of our active learning model, using multi-objective Bayesian optimization, against brute-force materials screening approach. Finally, we apply the active learning model to discover promising redoxmers with desirable properties from vast chemical space of 2 million molecular materials.

Fluorinated Dialkoxybenzene Based Catholyte Redoxmers for Redox Flow Batteries

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Redox flow batteries (RFBs), in which electric charge is stored in redox-active materials (redoxmer) dissolved in liquid electrolytes, show significant potential for grid-scale energy storage applications. Because of the liquid nature, RFBs feature remarkable flexibilities, including decoupled energy and power that is highly desired for adapting various scales of energy storage requirements. Aprotic organic solvents are extensively studied as they can significantly extend the electrochemical window, leading to higher cell voltage and energy density of RFBs. To that end, redoxmers with tunable redox potentials are actively pursued in order to realize the full potentials. In this presentation, a fluorinated dimethoxybenzene based high potential (catholyte) redoxmer will be discussed. By incorporating fluorinated substituents, the redox potential can be significantly increased while the new redoxmer still maintain excellent electrochemical behavior. Importantly, while bearing higher potential, the new redoxmer can deliver very stable cycling performance evidenced by the symmetric H-cell cycling. Kinetic study using electron paramagnetic resonance (EPR) also indicates impressive stability. DFT calculations reveal that while the introduced Fluorine atoms are helping to elevate the redox potential, they also depress major decomposing reactions of the charged redoxmer, affording excellent stability. This approach of utilizing strong electron withdrawing yet electron resonance Fluorine atoms seem very promising for constructing high potential and stable catholyte redoxmers for RFBs.

Towards Exascale Simulations in ICEs: Spray Modeling Using Nek5000

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A novel approach for modeling sprays from high-speed liquid injection is presented here. The liquid phase is modeled stochastically by Lagrangian parcels, while the gas phase is modeled in an Eulerian reference frame using the spectral-element code, Nek5000. Two-way coupling between the liquid and the gas is achieved using an interpolation/projection procedure. The framework was used to simulate nonevaporative and vaporizing sprays on thousands of MPI processes. Simulation results are compared quantitatively and qualitatively against experimental data from the Engine Combustion Network, showing good agreement with experiments. Some of the challenges and advantages of the current approach for modeling sprays are discussed. The aim of this work is to enable high-fidelity internal combustion engine simulations on Exascale systems, which requires porting the current modeling capabilities to GPU accelerated platforms. This will allow detailed analysis of in-cylinder processes, which will drive the design of cleaner and more efficient engines.

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Elucidating Interfacial Dynamics of Atomic Layer Deposition Coated Cathode Materials

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Current research in the field of lithium-ion batteries (LIB) is geared towards stabilization of the electrode-electrolyte interfaces to improve the cycling stability and efficiency. In this regard, atomic layer deposition (ALD) is a well-suited conformal method of coating a barrier layer on the surface of electrodes. While there are reports that demonstrate how these ultra-thin metal oxide/fluoride barrier coatings on cathodes influence the performance of LIBs, there is no systematic study to elucidate the interfacial compositional changes of cathode materials upon ALD coating. Therefore, this work aims at understanding the effect of ALD coatings on the surface electronic structure of the cathode materials.

Al₂O₃ and AlF₃ were employed as prototypical coatings due to their acid-resistive and charge-conductive nature. The cathode materials chosen for this study range from simplest transition metal oxides (e.g., NiO) to complex multi-element cathode materials such as NMCs. Surface-specific analysis on ALD coated cathode materials was performed using X-ray photoelectron spectroscopy (XPS), which shows significant compositional changes and selectivity upon ALD coating. Overall, this fundamental study will assist in the development of novel ALD barrier coatings that demonstrate highest sensitivity on multi-element cathode materials, which leads to the fabrication of robust electrode-electrolyte interfaces in LIBs.

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Machine Learning Force Fields for Li Ion Cathodes

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NMC (Lithium Nickel Manganese Cobalt Oxide) is a common choice cathode in Lithium ion batteries. However, it is susceptible to fracture at low Li content upon discharging, evidenced by a large change in the *c* lattice constant. We illustrate this collapse through a machine learning force field trained to 1 ps of *ab initio* molecular dynamics (AIMD) for the specific composition NMC-111 that contains equiatomic proportions of nickel, manganese and cobalt. We find the collapse occurs at a Li-content of 0.25% at 298 K in the O3 phase.

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Low Temperature Plasma Discharges for Lean Ignition

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Lean combustion is highly desirable in modern engines because of its associated lower emissions. However, it is challenging to attain stable operation of an engine that is operating lean, largely due to the difficulty of ignition (i.e., the self-sustained propagation of a flame) in these conditions. There is a strong correlation between ignition

failure and the so-called cycle-to-cycle variations (CCV) of an engine. Recently, low-temperature plasma discharge devices have been considered in solving this problem. In this presentation, we demonstrate the potential of such discharges by employing detailed numerical simulations of their electrochemical structure. Key results on flammability limits will also be shown.

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High Rate Li-Ion Batteries with Cation-Disordered Cathodes

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Cation disordering in electrode materials for Li-ion batteries is deemed as an undesired structural feature because it can disturb the formation of Li diffusion channel in structure. Therefore, extensive researches have focused on developing well cation-ordered structure. Here, we firstly show the potential of cation disordered compound for high power density and long cycle-life battery material. We developed a new class of cation-disordered material for high-power and long-term cycle batteries, by controlling the way of the cation distribution in structure.

Firstly, we demonstrated that cation disordering in triplite LiFeSO₄F could be activated by Li/Fe rearrangement during the 1st cycle. This re-arrangement decreases the amount of edge-shared FeO₄F₂ connection environments which can block Li diffusion channels. With this activation, triplite LiFeSO₄F exhibits several unexpected electrochemical features in subsequent cycles; the change in thermodynamic property, negligible volumetric change, enhanced Li diffusion, and facile phase transformation pathway.

Secondly, based on the understanding about the activation by re-arrangement of Li/Fe ions, we developed a new synthetic strategy to fully activate the electrochemical properties of triplite LiFeSO₄F. By changes in the synthesis temperature and the Li/Fe ratio, we reduced the amount of Fe edge-shared connection. Therefore, cation-disordered triplite LiFeSO₄F can deliver a substantially improved electrochemical performance. It exhibits a superior rate capability up to 100 C (36-s discharge) with ~60 mAh/g and excellent capacity retention for 2,500 cycles at 5 C charge/20 C discharge rate. These results extend the scope of electrode materials to include cation-disordered materials and provide new opportunities for designing them for high-performance Li-ion batteries.

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Exploration of Combustion Dynamics in a Multi-Mode Combustion Engine

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For gasoline fueled engines, diluted and low-temperature homogeneous charge compression ignition (HCCI) techniques have opened an affordable solution to maintain their attractiveness in low NO_x levels and rising demand of fuel efficiency. However, this approach is limited to a certain range of low-load engine conditions due to combustion instability and lack of autoignition controllability. To fulfill broad range of engine operating conditions while upholding such intrinsic benefits, controlled ignition techniques have been suggested to extend effectiveness of advanced compression ignition (ACI) regimes across more practical range of engine load.

Combination of the ACI with spark ignition (SI) combustion can provide a solution to meet this demand and hence arguably cover full-load range. Such a concept can be pursued in a multi-mode combustion strategy and hence requires engines to operate in two distinct combustion modes and transition between those when needed. This study utilizes the numerical simulations and explores the concept of multi-mode gasoline fueled engine by performing 3-D CFD simulations in a single cylinder GDI engine platform. The simulations are verified against the relevant experimental data available for ACI and SI mode strategies. Extended condition to reproduce mixed-mode condition was generated to assess the feasibility of multi-mode combustion strategy in a fashion of numerical experiment.

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Identifying the Delithiation Mechanisms for the Li-rich $\text{Li}_{1.3}\text{Fe}_{0.4}\text{Nb}_{0.3}\text{O}_2$ Disordered Rocksalt Cathode

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Interest in alkali-rich oxide cathodes has grown in an effort to identify systems that provide high energy densities through reversible oxygen redox. This effort has expanded beyond conventional layered structures with well-defined Li-diffusion pathways with the development of Li-rich disordered rocksalts. While substantial disorder is often thought to be detrimental to Li-diffusion, many of these systems have been found to display exceptional capacities and capacity retention. However, some of the most promising compositions such as those based solely on earth abundant elements, e.g., iron and manganese, suffer from poor capacity retention and large hysteresis. Here, we use the disordered rocksalt cathodes, $\text{Li}_{1.3}\text{Fe}_{0.4}\text{Nb}_{0.3}\text{O}_2$, as model systems to provide an in-depth insight into the delithiation mechanisms for this Fe-based system. Using a range of elementally specific spectroscopic probes, we identify the extent to which the delithiation is accounted for by iron redox, oxygen redox, and side-reactions (O_2 -gas release etc.). This work provides a clear baseline of signatures to look for when identifying the transition metal and oxygen contributions to the delithiation.

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Comparing Total Cost of Ownership of Battery Electric Vehicles and Internal Combustion Engine Vehicles

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The technological advance of electrochemical energy storage and the electric powertrain has led to a rapid growth in the deployment of electric vehicles. The high cost and the added weight of the batteries have limited the size (energy storage capacity) and therefore the driving range of these vehicles. But consumers are steadily purchasing these vehicles because of the fast acceleration, the quiet ride, and the greater energy efficiency of these vehicles. The higher pack-to-wheel efficiency and the lower energy cost per mile, as well as the less maintenance and repair

expense, translates to operating savings over conventional vehicles. This paper compares the battery electric vehicles with internal combustion engine vehicles on the basis of total cost of ownership. It is seen that the higher initial cost of the electric vehicle can be recovered within a few years, mostly within the average vehicle ownership of 8 years. This is especially true for the heavier electric vehicles with shorter driving ranges. Specifically, a 2,250 kg or heavier vehicle with an electric driving range of 200 miles may achieve cost parity with an equivalent internal combustion engine vehicle in less than 5 years.

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Probabilistic Machine Learning for Design of Multi-Physics Systems

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Mechanical systems often involve multi-physics interactions and complex nonlinearities due to which design optimization becomes challenging. The inherent complexity of the processes, along with limitations in data availability, mandate principled uncertainty estimates in modeling. Budget restrictions pose serious data limitations in the development and testing phases of the product pipeline, particularly in the presence of a hierarchy in the associated multi-physics process models with respect to their fidelity levels. This talk will focus on some fundamental developments and applications of probabilistic machine learning strategies in design optimization. For example, the advantages of variational inference in autoencoder frameworks in uncovering input sensitivity for flow structures inside automotive injectors will be presented. From the perspective of statistical learning, the advantages of MFM-based optimization over a single high-fidelity surrogate, specifically under complex constraints, will be discussed with benchmark optimization problems involving noisy data. Novel multi-fidelity surrogate modeling and optimization strategies will be discussed with respect to data-driven engineering design optimization problems, for example, process parameter optimization in additive manufacturing. The proposed framework is expected to accelerate design optimization tasks involving expensive simulations, particularly in data-scarce regimes.

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Regeneration of Lithium Ion Battery Cathodes Through Chemical Relithiation

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The demand for lithium-ion batteries (LIBs) has grown to meet the needs of the expanding electric vehicle market, but the supply and cost of the raw materials may soon become a limitation under current conditions. The major contribution to the cost comes from the metals used in the production of the LIB cathodes, which are primarily obtained from foreign sources. Recycling spent batteries and recovering the cathodes and other valued components provides an alternate feedstock and is critical for the future of the LIB market. The cathode from an end of life cell is typically 15-20% deficient in lithium content compared to pristine material. Relithiating the spent cathode through a direct chemical process will maintain much of the existing structure, while driving fresh lithium into vacancies. For this work, chemically delithiated $\text{LiNi}_{0.33}\text{Mn}_{0.33}\text{Co}_{0.33}\text{O}_2$ (NMC111) was used as the model for spent cathode. The delithiated powder was heated together with a lithium source within the thermal stability window as determined by TGA. The structure and composition of the relithiated cathodes were verified using XRD and GDOES. The performance was evaluated in half cell configurations and compared to pristine NMC111 cathodes.

A Neural Ordinary Differential Equations Approach to Modeling Chemical Kinetics

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The main bottleneck when performing computational fluid dynamics (CFD) simulations of combustion systems is the computation and integration of the chemical source terms. In recent times, machine learning has emerged as a promising tool to accelerate combustion chemistry, involving the use of regression models to predict the chemical source terms as functions of the thermochemical state of the system. However, combustion is a highly nonlinear phenomenon, and this leads to divergence from the true solution when the neural network representation of chemical kinetics is integrated in time. This is because these approaches minimize the *a priori* error during training without guaranteeing successful integration with ordinary differential equation (ODE) solvers. In this work, a neural ODE approach to combustion modeling is developed to address this issue. The source terms predicted by the neural network are integrated during training, and by backpropagating errors through the ODE solver, the neural network weights are adjusted accordingly to minimize the difference between the predicted and actual ODE solutions. It is shown that even when the dimensionality of the thermochemical manifold is trimmed to remove redundant species, the proposed approach accurately captures the correct physical behavior and reproduces the results obtained using the full chemical mechanism.

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Quantification of Local and Global Degradation Mechanisms During Extreme Fast Charging in Lithium Ion Batteries

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With an ever-increasing demand for electric vehicles, there is an urgent need for Li-ion batteries (LIBs) with extreme fast charging (XFC) capabilities. The need arises from making recharging times for commercial electric vehicles comparable to traditional refueling times. However, such XFC rates are associated with a drastic decrease in performance, as well as safety hazards, for which the primary contributor is parasitic Li plating on the anode. Here, high-energy X-ray diffraction (XRD) is presented as a way to study Li plating and tie it to the battery degradation, in a *quantitative* and *in-situ* manner, across length scales. Firstly, XRD provides a way to quantify the *total* amount of Li plating, as well as other loss mechanisms, and tie them to the *global* cell performance after XFC cycling. Second, the *local* heterogeneities in the cathode and anode degradation are explored and correlated to *local* heterogeneities in Li plating.

In this work, single layer LIBs with a porous graphite anode, NMC ($\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$) cathode and EC:MC (with LiPF_6 additive) electrolyte were charged at different rates within the XFC regime (10-15 min charge) and characterized using in-situ XRD. Locally, the regions with local lithium plating are shown to be correlated to the local state of charge and loss of active surface area in the cathode and anode. Globally, the capacity fade of the cycled cells is correlated to the amount of dead Li, with separated contributions from various loss of lithium mechanisms, including Li plating. Additionally, the local characteristics of plated lithium crystallites such as their preferred crystallographic orientations are analyzed. Based on this knowledge of the properties of lithium plating and the conditions that favor it, as well as its effect on overall battery performance, new approaches towards

designing batteries can be realized, such that irreversible Li plating, and in turn cell degradation is minimized. This step will in turn help to guide the rational design of the next generation of XFC capable LIBs with a consistent and safe performance.

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Hydro-Economics Tradeoff Surfaces to Guide Unit Commitment in Production Cost Models

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The hydropower industry is concerned about the fidelity and computational burden of hydropower representation in Production Cost Models (PCMs). The objective of this paper is to innovate and find an appropriate tradeoff between accuracy and computational speed in large-scale power system models representing hydropower plants. In general, models that represent large-scale power systems can only represent hydropower plants in a simplified way for computational reasons, whereas accurate hydropower plant models are often limited to a limited footprint. To achieve a good tradeoff between computational speed and accuracy, this paper explores a new method that take advantage of both types of models. Specifically, an accurate hydropower model is first used to generate surfaces representing several hydropower output data (maximum and minimum power capacity, and maximum ramp) based on numerous water releases and forebay elevation scenarios. Then, these surfaces are used into the large-scale power system model to provide a more accurate representation of hydropower output at a negligible computational cost. This method drastically increases the accuracy of hydropower plants in large-scale power system models at a virtually null additional computation cost.

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Artificial Intelligence Enabled Lithium-Ion Battery Health Management

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Lithium-ion batteries represent complex electrochemical-mechanical systems and hence their performance and degradation are difficult to model. With the advancements in artificial intelligence techniques and the availability of large battery testing datasets, there is an opportunity to solve some of the issues central to battery health management using black-box and grey-box approaches. In this presentation, I will present two key application studies of machine learning in battery research from my PhD and Postdoctoral research. These studies include the capacity estimation of batteries in battery management systems using features from voltage and current sensors data and representation of the battery charge-discharge open circuit voltage curves using variational autoencoders in reduced dimensional space. Models from these studies can be used for tracking the battery health in real-life applications and understanding the effects of degradation on battery parameters and performance.

Statistical Modeling for Charging Behavior of Plug-in Electric Vehicles using Large-scale Charging Data

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The market share of plug-in electric vehicles (PEVs) are increasing over the past decade. Understanding how the PEV drivers charge their vehicles is imperative in charging infrastructure planning, power system operation, and energy impacts analyses. This research aims to quantify the impacts of different factors that play significant roles in PEV charging behavior. In particular, we develop statistical models to understand when, where, and how long do PEVs plugin, and identify predictive factors, such as vehicle types, driver characteristics, charger features, and charging prices. Data for more than 189,000 charging sessions in the State of Illinois for a 13-month period were collected from ChargePoint, one of the leading charger network providers in Illinois. This study provides an in-depth statistics analysis of this data by developing six linear and logistic regression models to estimate the impacts of different influencing factors on charging behavior, including the location of a charging session, state of charge (SOC) at the beginning of the session, charger type used, etc. Our results based on a unique dataset from supply-side and statistical models highlight the essential roles that different charger and vehicle attributes play in PEV's charging behavior.

Two Lithium Intercalation Reaction Of ϵ -VOPO₄ for Lithium-Ion Batteries

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ϵ -VOPO₄ has been optimized as a cathode material for lithium-ion batteries to reversibly intercalate two Li-ions to reach the full theoretical capacity at least 50 cycles with a coulombic efficiency of 98%. This material adopts a stable 3D tunnel structure and can extract two Li-ions per vanadium ion, giving a theoretical capacity of 305 mAh/g, with an upper charge/discharge plateau at around 4.0 V, and one lower at around 2.5 V. As ϵ -VOPO₄ is capable of reversibly intercalating more than one lithium ion into the structure, it stores and delivers more energy than current batteries in the market. Compared to LiFePO₄, ϵ -VOPO₄ has a higher electronic conductivity and higher energy density with the insertion of one Li-ion, 159 mAh/g at 4.0 V vs 170 mAh/g at 3.45 V. Here we show the facile preparation of nano-sized ϵ -VOPO₄ particles and demonstrate the enhanced electrochemistry and cyclability for potential applications in lithium-ion batteries.

High-Fidelity Simulations of Motored Sandia DISI Engine Using Nek5000

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Engine manufacturers currently use commercial codes that have inherent limitations in predictive capability and

to massive parallelization. Our group has been leveraging Argonne's massively parallel open-source CFD platform, Nek5000, to perform multi-cycle large eddy simulations (LES) of motored internal combustion engines (ICE). This code is based on the high-order spectral element method framework and has demonstrated minimal numerical errors and high scalability on a variety of leadership computing platforms. Nek5000 also has a wide user base and allows moving piston/valve simulations with more advanced turbulence modeling capabilities compared to current ICE simulation software. In this project, LES of the motored Sandia optical direct injection spark ignition (DISI) engine was performed using Nek5000. Complex geometrical features of the piston surface were fully incorporated in the mesh generation developed using CUBIT with in-house techniques. Closed-cycle simulations with a flat top surface and motored piston were first conducted using Nek5000 to investigate in-cylinder motions and the performance of mesh deformation under various flow conditions. Then, complete engine features will be introduced, and open-cycle simulations will be performed to simulate full engine cycles. The high-fidelity simulation data will be validated against PIV measurements from Sandia and used to understand the dynamics of the in-cylinder flow and cycle-to-cycle variabilities. It enables us to improve wall-modeling techniques and develop data-driven models for future exascale platforms.

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Numerical Evaluation of Cold Start Strategies on Gasoline Compression Ignition during Cold Idle Operation in a Heavy-Duty Diesel Engine

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The operation of compression ignition engines can be challenging under cold conditions. Among the factors that inhibit robust combustion in traditional diesel engines are insufficient fuel vaporization, heavy wall impingement, thick wall films, and low ignitability conditions for the fuel. For gasoline compression ignition (GCI) engines to become viable in a real-world environment, it is important to understand and optimize combustion under cold start conditions. In the current project, a comprehensive study was conducted to use Computational fluid dynamics (CFD) to accurately predict the ignition and combustion processes in a cold-started GCI engine. This study aimed to better understand the combustion physics of engine cold start to achieve a faster, numerically-derived calibration. Based on the understanding of the spray, ignition and combustion processes for a GCI engine under cold conditions, the study further focused on evaluating different cold starting aids for their effectiveness on GCI cold combustion performance.

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Whither Mn Oxidation in Mn-rich Alkali-Excess Cathodes?

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Lithium-rich NMC (LR-NMC) compounds exhibit high capacities beyond the traditional redox, but it remains unclear whether the anomalous charge compensation mechanism is due to oxidized lattice oxygen or migration

assisted Mn oxidation. We compare LR-NMC with a model Mn^{7+} system (KMnO_4) using a combination of RIXS irradiation studies and operando XAS/XRD to quantify transition metal migration, Mn oxidization, and beam-induced effects. We reveal how for KMnO_4 it is possible to observe beam-induced Mn reduction resulting in trapped molecular oxygen. For LR-NMC, we observe limited oxidation beyond Mn^{4+} and the corresponding O K-edge RIXS spectra are distinctly different from those of molecular oxygen. The observed transition metal migration into the Li-layer in LR-NMC is instead strongly correlated with a reduced transition metal environment (TM^{4+}). Overall, LR-NMC displays neither migration assisted Mn oxidation nor beam-induced molecular oxygen in LR-NMC but rather provides further support for oxidized lattice oxygen.

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Atomistic and Continuum Modeling of Liquid-Vapor Phase Change Processes

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Multiphase fluid phenomena involving phase transformations are not only abundant in nature but also prevalent in various engineering applications. Such liquid-vapor phase change processes (evaporation/condensation) have been studied over several decades but certain important aspects are yet to be understood. For instance, quantitative theories which accurately predict mass fluxes or characterize the temperature jump at liquid-vapor interfaces during phase transformations are still subjects of active research. Along with better fundamental theories for describing evaporation/condensation processes, continuum numerical methods capable of utilizing these ‘theories’ to model macroscopic phenomena are essential. In this talk, I will address some of the fundamental questions regarding liquid-vapor phase transformations using molecular dynamics simulations. Simultaneously, I will discuss how finite element-based continuum numerical methods for modeling multiphase flows can be augmented with information uncovered from atomistic simulations.

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Exploring Chemically Active Sites on Ceria-Supported Pd Single-Atom Catalysts from Experiments and First Principles

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Active sites for single-atom catalysts (SACs) remain highly debated, and fundamental insights are limited due to experimental challenges where only the “resting states” of SACs are likely to be detected. We used CO oxidation over Pd single atoms supported on ceria as a probe for understanding the active Pd states, oxidation states, and reaction mechanisms which are crucial in understanding site stability and predicting catalytic performance. Density Functional Theory (DFT) calculations in conjugation with spectroscopic experimental techniques examine and identify the synergy between Pd atoms and the ceria support towards CO oxidation. We also developed a first principles microkinetic model to provide further insights into Pd dynamic states under CO oxidation reaction conditions. Further on, Bayesian statistics was used to calibrate the microkinetic model as well as narrow the search towards reasonable Pd/ceria model and identify dominant reaction networks that match experimental observables.

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Maximizing Selectivity: An Analysis of Isoporous Membranes

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Membranes are compelling candidates for many separation-based industrial processes. However, all synthetic membranes are subject to well-recognized permeability-selectivity tradeoffs that hinder their use in advanced applications. Having uniform nanoscale pore size, isoporous membranes have attracted wide research interest. However, quantitative analysis of their separation performance is lacking – particularly at macroscopic system-level scales. In this study, an analytical model is built to investigate how membrane pore-size distribution affects the solute separation efficiency (i.e., selectivity). The model accounts for microscopic and macroscopic transport mechanisms and explores effects on separation from the solute-to-pore-size ratio and stage cut (i.e., percent recovery). At the module level, our analysis suggests that a notably sharper rejection vs. solute size curve can be obtained as the pore-size distribution becomes narrower. As the stage cut increases, the rejection of a solute is maintained at a high level using isoporous membranes while the rejection drops rapidly for membranes that possess a disperse pore-size distribution. Furthermore, in the separation of mixed solutes, isoporous membranes achieve a large selectivity with a modest loss of permeability. Overall, this study elaborates on the unique role that isoporous membranes play within the permeability-selectivity trade-off relations and identifies the most exciting opportunities for their future applications.

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Insights into Coordination Complexes and Supramolecular Architecture within Solvent Extraction Systems of Diglycolamide and Organophosphorus Acidic Ligands

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Nowadays selective separation processes are sought after more than ever before. They are indispensable to meet the growing demand for individual rare earth elements and minor actinides partitioned from advanced nuclear fuel cycles. This multifaceted research focuses on such separation techniques as solvent extraction which is currently the dominant technology in hydrometallurgy. In terms of the development of solvent extraction processes in hydrometallurgy, multiple approaches have been explored worldwide to address the chemically challenging separations. As part of those efforts we explored the structure-property relationship within a mixture of ligands, accounting for extraction synergy. Through systematic variation of the aqueous phase acidity and extractant concentration and extractant combination, we provided a metrical, morphological and structural information on coordination environment of the trivalent 4f ions within multi-scale aggregates formed by neutral diglycolamide and acidic organophosphorus extractants. The structural organization of aggregates and metal extraction efficiency was probed with small-scale solvent extraction tests using radiotracers, FT-IR spectroscopy, small-angle X-ray scattering, tensiometry, and various titrations quantifying the transfer of solutes. The distribution ratios of metal, water, and counterions were linked to structural changes of reverse-micellar aggregates within complex liquids at the concentration range of practical conditions of solvent extraction.

Generic Coarse-Grained Model for Mixed Conducting Systems

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Organic mixed ion-electron conducting (OMIEC) polymers exhibit transport of both electrons and ions. This unique functionality underpins many emerging applications including biosensors, organic electrochemical transistors, neurocomputing devices, and batteries. OMIEC design is incipient, and the few materials that have been synthesized have been based on electron conducting units and ion conducting units from adjacent applications in organic semiconductors and polymer electrolytes, respectively. Although this modular approach has produced materials exhibiting mixed transport, further progress is frustrated by incomplete knowledge of how ionic and electronic transport are coupled in these materials and the absence of design rules specific to OMIECs. In this work, we develop a general coarse-grained model which can effectively explore the slow dynamics and nanoscale features of these systems. The model is extremely flexible and enables variation of backbone anisotropy, persistence length, side-chain density, hydrophilicity, and patterning, that can be used to interrogate how these general properties affect OMIEC behavior and electronic ionic coupling. We present our findings on the emergent OMIEC physics upon variation in sidechain composition and further, suggest novel design rules.

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Oil Spill Proliferation by Gentle Drop Impact

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Leakages from tankers aboard maritime vessels can have paralyzing consequences for marine lifeforms besides contaminating pathways of our sources of food and water. Small drops emanating from spraying oil jets are especially difficult to contain since their proliferation is closely linked to the coalescence dependent spreading and therefore warrant a detailed investigation. To this end, we examine the model problem of gentle deposition of a single drop of oil on a pool of water, representative of an oil spill scenario. Through a methodical study of 11 different *n*-alkanes, polymers and hydrocarbons typically present in crude oils we devise a regime map, scaling laws for deformation features and spreading behavior. We report the existence of a previously undocumented regime of coalescence. Our studies also unearth the crucial dynamics of initial time spreading which is markedly different from the extensively documented late time spreading and deeply connected to the coalescence behavior. These findings can be readily extended to different two-phase interactions which include (but not limited to) emulsions, enhanced oil recovery, CO₂ sequestration and sea sprays.

Simulation of Finite-sized Particle Transport through Porous Media

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Understanding the transport of finite-sized particles comparable to pore or throat diameter through a porous medium is important in many industrial and natural processes, including oil recovery, drug delivery, and ground water contamination and remediation. Theoretical and computational studies of pore-scale transport have often focused on the dispersion of infinitesimally small particles in which steric and hydrodynamic interactions of particle with the porous medium do not play an important role in the dispersion. Here, we employ the Stokesian dynamics method to investigate the effect of steric and hydrodynamic interactions on flow-driven transport of finite-sized nanoparticles within a porous medium. We model the porous medium as an ordered array of nanoposts. We vary the flow conditions to access Péclet numbers from 0 to 40 and the spacing between nanoposts to access dimensionless confinements from 0.05 to 0.5. Using this model, we calculate diffusion coefficients in quiescent conditions and dispersion coefficients in flow conditions. Under quiescent conditions, the diffusivity of particles that interact with the posts only through steric exclusion linearly decreases with increasing confinement due to the higher frequency of collisions with nanoposts. Inclusion of lubrication and far-field hydrodynamic interactions (HI) further reduces particle diffusivity, largely for strong confinement due to increased viscous drag from nanoposts. Under flow conditions, with steric interactions alone, the longitudinal dispersion coefficient increases slightly as a function of Pe due to increases in collision frequency with nanoposts and in the width of collision frequency distribution. Inclusion of lubrication and far-field HI, however, leads to a power-law increase in the longitudinal dispersion coefficient as a function of Pe, due to spatial variations in the fluid velocity induced by nanoposts. Improved understanding of the effects of steric and hydrodynamic interactions on particle transport under quiescent and flow conditions will help to improve the design of particles for transport through porous media and the design of periodic microstructures for separations of nanomaterials.

Chemically Specific Modeling Approaches to Accelerate Organic Photovoltaics Design

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The presentation will discuss chemically specific modeling approach leveraging computational approaches such as molecular dynamics and coarse-graining. Optimizing morphology of typical photoactive layers of organic solar cells for the targeted properties, such as - the performance and stability, are challenging due to the inherent complex correlation. This presentation intends to establish a high-throughput computational framework which will connect data-enabled predictive modeling with chemically specific multi-objective optimization approaches in aim to accelerate the organic photovoltaics design. Alongside the discussion on the computational modeling approaches the presentation will provide perspective into the collaborative approaches to leverage theoretical knowledge gained from computer simulations to augment experimental design and characterization processes.

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Multi-Dimensional Non-Linear Spectral Vanishing Viscosity for Stabilization of Hyperbolic Problems within the CG Spectral Element Framework

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In this work we present the implementation of a novel spectral vanishing viscosity (SVV) operator in the spectral element code, Nek5000, for the stabilization of pure linear/non-linear hyperbolic problems. The multidimensional SVV convolution kernels, which, in essence, have a similar effect as a high pass filter applied to the derivatives, are formulated by exploiting the tensor product form, analogous to the construction of the usual Laplacian matrix system. The resulting kernels are orthogonal and subsequently ensure a symmetric positive definite diffusion operator. Further, a non-linear viscosity coefficient is formulated for scaling the SVV term, which provides a reliable mechanism for detecting sharp gradients in the solution or its derivatives and amplifying the SVV magnitude. The overall formulation is demonstrated to provide a robust stabilizing mechanism through challenging linear and non-linear hyperbolic problems, including, shock capturing for 1D Burger's equation, Zalesak rigid body problem and the level-set re-distancing problem. Detailed analysis of the results elucidates the behavior of both linear and non-linear SVV constructions for smooth solutions and near the shock/discontinuity. While the linear SVV construction provided a robust mechanism for capturing discontinuities, it manifested severe undershoots and overshoots in its immediate vicinity. The non-linear viscosity coefficient is shown to be effective in ameliorating this problem, while simultaneously enhancing the solution profile in the smooth regions.

ENVIRONMENTAL SCIENCE

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Simulating Wind Velocity Deficit and Turbulence Characteristics in Urban Areas

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Atmospheric boundary layer (ABL) simulations allow for the optimization of the design and operation of wind turbines and wind farms. Distributed wind turbines can be used in urban or suburban areas for covering energy needs using a sustainable energy solution. The simulation of high Reynolds number turbulent ABL flows past obstacles can be used for the prediction of velocity deficit and turbulence characteristics (e.g. turbulent kinetic energy or turbulence intensity) downstream of building-like obstacles, thereby allowing for the estimation of power losses and fatigue loads in wind turbines. Our current study focuses on predicting the complex flow patterns in the wake of cuboids, which represent buildings, using a hierarchy of flow modeling techniques – ranging from DNS to RANS. More recently, we have also been exploring the use of overset grid method to perform an extensive parametric study to characterize the effects of building aspect ratios and building orientation, surface roughness, and temperature and on the velocity and turbulence profiles. The flow data sets and analysis of our simulations will then be used to inform the development of subgrid models, via AI/ML techniques, to predict the interactions of ABL flow with buildings on complex terrains.

Convection Resolved Climate Simulations

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An increase in precipitation intensity has been occurring in the continental United States (CONUS) (Chang et al., 2016). A strong correlation exists between the increase in temperature and precipitation intensity which is also expected in future in warming trends. The impacts of these precipitation patterns include electric and gas providers as well as water treatment and drainage systems (Argonne Climate Resiliency Workshop). Precipitation forecasts are improved through the use of convection-resolved scale simulations that use dynamically downscaled regional climate models (Chang et al., 2018). In order to advance the understanding of this increase in precipitation, this type of simulation needs to be conducted. For this study, the WRF model with 4km grid resolution is used to examine model performance of precipitation patterns with the ERA5 data. Several years of data are simulated for the purpose to examine bias. These results are part of a much larger and growing dataset of convection resolved climate simulations to fully understand the improvement of forecasts with dynamic downscaled regional climate models.

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MATERIALS SCIENCE

In Situ Measurement of Atomic Layer Deposition Reaction Heats using Pyroelectric Calorimetry

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Atomic layer deposition (ALD) is used in applications such as semiconductor devices and nanomaterial synthesis. It is characterized by sequential self-limiting reactions of gas phase precursors on a substrate surface. Film and interface properties such as defects, stoichiometry, and crystallinity depend on this surface reaction, but typically the process is empirically optimized without detailed understanding of the reaction pathways. This is particularly true for ALD nucleation on non-ideal or heterogeneous substrates which can vary greatly from steady state growth. Pyroelectric calorimetry has been developed as an *in situ* method to measure time resolved heat generation in ALD reactions. This work presents the first calibrated measurements of ALD reaction heats and provides greater sensitivity and time resolution compared to complementary techniques such as quartz crystal microbalance, spectroscopic ellipsometry, and infrared spectroscopy. We demonstrate that ALD calorimetry can resolve the heat from fractions of an ALD half-cycle reaction with < 0.5 ms sampling. A foundation for this technique is established with the measurement of the trimethylaluminum and water reaction, as this is the most widely studied ALD reaction with the greatest resource of computational modeling results. Opportunities for future work include selective deposition for defect passivation and reaction inhibition for area-selective ALD.

Atomic Layer Deposition for Microchannel Plate Applications

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Microchannel plates (MCPs) are a continuous 2d array of 10^4 to 10^7 micron-sized pores, which act as electron amplifiers. These channels display high sensitivity to incoming electrons generated from the photocathode. These electrons undergo secondary electron emission as they propel towards the anode. MCP-based photodetectors exhibit high gain, high spatial and timing resolution, and very low background noise with applications in low-level photon signal detection, secondary electron microscopy, and time of flight detection.

In the advanced ALD-MCP technology, electrical resistance and the secondary electron emission can be adjusted independently unlike conventional toxic lead oxide glass based MCPs. Atomic layer deposition (ALD) is a robust thin film deposition method involving alternation of precursor and purge gas exposures allowing deposition of conformal, stoichiometric films inside pores. We have developed ALD processes where the resistivity can be tailored by adjusting content of W and Mo in the nanocomposite $W:Al_2O_3$ and $Mo:Al_2O_3$ resistive films. Next, the high secondary electron emission layer of MgO is deposited by ALD, which results in high MCP gain. This technology can be used to coat large area MCP substrates with very conformal pinhole free resistive and emissive films.

First-Principles Study of the Electro-Mechanical Modification of 2D Materials

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The non-trivial properties of low-dimensional (LD) materials due to quantum confinement effect miraculously advance our understanding of the fundamental physics principles of nature. This work explores the electronic and mechanical properties of LD materials through employing state-of-art computational method of first principles calculations, especially density functional theory (DFT). Regarding electronic and mechanical properties, band gap transitions of MoS_2 and WS_2 , anisotropy of phosphorene. Firstly, accurate band gaps as a function of homogeneous biaxial strain in monolayer transition metal dichalcogenides were investigated, in consideration of various perturbative corrections to the DFT electronic structure, e.g. GW, spin-orbit coupling, as well as many-body excitonic and trionic effects. We show that all of these corrections are of comparable magnitudes and need to be included in order to obtain an accurate electronic structure. Secondly, the effects of uniaxial stress along an arbitrary direction on mechanical and electronic properties of phosphorene were explored, resulting in the enhancement of inherent anisotropy.

Quantum Inspired Ultrafast Imaging and Spectroscopies

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Ultrafast Imaging and spectroscopies are powerful tools to explore transient events in the field of energy, environment, and national security. Conventional ultrafast imaging and spectroscopy techniques are limited in the aspects of detection efficiencies, environment obstructions and detector technologies. To overcome the limitation of conventional techniques, we propose a series of quantum inspired ultrafast imaging and spectroscopy techniques, i.e., ghost imaging second harmonic generation, time-resolved photoluminescence ghost imaging and hyperspectral transient absorption ghost imaging. With these proposed techniques, we show that firstly are we able to speed up the imaging speed by an order of magnitude, secondly, we can image through scattering environments, and the last, we can eliminate the usage of special focal plane array detectors which are not cost-effective.

MATHEMATICS & COMPUTER SCIENCE

Improving Application Performance on Supercomputers using Flexible Bandwidth Allocations

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Many essential research activities rely on supercomputers to solve complex problems, such as climate modelling, simulating galaxies in the universe, and developing Covid19 vaccines. These supercomputers use thousands of small compute nodes and rely on very high-speed networks to efficiently move data among the different compute nodes. However, running multiple applications at the same time causes network interference, resulting in unpredictable performance slowdown as the applications compete for network bandwidth.

Quality-of-service (QoS) classes can allocation bandwidth per application to manage competition and interference, but most solutions use coarse-grain bandwidth allocations that are unsuitable for dynamic workloads. We propose a flexible method of allocating bandwidth that adapts to changing application demands. By defining QoS classes with two bandwidth limits, an assured bandwidth limit and a peak bandwidth limit, we can guarantee the minimum amount of bandwidth required by the application as well as control how applications access bandwidth above their guaranteed amounts. Evaluations prove that our solution can effectively regulate bandwidth allocation for varying traffic loads to control the impact of interference and improve application performance. This enables multiple applications to share the network without excessive slowdown due to interference.

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Multiobjective Optimization of Simulations with PARMOO

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Multiobjective optimization (MOO) problems are ubiquitous in science and engineering. In MOO, the optimization algorithm must balance the tradeoffs between multiple potentially conflicting objectives. For many of these problems, the underlying cost function is derived from a computationally expensive numerical simulation. In such situations, the computational cost of solving the MOO problem can be prohibitive. In this talk, we will discuss our ongoing work on PARMOO, a MOO framework that is designed to take advantage of parallel resources and exploit properties of the simulation.

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Stochastic Epidemic Model Calibration using Quantile Based Emulation

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We present a calibration approach based on Gaussian process emulation for large scale stochastic computer models. As opposed to deterministic computer simulations, output from repeated runs of stochastic computer model at same input yields random realizations from an unknown distribution. The proposed approach uses quantile regression strategy [M. Plumlee and R. Tuo, *Technometrics*, 56 (2014), pp. 466–473] to emulate the multivariate stochastic output from an agent based epidemic model. Such an emulator is then used within a Bayesian model calibration framework to calibrate the large epidemic model and to make future predictions with associated uncertainties. Illustrations are taken from an Ebola epidemic workshop from 2015 and the ongoing Covid19 pandemic.

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Application-Specific Lossy Compression Algorithms for Scientific Data

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With the improvements in high-performance computing (HPC), many scientific applications have gained access to work on much larger datasets than before, which shifted the bottleneck to the memory and storage systems. Our work focuses on helping helps to overcome these bottlenecks by developing application-specific lossy

compression algorithms when the conventional lossless or general-purpose algorithms are not efficient enough.

Our award-winning compression algorithm PaSTRI [1] helps improving the performance of GAMESS [2], an important quantum chemistry application that is also a part of ECP[4]. We have observed that there are repeating patterns in each block, which we have exploited to develop an efficient algorithm to compress the data with the same error bound used in the original GAMESS application.

We are also developing another compression algorithm called ROI-Comp that helps ExaFEL [4] project, another ECP project that analyzes x-ray free electron laser data. The ExaFEL data has different regions based on their importance, which we treat differently in our algorithm, and achieve better compression ratios than other compressors without compromising the data quality. Consequently, we have showed that our lossy compression techniques can help achieving the desired compression ratios and rates on important ECP applications without affecting their output quality.

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Implicit-Explicit (IMEX) Methods for Coupled Compressible Navier-Stokes Equations

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Earth system models require to couple various components including atmosphere, ocean, and land. For decades, each component has been well-developed and continuously improved. When it comes to coupling, we need to address several challenges such as matching different grids at the interface and treating different time scales arising from each model. In this study, we focus on the coupling strategy in the sense of stable time integration methods. In particular, explicit coupling, partially-implicit coupling, and implicit-explicit (IMEX) coupling strategies are explored to handle different time scales. For a simplified model for air-sea interaction problem, we consider a coupled compressible Navier-Stokes equations with an interface condition. Under the rigid-lid assumption, horizontal momentum and heat flux are explicitly exchanged through the interface. Several numerical experiments are conducted to demonstrate the stability of the couplings schemes.

Model-Based Reinforcement Learning for Predictive Synthesis of MoS₂

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Designing conditions for experimental synthesis is the primary bottleneck for the realization of new functional quantum materials. Current strategies to synthesize new promising materials with desired properties are based upon a trial and error approach, which is a time-consuming process and does not generalize to different materials. Here, we use deep reinforcement learning (RL) to learn synthesis schedules, which are time-dependent synthesis conditions of temperatures and reactant concentrations for a prototypical quantum material, monolayer MoS₂ via chemical vapor deposition (CVD). The RL agent is coupled to a deep generative model that captures the probability density function of MoS₂-CVD dynamics and is trained on 10,000 computational synthesis simulations. After training, the RL agent successfully learns the optimal policy in terms of threshold temperatures and chemical potentials for the onset of chemical reactions and provides mechanistic insight to predict new synthesis schedules that produce well-sulfidized crystalline and phase-pure MoS₂ in minimum time, which is validated by reactive molecular dynamics simulation.

Towards CAD-Based Geometry Modeling with The Random Ray Method for Radiation Transport

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The Advanced Random Ray Code (ARRC) is a high-performance computing application capable of high-fidelity simulations of full core nuclear reactor models. ARRC leverages a recently developed stochastic method for neutron transport, known as The Random Ray Method (TRRM), which offers a variety of computational and numerical advantages compared to existing methods. TRRM has been shown to be capable of efficient simulation of explicit three-dimensional geometry representations without assumptions about axial homogeneity. To date, ARRC has utilized Constructive Solid Geometry (CSG) combined with a nested lattice geometry which works well for typical pressurized water reactors but is not sufficient for arbitrary geometries.

To facilitate simulation of arbitrarily complex geometries in ARRC, we propose performing transport directly on Computer-Aided Design (CAD) models of the geometry. In this study, we utilize the Direct-Accelerated Geometry Monte Carlo (DAGMC) toolkit which tracks particles on tessellated CAD geometries. Additionally, we present a method for automatically subdividing the large CAD regions into smaller mesh cells required by random ray to achieve high accuracy. Finally, we test the DAGMC geometry implementation in ARRC on several test problems, including a 3D pincell, 3D assemblies, and an axial section of the Advanced Test Reactor at Idaho National Laboratory.

Scalable and Accurate Multi-GPU Based Image Reconstruction of Large-Scale Ptychography Data

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Ptychography is a coherent imaging technique that can be used to image materials at nanoscale resolutions. The ptychography experiments can yield hundreds of Gigabytes to Terabytes scale datasets that are far beyond a single GPU's capacity. In this work, we propose a multi-GPU based fine-grained parallelization of maximum-likelihood (ML) based ptychographic reconstruction in this work. Our design aim to improve the performance of conjugate-gradient (CG) solver in the ML method. In contrast to the existing works that parallelize an algorithm (e.g., the ePIE) at coarse level, our work designs an advanced hybrid parallelization technique that applies different approaches for different CG solver steps in accordance with their respective performance bottlenecks. This design can diminish the inter-GPU synchronization and communication overhead while fully preserve the original algorithm's accuracy. We implement our optimizations in a software package, PtyGer, and comprehensively evaluate it using various phantom and experimental datasets. The experimental results show that PtyGer can provide accurate reconstruction with outstanding multi-GPU scalability. We believe the interested parties can use our software package to reconstruct their experimental datasets or apply our optimizations to their own ptychographic reconstruction algorithms.

PHYSICS & HIGH ENERGY PHYSICS

Picosecond Timing Resolution Measurements of Low Gain Avalanche Detectors with a 120 GeV Proton Beam for the TOPSiDE Detector Concept

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The Timing Optimized PID Silicon Detector for the EIC (TOPSiDE) is Argonne's proposed central detector concept for the Electron-Ion Collider, with its physics goals of perturbative and non-perturbative Quantum ChromoDynamics (QCD) studies of the structure of nucleons and nuclei. It requires high precision tracking, good vertex resolution, and excellent particle identification with a timing resolution of around 10 ps or better. TOPSiDE uses Ultra-Fast Silicon Detectors (UFSD) based on the Low-Gain Avalanche Detector (LGAD) technology. The speaker will present the work on the characterization and testing of the LGAD silicon sensors at Argonne [1].

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Search for Michel Electrons in ProtoDUNE

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The Deep Underground Neutrino Experiment (DUNE) is a cutting-edge experiment for neutrino science and proton decay studies. The single-phase liquid argon prototype detector at CERN (ProtoDUNE) is a crucial milestone for DUNE that will inform the construction and operation of the first and possibly subsequent 17-kt DUNE far detector modules. I will present the current status of reconstructing Michel electrons from the decays of 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 selection tools to identify such Michel electrons which could benefit any LArTPC experiment generically.

SYNCHROTRON RESEARCH

Observation of Double-Core-Hole Continua and Fragmentation Patterns of the Formamide Molecule after Irradiation by Intense Femtosecond X-ray Pulses

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The development of third generation synchrotron radiation (SR) facilities, as well as the intense femtosecond pulses provided by an X-ray Free Electron Laser (XFEL), made the experimental observation of the elusive double-core-hole (DCH) states feasible [1,2]. DCH states are electronic states of matter, created either by the ejection of two core-shell electrons to the continuum [3], by a core-ionization core-excitation mechanism [4], or by a double core-excitation.

Experimental results on the observation of DCH states, involving the K-shells of all C, N and O atoms in formamide, the simplest bio-molecule, have been acquired by our group, and interpreted by the aid of state-of-the-art *ab initio* quantum chemical calculations [5]. Both single-site (ss) K^{-2} and two-site (ts) $K^{-1}K^{-1}$ DCH

fingerprints are present in the measured spectra, where in the latter case, two different atoms in the molecule possess a K-shell vacancy each. Finally, using an ion time-of-flight (TOF) spectrometer, different fragmentation pathways of the molecule have been observed, while several photons absorption is taking place as can be seen by the high mass over charge states (C^{3+} , N^{4+}) in the spectrum.

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Are you preparing for an academic job search? Do you have questions about preparing for faculty interview positions or preparing your application materials? Are you looking for general information on what a faculty career entails? Professor Walter Henne of Governors State University, Chemistry, will be on hand to offer advice and answer your questions about academic careers. Dr. Henne has mentored several Argonne postdoctoral alumni through successful academic searches. Dr. Henne received his Ph.D. in Chemistry from Purdue University with a special focus in bio-

analytical chemistry and chemical biology. His current research interests center around the use of low molecular weight, high affinity ligands/probes for the development of targeted drug therapies and medical diagnostic assays. Areas span infectious disease, cancer and inflammatory disorders. He is the author of more than 20 peer-reviewed research papers and patents and has received several awards for excellence in teaching.



Advanced Material Pandemic & Future Preparedness Taskforce (AMPT) is an independent international, public benefit organization committed to facilitating the global use of advanced materials to solve some of humanity's most immediate challenges. The taskforce engages thought leaders from academia, industry and policy making organizations to create an international "Future Preparedness" infrastructure and to shape national and international agendas that will maximize the IMPACT of advanced materials on society and human life. Currently with over 15 country chapters, 10 working groups, and over 30 institutions, AMPT is set to establish a comprehensive roadmap, library of knowledge and map of user-centric needs to deliver a framework to devise strategies, coordinate global activities and fast track solutions to address the technological and societal needs of the post pandemic world. www.amptnetwork.com

[Looking for](#) PhD in condensed matter, material science, bioelectronics, polymer and composites



Data Discovery and Decision Science (D3) is the research and analytics organization at **Allstate Insurance Company**. We are solving some of today's most complicated analytics problems, making the lives of our Allstate colleagues easier and more productive, and driving our mission to deliver perfect insurance solutions to our customers. We are avid about learning and applying new tools and techniques to get the most value from our massive data resources. In partnership with technology and the business, we are incorporating analytics into every aspect of the enterprise. www.allstate.com

Degrees/Areas of interest: Master's or Ph.D. degrees are preferred, and research areas include advanced machine learning techniques/predictive modeling, including natural language processing and computer vision.



Aramco Americas provides new thinking, new approaches, and new solutions for the future of energy. We operate as a vital link between people and partners in the Americas and our parent company, Saudi Aramco, the world's leading energy company. From engineers and scientists to specialists in procurement and R&D, our team members embody the highest standards of safety and professional conduct. Our work not only applies to the oil and gas industry but also has far-reaching implications for other industries. We are developing innovative solutions to today's operational challenges while also looking ahead to create the energy breakthroughs

that will power the future.

Aramco is a leading producer of energy and chemicals. At its research & innovation centers around the world, Aramco's transport technologies team is working with leading automakers to develop and demonstrate new fuel and engine solutions that improve efficiency and address environmental challenges. <https://americas.aramco.com/>

Degrees/Areas of interest: M.S./Ph.D., Advanced engine/fuel technologies, including engine combustion, CFD, design optimization, vehicle modeling, and fuel chemistry etc.



Arity is a data and analytics company focused on improving transportation. We collect and analyze enormous amounts of data, using predictive analytics to build solutions with a single goal in mind: to make transportation smarter, safer and more useful for everyone. We believe the future of mobility is about more than just how we get from A to B—it's about what moves us forward. Emerging technologies and business models, like ridesharing, are disrupting existing systems and rapidly changing the way people get around. Born from Allstate Insurance, Arity is uniquely positioned to predict and manage risk through data and behavioral insights. We find the meaning in mobile and vehicle telematics data so businesses can make smarter decisions and grow their business well into the future. <https://www.arity.com/>

Common degrees we look for in Analytics candidates include but are not limited to statistics, mathematics, computer science, data science, and predictive analytics. <https://www.builtinchicago.org/company/arity>



ASM is a leading, global supplier of semiconductor wafer processing equipment. Our smart and ambitious team is dedicated to delivering innovative technology solutions to the world's leading semiconductor manufacturers. We have over 2,200 employees based in 16 countries, including Belgium, Japan, Netherlands, South Korea, Singapore, Taiwan, and the United States. Together we work to develop Epitaxy, ALD, PEALD, Vertical Furnaces and PECVD thin-film deposition technologies for our customers. Our goal is to remain an industry leader by being ahead of what's next. We accomplish this by focusing on finding collaborative solutions to make integrated circuits, or chips, smaller, faster and even more powerful. <https://www.asm.com/>

Interested degrees: Electrical Engineering, Material Science, Mechanical Engineer, Chemical Engineering, and Physics



Brookhaven National Laboratory (BNL) delivers discovery science and transformative technology to power and secure the nation's future. Primarily supported by the U.S. Department of Energy's (DOE) Office of Science, Brookhaven Lab is a multidisciplinary laboratory with seven Nobel Prize-winning discoveries, 37 R&D 100 Awards, and more than 70 years of pioneering research. <https://www.bnl.gov/world/>

We advance fundamental research in nuclear and particle physics to gain a deeper understanding of matter, energy, space, and

time; apply photon sciences and nanomaterials research to energy challenges of critical importance to the nation; and perform cross-disciplinary research on computation, sustainable energy, national security, and Earth's ecosystems.



Cerebras Systems is a team of pioneering computer architects, computer scientists, and deep learning researchers. We have come together to build a new class of computer system that accelerates artificial intelligence by orders of magnitude beyond the current state of the art.

At Cerebras, we are always looking for extraordinary people. We value integrity, passion, problem-solving ability, and a sense of humor. Interested in joining our team? We have specific opportunities across software and hardware engineering, and machine learning research. We are looking for talented individuals with various education backgrounds (bachelor through Ph.D.) and experience. Find more about our current openings at www.cerebras.net/careers .



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innovative technologies and solutions, backed by a talented and dedicated team of employees. <https://www.donaldson.com/en-us/>

Looking for B.S., M.S., and Ph.D. in chemistry, physics, chemical engineering, materials science, electrical engineering, and mechanical engineering.



Exelon is a FORTUNE 100 company that works in every stage of the energy business: power generation, competitive energy sales, transmission and delivery. As the nation's leading competitive energy provider, Exelon does business in 48 states, D.C., and Canada and had 2018 revenues of \$35.9 billion. We employ approximately 33,400 people nationwide. To thrive in an industry undergoing fundamental change, Exelon has cultivated a culture of innovation that promotes early adoption of promising new technologies and processes.

Exelon's mission is to be the leading diversified energy company - by providing reliable, clean, affordable and innovative energy products. At Exelon, we believe that reliable, clean, and affordable energy is essential to a brighter, more sustainable future. That's why we're committed to providing innovation, best-in-class performance and thought leadership to help drive progress for our customers and communities.



The **International Atomic Energy Agency (IAEA)** in Vienna, Austria is the world's center for cooperation in the nuclear field committed to promoting safe, secure and

peaceful uses of nuclear technology. The IAEA offers opportunities to engage current, meaningful issues of global peace, security and development while working in a multicultural environment. Working at the IAEA is a rewarding experience and provides an opportunity to contribute to the promotion of peaceful uses of nuclear technology and to sustainable development. As the largest contributor to IAEA programs, the U.S. is committed to encouraging well-qualified Americans to apply for professional posts at the IAEA. The IAEA employs professionals from a variety of scientific and policy backgrounds. The IAEA offers different types of employment opportunities: for professional and general service posts; consultants and experts; junior staff, through internships; and the Junior Professional Officer program. IAEA Programs at Argonne offers U.S.-sponsored internship and Junior Professional Officer positions for recent graduates and professionals. There are also programs to offer senior professionals an opportunity to temporarily join the IAEA's workforce as Cost-Free Experts. Please check out our brochures *Careers at the IAEA* and *Jump-Start Your Career at the IAEA* to learn more about how to apply, benefits, employment opportunities, and to read testimonies from previous Junior Professional Officers and Interns. If you would like to contribute to the IAEA at an overseas assignment in Vienna, Austria or Monaco, you can read more at: <http://international.anl.gov/careers>

Areas of interest: Nuclear science, nuclear engineering, physics, chemistry, biology, oceanography, environmental science, environmental radioactivity, computer modeling, scientific or engineering discipline relevant to nuclear safety, social sciences, and international relations.



Idaho National Laboratory (INL) is part of

the U.S. Department of Energy's complex of national laboratories. The laboratory performs work in each of the strategic goal areas of DOE: energy, national security, science, and environment. INL is the nation's leading center for nuclear energy research and development. INL is managed by Battelle Energy Alliance for the Department of Energy's Office of Nuclear Energy. <https://inl.gov/>

INL is the nation's lead laboratory for nuclear energy research, development, demonstration and deployment, and we are engaged in the mission of ensuring the nation's energy security with safe, competitive and sustainable energy systems and unique national and homeland security capabilities. Nuclear energy, advanced manufacturing, hybrid batteries, energy systems and storage, hydrogen energy systems, grid infrastructure protection, cyber security, wireless technology, grassy bio fuels, computation modeling and simulation engineering and science nuclear, materials, chemical, mechanical, electrical, chemistry, computation, AI & ML, operations research.



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Jinetics Inc. is a spin-off from Stanford University working on hydrogen-related electrochemical solutions. Leveraging the synergy between deep-tech R&D and applicational innovations, Jinetics aims at becoming a top enabler of the hydrogen economy. We identify decarbonization opportunities in multiple sectors (transportation, healthcare, and the built environment) and develop hydrogen-related solutions. We are on the lookout for the person who shares the passion for a hydrogen future and eager to carry out research results into practical solutions. <http://www.jinetics.com/>

Preferred degrees: M.S. and Ph.D. Research area: fuel cell/electrochemical synthesis



The National Renewable Energy Laboratory (NREL) is a leader in the U.S. Department of Energy's effort to secure an energy future that is both environmentally and economically sustainable. From breakthroughs in fundamental science to new clean technologies to integrated energy systems that power our lives, NREL researchers are transforming the way the nation and the world use energy.

Areas of interest: advanced manufacturing, bioenergy, buildings, chemistry and nanoscience, computational science (including HPC), energy analysis, energy storage, energy system integration,

geothermal, grid modernization, hydrogen and fuel cells, materials science, transportation and renewable energy sources (hydro, wind, solar).



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We hire mostly people with degrees in physics (especially nuclear or particle) or biomedical engineering.



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Spectral Sciences, Inc. is looking for candidates with degrees in the physical sciences (physics, atmospheric sciences, image science, optics, etc.) or engineering (electrical, aerospace, mechanical, etc.). Research areas include the development of fundamental physical models for (1) electro-optical data analysis, (2) sensor concepts for remote sensing (3) spectral image processing, (4) hyperspectral and multispectral imaging, (5) molecular spectroscopy, (6) gas and fluid dynamics, and (7) radiative transfer phenomena.

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