11TH ANNUAL
OAK RIDGE POSTDOCTORAL ASSOCIATION RESEARCH SYMPOSIUM

IN-PERSON WITH VIRTUAL OPTIONS AT

OAK RIDGE National Laboratory

TENNESSE ROOMS
MAY 18–19, 2023

Foreword by Laboratory Deputy Director for Science and Technology

I want to start by thanking the Oak Ridge Postdoctoral Association (ORPA) Executive Committee for their leadership and organization of the 11th Annual Research Symposium. This two-day event provides an opportunity to discuss a snapshot of recent progress associated with the extraordinary Oak Ridge National Laboratory (ORNL) science and technology portfolio by bringing together people from across the institution and our partner universities. I am excited to take part in and engage with many of you at this event.

I was fortunate to be exposed to team science and access powerful research infrastructure through my engagement with a national laboratory during my PhD. The experience of working closely with colleagues having diverse expertise to tackle important national challenges that required convergence was intoxicating, and forever changed my career trajectory. Over the next couple of days, you will have an opportunity to meet many new colleagues while growing your understanding of ORNL team science. I encourage you to talk with those outside your area to better understand the challenges they are working on and consider how you could potentially collaborate. The connections and network you create now could have an outsized impact on your future career, your research, and its impact.

This year's symposium also provides an occasion to recognize ORNL's 80th anniversary, and how we continue to build upon the Laboratory's foundational breakthroughs. In 1943, the Laboratory was established as part of the Manhattan Project. Through the years, we have discovered elements, built the fastest supercomputers in the world, operated 13 nuclear reactors, and much more. Although our mission has evolved, the fact remains—ORNL continues to tackle the most challenging and pressing scientific challenges of our time. Examples today include mitigating climate change, enabling the transition to clean energy, and enhancing national security. It takes each of us working together to turn ideas into real-world solutions, and this event is crucial to making that happen.

I hope you enjoy the next few days of learning and networking.

Dr. Susan Hubbard

Foreword by Office of Research Director

I'm pleased to welcome you to ORNL's 11th annual ORPA Research Symposium! The Oak Ridge Postdoctoral Association Executive Committee has planned a fantastic program that will allow all of you to share your research and hear about the research of others. It's exciting to note that more than 100 presentations and posters will be shared at this event—a number that speaks to both ORPEX's commitment to deliver a robust scientific program and your interest in sharing your science. I wish to express my sincere gratitude to ORPA's Research Committee chairs, Athena Chen and Johnson Lu, for their organizing efforts; all our postdoc and postdoc ally volunteers, who have helped bring this program to the ORNL community; and the ORNL staff members who are serving as judges.

ORPA and the Executive Committee help foster a strong scientific community at ORNL through activities aimed at welcoming new postdocs, providing timely and important information to our postdoc community, creating a sense of community among postdocs with social gatherings of many kinds, promoting a sense of connection with the community outside campus by sharing volunteer opportunities, and facilitating career development opportunities through programs such as the annual Research Symposium. Other key events in this year's postdoc calendar include R U Feeling OK? activities on May 24 and 25, the Your Science in a Nutshell competition on June 22, and Postdoc Appreciation Week on September 18−22. From community building and wellness to opportunities to learn about career paths and research going on at ORNL, ORPA implements an integrated strategy to develop and prepare postdoctoral researchers for the next stage in their career and to actively engage them while they're with us at ORNL.

This year's Executive Committee has made it their mission to connect with postdoc associations at other national laboratories, and they're developing strong ties with Los Alamos and Argonne National Laboratories in particular. Their efforts are to be commended, as these connections will certainly continue to broaden over time and bolster the connectedness and programmatic success that are hallmarks of our postdoc community. ORPA's ongoing efforts help sustain ORNL's reputation as one of the best places in the world for postdoctoral research—a place where you can become a leader in your field and develop professional relationships beyond your own areas of expertise—and the quality of ORNL's postdoc experience has a direct correlation to ORNL's position as a world-leading research institution. I'm looking forward to hearing from ORNL's postdoc community as you share your science at this year's Research Symposium and to watching you connect with each other as you celebrate postdoc research at ORNL.

Best wishes,

Dr. Moody Altamimi

Foreword by the ORPA President

Welcome to the 11th Annual Research Symposium, hosted by Oak Ridge Postdoctoral Association (ORPA). The Symposium provides postdoctoral researchers and early career scientists with the opportunity to present their work to ORNL's research community through a day of presentations, posters, and networking receptions. This wonderful annual event brings together scientists from all directorates at ORNL, hopefully fostering many stimulating discussions and possibly future collaborations.

As an association, ORPA works closely with ORNL management to facilitate research, career, and social development of the postdoctoral associates at the laboratory. The social and networking events organized by ORPA are open to all ORNL employees. This year's Research Symposium is special because we have increased participation by 300% compared to last year.

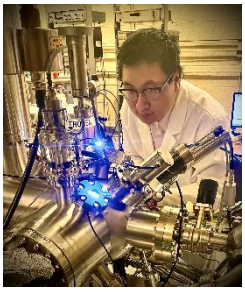
The Symposium also would not have happened without the guidance and support of Dr. Moody Altamimi, Director of the Office of Research Excellence (ORE), and Laurie Varma, Early Career Programs Specialist in ORE. We are very grateful for their interest in and involvement with ORPA.

Thank you for attending the 11th Annual ORPA Research Symposium and for supporting the postdoctoral researchers at ORNL.

Respectfully,

Indranil Roy

Foreword by Research Committee Chairs, Oak Ridge Postdoc Association



Welcome to the 11th Annual Research Symposium, hosted by the Oak Ridge Postdoctoral Association (ORPA). The symposium is designed as a unique platform to highlight research from ORNL postdocs and early-career staff and to enable postdocs and early-career staff to network with the broader ORNL community and explore potential collaborations. The symposium is taking place on May 18–19, 2023, at Tennessee Rooms A & B (oral presentations) and second-floor lobby (posters).

This year we are very excited to feature four keynote speakers: Dr. Michael Zachman, Dr. Sang Soo Lee, Dr. Mina Yoon, and Dr. Mark Lumsden. Dr. Michael Zachman is a staff scientist in the Center for Nanophase Materials Sciences at ORNL and will discuss Advanced Electron Microscopy for Energy Storage and Conversion Materials Research. We are delighted to have Dr. Sang Soo Lee, who is a geochemist from the Chemical Sciences and Engineering Division at Argonne National Laboratory, join our symposium in person, despite having traveled a long distance. Dr. Lee will be presenting on the topic of Intrinsic Complexity of Solid–Water Interfaces Deciphered by Synchrotron X-Ray Reflectivity. Dr. Mina Yoon is a senior R&D staff who leads the Microstructural Evolution Modeling Group in the Materials Science and Technology Division at ORNL. She will present her recent research regarding 2D Materials – Opportunities and Challenges. Dr. Mark Lumsden, who is Spectroscopy Section Head in the Neutron Scattering Division at ORNL, will captivate us with his presentation on the evolution and potential of neutron spectroscopy: Neutron Spectroscopy – Past, Present, and Future.

We invite you to join us in honoring the the breadth of science being undertaken at ORNL with more than 100 presentations and posters, which represent all major areas of study within the laboratory! ORPA'sResearch Committee, with the aid of the Executive Committee and ORNL volunteers, have worked hard to plan and organize this spectacular event. We extend our heartfelt gratitude to all members of both committees for their unwavering commitment to ensuring the success of the Research Symposium. We would also like to acknowledge and appreciate the invaluable contributions of Dr. Moody Altamimi, Director of the Office of Research Excellence; Laurie Varma, ORNL Early Career Programs Specialist, and Caitlyn Wakefield, Administrative/Project Support to Dr. Altamimi, without whom this symposium would not have been possible.

Thank you for attending the 11th Annual ORPA Research Symposium and for supporting early-career researchers at ORNL.

Si Athena Chen and Qiangsheng (Johnson) Lu

Acknowledgments

The Oak Ridge Postdoctoral Association (ORPA) and Research Committee would like to thank lab leadership, all volunteers, admins, and the ORNL community as a whole for their continued support of this year's Research Symposium. This event would not have been possible without your continued commitment!

We are very grateful to our four keynote speakers for their support of ORPA and the Research Symposium: Dr. Michael Zachman, Dr. Sang Soo Lee, Dr. Mina Yoon, and Dr. Mark Lumsden.

We would like to thank Laurie Varma, ORPA advisor and ORNL Early Career Programs Specialist, for her fruitful collaboration, guidance, and support on the Research Symposium. Our special thanks go to Dr. Moody Altamimi, Director of the Office of Research Excellence, for her guidance and support for the Postdoctoral Program and ORPA over this past year. Further thanks go to Caitlyn Wakefield, administrative/project support to the Office of Research Excellence, for her support with logistics and advertising.

We would furthermore like to thank the Douglas Edwardson, Web Developer in the Information Technology Service Division, Mark Robbins, Graphic Designer in the Communications Division, as well as Bill Cabage and Sean Simoneau in Laboratory Communications.

Finally, we would like to express our gratitude to all the volunteers for their dedicated efforts in assisting us with the organization of the 11th annual Research Symposium:

Arpan Biswas
Biva Talukdar
Briana Schrage
Ehab Hassan
Janet Meier
Josh Cunningham
Lu Yu
Lynda Amichi
Manjula P Senanayake Mudiyanselage
Marm Dixit
Michael Melesse Vergara
Moataz Harb
Pratishtha Shukla
Selda Nayir
Subhamay Pramanik
Tomas Grejtak
Yawei Gao
Zewen Zhu

Volunteers for the 11th annual Research Symposium included (b**ack, left to right):** Subhamay Pramanik (ORPA Vice-President), Qiangsheng (Johnson) Lu (ORPA Research Co-chair), Zewen Zhu, Arpan Biswas, Ehab Hassan, Michael Melesse Vergara, and Tomas Grejtak (ORPA Outreach Chair). **Front (left to right):** Janet Meier, Lynda Amichi, Si Athena Chen (ORPA Research Co-chair), Biva Talukdar (ORPA Communications Chair), Selda Nayir, Briana Schrage (ORPA Secretary), Laurie Varma (ORPA advisor), Pratishtha Shukla (ORPA New Hire Chair). Not pictured: Josh Cunningham, Yawei Gao, and Lu Yu.

Our volunteers took on many tasks.

Abstract book organizers:
Manjula P Senanayake Mudiyanselage, Selda Nayir, Laurie Varma

Invited speaker organizers and Research Symposium official website:
Si Athena Chen, Qiangsheng (Johnson), Zewen Zhu

Judge organizers:
Tomas Grejtak, Moataz Harb, Biva Talukdar, Pratishtha Shukla, Lu Yu

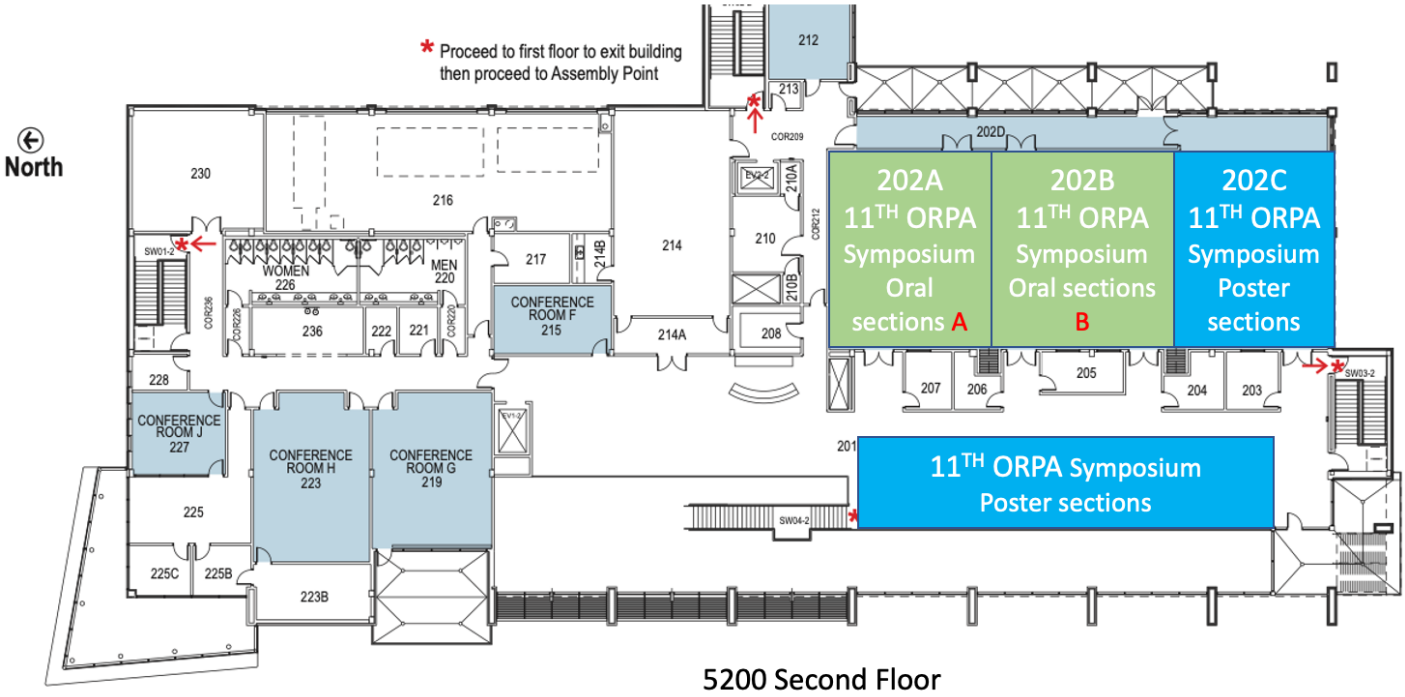
Oral session organizers:
Bioscience: Michael Melesse Vergara
Computer Science: Ehab Hassan
Earth and Environmental Sciences: Biva Talukdar
Energy Science: Marm Dixit, Moataz Harb
Material Science: Lynda Amichi, Arpan Biswas, Tomas Grejtak, Janet Meier, Subhamay Pramanik
Neutron and Nuclear Sciences: Manjula P Senanayake Mudiyanselage

Poster session organizers:
Pratishtha Shukla, Briana Schrage, Lu Yu

Online streaming moderators:
Josh Cunningham, Yawei Gao

Oak Ridge Postdoctoral Association
11th Annual Research Symposium Agenda

Event contact	Si Athena Chen (chens1@ornl.gov) and Qiangsheng (Johnson) Lu (luq1@ornl.gov)
Location	ORNL Conference Center, Building 5200, Tennessee Rooms (A&B&C) and 2nd Floor Lobby
May 18–19, 2023	



5200 Second Floor

May 18, 2023			
9:00–9:10 am	**Welcome Remarks (Room 202A)**	Susan Hubbard, (*ORNL Deputy for Science and Technology)*	
9:10–9:20 am		Moody Altamimi, (Director of ORNL Office of Research Excellence)	
9:20–9:30 am		Athena Chen & Johnson Lu (ORPA research co-chair)	
9:30–10:30 am	**Keynote Speaker 1 (Room 202A)**	**Michael Zachman, Advanced Electron Microscopy for Energy Storage and Conversion Materials Research**	
10:30–10:40 am	Break		

	10:40-12:40	**First Round of Talks (Thursday morning)**	
No.	*Name*	*Talk Title*	*Session Title*
1	Indranil Roy	Understanding microstructure evolution of Al-alloys during solidification through meso-scale modeling	Material Science in Separation and Energy Materials *10:40-11:40 am* **(Room 202A)**
2	Jaeyun Moon	Characterization of complex atomic degrees of freedom in liquids and glasses: Application to heat capacity	
3	Yu Lu	Efficient Cathode Recycling Process for Cobalt Recovery via Dual-function Green Solution	
4	Panagiotis Christakopoulos	Thin films of ionic polymers in applied electric fields	
5	Veronica Bradley	Single-particle inductively coupled plasma-mass spectrometry for automated, reproducible elemental and isotopic analysis of nanoparticles	
6	Sandeep Kaur	An efficient extraction of rare earth elements by using versatile Diglycolamide-based ligands	
7	Amith R Devireddy	Overexpression of a member of the Cation/H^+ exchanger gene family CHX20 confers drought tolerance in Arabidopsis thaliana and hybrid poplar	Genetics and Structural Biology 10:40-11:30 am **(Room 202B)**
8	Victoria Drago	Visualizing protonation states in serine hydroxymethyltransferase with neutron crystallography	
9	Yang Liu	Plant Synthetic Biology to Enable Safe Biodesign of Novel Plant-Microbe Interactions	
10	Alan Hicks	Disordered domain of companion of cellulose synthase 1 bundles microtubules into hexagonal assemblies	

11	Briana Schrage	Chelating antimony(V) for Sb-119 targeted Auger therapy	
	1:40–1:50 pm	Lunch Break	

12:40–1:40 pm	**Keynote Speaker 2 (Room 202A)**	**Sang Soo Lee, Intrinsic complexity of solid–water interfaces deciphered by synchrotron X-ray reflectivity**
1:50–5:00 pm	**Second Round of Talks (Thursday afternoon)**	

No.	*Name*	*Talk Title*	*Session Title*
12	Si Athena Chen	Strontium Incorporation to Single Crystal Calcite Growth: In Situ Measurements Coupled with Multiscale Chemical Imaging	Earth and Environmental Science 1:50 - 2:50 pm **(Room 202A)**
13	Tingting Liu	Molecular Understanding of the Influence of Electrolyte Species on Boehmite Particle Aggregation using Rare Event Simulations	
14	Matthew Berens	Evolving phosphorus biogeochemistry in an emerging coastal delta	
15	Yaoping Wang	Water, Thermal, and Land Cover Factors Led to Contrasting Urban and Rural Vegetation Resilience to Heat Waves	
16	Ryan Jacobson	Wildfire Fuels Mitigation Biomass Estimates	
17	Mengjia Tang	Performance of hemp insulation as a low embodied carbon substitute for fiber glass in building envelope systems	
18	John Lagergren	Few-shot learning enables population-scale analysis of leaf traits in Populus trichocarpa	Computational Biology 1:50 - 2:30 pm **(Room 202B)**
19	Bryan Bozeman	The ecological effects of sub-daily flow variability on riverine fishes: a systematic review	
20	Paul Inman	A Computational Multiscale Framework for Simulated Radiotherapy of Multicellular Tumor Models	
21	Kazi Masel Ullah	Evaluating the Incentive for Soil Organic Carbon Sequestration from Carinata Production in the Southeast United States	
	2:30–2:40 pm	Break	

22	Fengqi Li	Infomorphism: An Urban Planning Framework for Local Renewable Energy Integration	Grids and Machines 2:40 - 3:40 pm **(Room 202B)**
23	Qianxue Xia	Enhancing Efficiency and Stability in Multi-Port Autonomous Reconfigurable Solar Power Plants (MARS) through Advanced Control Methods	
24	Maximiliano Ferrari	Voltage Source Inverter (VSI) with Enhanced Short-Circuit Fault Current Contribution to Enable Legacy Overcurrent Protection in Islanded Microgrids	
25	Melrose Pan	Identifying travel patterns of low-income populations in New York State	
26	Saad Ayub Jajja	Implementing Low Global Warming Potential Refrigerants in the Next Generation of Condensers	
27	*Himel Barua*	Mechanical Stress, Vibration, and Rotodynamic Analysis of High-Speed Electric Motors	
	2:50–3:00 pm	Break	
28	*Lucas Pressley*	Metastable access to Kitaev quantum spin liquid candidates: a chemistry approach	Functional and Advanced Materials *3:00 - 3:50 pm* **(Room 202A)**
29	*Matthew Chambers*	Energy landscape of LixLa2/3–x/3TiO3 (LLTO) synthesis explored via structurally similar precursors	
30	*Abhijeet Dhakane*	Understanding Dynamics of Heterogeneous Ferroelectric Oxides at the Nanoscale using Graph Neural Networks on Reactive Force-Field Simulations	
31	*Qiangsheng (Johnson) Lu*	Discovery of two-Dimensional Weyl Semimetal	
32	*Anuj Bisht*	Pressure and Temperature: Tuning Knobs for a Practicing Solid-State Battery Researcher	
	3:40–3:50 pm	Break	
33	*Nolan Hayes*	A real-time evaluator to enable faster and more affordable building envelope retrofits	Building Energy and Efficiency Research *3:50 - 4:50 pm* **(Room 202B)**
34	*Zhenglai Shen*	Coupling thermal energy storage with thermally anisotropic building envelope for demand side management of HVAC loads	
35	*Jyothis Anand*	Let's use buildings to cool down our cities.	

36	*Rui Zhang*	Low-cost Natural Fibers for Vacuum Insulation Panels Core Materials	
37	*Pratishtha Shukla*	Transformer Failure Probability Modeling under Geomagnetic Disturbances	
38	*Archana Ghodeswar*	Quantifying the Economic Costs of Power Outages due to Natural Disasters: A Systematic Review	
	3:50–4:00 pm	Break	
39	*Colin Sarkis*	Magnetic Properties of disordered Co-Honeycomb materials Na_2Co_2-x$Mg_x$$TeO_6$ and Na_2Co_2-x$Zn_x$$TeO_6$	Magnetic Materials and Spintronics *4:00 - 5:00 pm* **(Room 202A)**
40	*Madalynn Marshall*	Field-Induced Partial Disorder in a Shastry-Sutherland Lattice	
41	*Raju Baral*	Magnetic pair distribution function analysis of 2D van der Waals antiferromagnetic material $MnPSe_3$	
42	*Yiqing Hao*	Field-induced magnetic disorder in the Kagome-stripe-lattice $Na_2Co_3(VO_4)_2(OH)_2$	
43	*George Yumnam*	Doping induced magnetic anisotropy in an antiferromagnetic semiconductor	
44	*Abdulgani Annaberdiyev*	The role of electron correlations in the electronic structure of putative Chern magnet $TbMn_6Sn_6$ using correlated methods	

May 19, 2023

	9:00-9:10 am	Opening talk by Si Athena Chen & Johnson Lu (ORPA research co-chair)	**(Room 202A)**
9:10–10:10 am	**Keynote Speaker 3 (Room 202A)**	**Mina Yoon, 2D Materials– opportunities and challenges**	
10:20–12:00 pm	**Third Round of Talks (Friday morning)**		
	10:10-10:20 am	Break	
No.	*Name*	*Talk Title*	*Session Title*
45	*Tomas Grejtak*	Lightweight high-temperature aluminum alloy rotors for EV Regenerative Braking	

46	*Janet Meier*	Development of a lean electrically conductive Al-Zr alloy through Sn micro-alloying	Mechanical Engineering/ Metallurgy *10:20 - 11:10 am* **(Room 202A)**
47	*Selda Nayir*	Processing Parameters Effect on Powder Bed Fusion Processed 316L	
48	*Qing-Qiang Ren*	Grain boundary chemistries of an additively manufactured Ni-based superalloy: as printed vs after hot isostatic pressing	
49	*Subhamay Pramanik*	Preorganized Ligands for Efficient Separation of Rare Earths	
50	*Stefan Schnake*	A Predictor-Corrector Strategy for Adaptivity in Dynamical Low-Rank Approximations	Computational and Statistical Methods *10:20 - 11:10 am* **(Room 202B)**
51	*Aditya Kashi*	Can a deep learning model predict the solution of a partial differential equation given the boundary values? An initial exploration	
52	*Sarah Chehade*	How many unitaries does it take to reach a good solution state?	
53	*Benjamin Russo*	System Identification and Surrogate Modeling	
54	*Elaine Wong*	A Short Software Demonstration for Symbolic Combinatorics	
	11:10-11:20 am	Break	
55	Holden Hyer	Distributed Strain Measurements in Additively Manufactured SS316 with Embedded Fiber-Optic Sensors	Nuclear Energy *11:20 - 12:00 pm* **(Room 202A)**
56	Rabab Elzohery	SCALE Non-Light-Water Reactor (Non-LWR) Fuel Cycle Demonstration for a High-Temperature Gas-Cooled Reactor	
57	Shahinul Islam	Towards an MPEX Digital Twin: Validation studies using Proto-MPEX and SOLPS-ITER	
58	Yuqiao (Joy) Fan	Helium Flow Visualization Simulation for Fusion Reactor First Wall Cooling	
59	Raymond C Borges Hink	Securing Distributed Energy Resources (DERs) through Data and Device Verification	Pattern Identification and Threat Detection *11:20 - 12:00 pm* **(Room 202B)**
60	Aaron W. Werth	Cyber-resilience of Blockchain for the Electric Grid	
61	Ashok Tiwari	Absorbed doses from accidental extravasation of radiotracers in PET imaging	

62	Ashok Tiwari	Validating Monte Carlo simulations experimentally to quantify DNA damage in breast cancer cells following exposure to 225Ac	
	12:00-01:00 pm	Lunch Break	

01:00–02:00 pm	**Keynote Speaker 4 (Room 202A)**	**Mark Lumsden, Neutron Spectroscopy – Past, Present, and Future**
2:10–2:50 pm	**Fourth Round of Talks (Friday afternoon)**	

	02:00-02:10 pm	Break	
No.	*Name*	*Talk Title*	*Session Title*
63	Matthew Loyd	Optimizing Spatial Resolution and Gamma discrimination of Neutron Anger Cameras	Neutron Detection and Instrumentation *2:10 - 2:50 pm* **(Room 202A)**
64	Austin Hoover	High-dimensional phase space measurements for halo-level hadron beam control	
65	Yadukrishnan Sasikumar	Studying the respirable airborne contamination from spent nuclear fuel fractures	
66	Breanna King Vestal	Low Temperature Liquid-Based Chlorination of Zirconium Alloys	
67	Qianli Ma	CrysFieldExplorer: a software for rapid optimization of crystal field Hamiltonian	Computational Material Science *2:10 - 3:10 pm* **(Room 202B)**
68	Arpan Biswas	A Bayesian optimized human assessed spectral recommender system for added flexibility of real-time decision making in Automated Experiments	
69	Arpan Biswas	Towards meaningful latent space learning via Variational autoencoder with physical constraints	
70	Deepak Kumar Pokkalla	Inverse design of architected materials with prescribed nonlinear responses using deep learning	
71	Bokyung Park	Synthesis of high-performance thermal insulation materials guided by multi-scale simulations	
72	Malgorzata Makos	Reaction Pathways Search Using Adaptive-Learning Global Optimization Algorithm	

3:00–5:30pm	**Poster Session** **Odd numbered posters presented from 3:00 – 4:30 p.m.* **Even numbered posters presented from 4:00 – 5:30 p.m.*

Poster Session

Room 202C & 2nd Floor Lobby

No.	*Name*	*Poster Title*	*Session Title*
73	Lynnicia Massenburg	Structure Determination of Moss Cellulose Synthase 5 (PpCesA5) Trimer	Bioscience
74	April Armes	Unraveling network connections in a 3-member microbial synthetic community	
75	Manjula Senanayake	Effects of 3-dehydroshikimate dehydratase expression levels in the organization of cellulose microfibrils in poplar mutants for efficient production of sustainable energy	
76	Kelsey Carter	Using hyperspectral imaging to predict plant resilience traits	
77	John Holmen	Performance Portability at the NCCS	Computer Science
78	Matthias Maiterth	MCHound - Telemetry Collection in Userspace	
79	Naw Safrin Sattar	Leveraging Multi-GPU Power for Large-scale Graph Analytics on Frontier	
80	Jordan Miller	Can expert-provided lexicon help classify pediatric anxiety? A random forest-based approach	Computer Science
81	Nolan English	Towards PBPK informed Generative Modeling in Drug Design	
82	Agniva Chowdhury	Faster Randomized Interior Point Methods for Tall/Wide Linear Programs	
83	Shuvodeep De	Interactive Distortion Compensation of Large-Size Component Fabricated by Wire-Arc Direct Energy Deposition	
84	Shannon Jones	Improving biogeochemical modeling of coastal regions in a land surface model by representing mangrove hydrology and ecosystem functions	Earth and Environmental Sciences

85	Md Arifuzzaman	Precision Deconstruction of Mixed Plastics by a Tailored Organocatalyst	Energy Science
86	Ozgur Alaca	A Novel Spectral Correlation Function Based Detection Method for Grid-Signal Distortions	
87	Elizabeth Piersall	Comparison of Analysis Approaches for Time Series Sensor Data	
88	Kyra Owensby	Lithium Morphology Evolution Through Crosslinked Poly(ethylene oxide) Solid Polymer Electrolyte	
89	Ivan Paradela Perez	Analysis of power and momentum transport and removal in spherical tokamaks using SOLPS-ITER	
90	Dengpan Dong	Design of Future Batteries: Insights from Molecular Simulations	
91	Su-Ann Chong	Microchannel Plates with Quad Timepix3 Readout (MCP/TPX3) Detector for High Spatial ResolutionNeutron Imaging with Time-of-Flight Capability	Neutron and Nuclear Sciences
92	Teagan Sweet	Raman Spectroscopic Investigation of Uranyl Phosphates and Arsenates	
93	Wenbo Wang	Eco-friendly and Anti-wear Ionic Liquids Additives in Marine Turbomachinery Lubricants	Material Science
94	Jenn Neu	Nanoscale Interrogation of Metallic Nuclear Materials: Atomic Force Microscopy and Magnetic Force Microscopy	
95	Lynda Amichi	Investigation of nanoparticle degradation in hydrogen fuel cell systems through automated electron microscopy	
96	Yawei Gao	Multiscale Computational Modeling for Predicting Mechanical Behavior of Binder Jet 3D-Printed Structures	
97	Eleanor Clements	Magnetothermal transport in the kagome van der Waals compound $Pd_3P_2S_8$	
98	Jopaul Mathew	Innovative family of guanidium-based aqueous complexants for technetium management	Other
99	Layla Marshall	Audio-Based Lossy Compression of Power Line Signals	

100	Darren Driscoll	From Local Chemistry to the Macrostructure: Characterization of Emerging Materials for the Separation and Extraction of Rare Earth Elements	Physic Science
101	Debmalya Ray	Understanding CO_2 Release and Regeneration Mechanism of Methyl-glyoxal-bis-imminoguanidine (MGBIG) Linkers	
4:00–4:45pm	**Closing Remarks & Awards**		

Keynote Speaker Bios and Abstracts

Advanced Electron Microscopy for Energy Storage and Conversion Materials Research

Michael J. Zachman

R&D Staff, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Bio

Michael Zachman is a Staff Scientist in the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory. He received his B.S. in Physics from Purdue University in 2012 and his Ph.D. in Applied Physics from Cornell University in 2018. Michael's research interests lie in advancing electron microscopy techniques to provide an understanding of the structure and properties of energy and quantum materials down to the atomic scale. His doctoral work concentrated on developing cryogenic focused ion beam (cryo-FIB) and scanning transmission electron microscopy (cryo-STEM) techniques to study processes at solid-liquid interfaces at high resolution with liquids and reactive materials intact. Michael's postdoctoral research focused on developing and applying four-dimensional STEM techniques to battery and two-dimensional materials to access to new aspects of their structure at nanometer and atomic scales. As a staff scientist, Michael has worked to advance hydrogen generation and conversion materials through techniques such as these in combination with automation strategies to increase the robustness and reliability of generated results.

Abstract

Development of enhanced energy storage and conversion devices is critical for accelerating our transition to a sustainable future. The performance, durability, and safety of these devices often depend highly on the nano- to atomic-scale properties of the materials and interfaces within them, making an understanding of their local properties critical for enabling progress. While a variety of characterization techniques are available that can provide a wealth of information, many lack the spatial resolution required to directly capture heterogeneities at these scales. High-resolution scanning transmission electron microscopy (STEM) and spectroscopy are therefore valuable tools for directly probing local structural and electronic properties of materials in real space. The high-energy electron beam, high-vacuum sample environment, image contrast mechanisms, and typical low fields of view (FOVs) of conventional techniques can limit the types of materials that can be characterized and the robustness of measurements performed, however. In this talk, I will describe advanced electron microscopy techniques designed to address these limitations by providing access to new materials and increasing the quantity and quality of information obtainable. First, I will show how cryogenic techniques enable the structure and chemistry of solid-liquid interfaces, such as electrode-electrolyte interfaces in Li-metal batteries, to be explored at the nanoscale with liquids and reactive materials intact. Next, I will discuss how "four-dimensional" STEM imaging techniques allow the structure of battery and fuel cell materials consisting of a range of elements to be visualized at the atomic scale in a directly interpretable manner. Finally, I will demonstrate how automation enables orders of magnitude more information to be acquired in a single experiment, allowing measurements to be performed across large FOVs, such as entire electrode cross sections, while maintaining high spatial resolution. Techniques such as these provide critical insights into the local properties of energy conversion and storage materials and devices, advancing progress toward next-generation devices important for enabling a sustainable future.

Intrinsic Complexity of Solid–Water Interfaces Deciphered by Synchrotron X-Ray Reflectivity (and Then Handed Over to a Geoscientist)

Sang Soo Lee

Geochemist, Interfacial Processes Group, Chemical Sciences and Engineering Division, Argonne National Laboratory

Bio

Sang Soo Lee is a Geochemist in the Chemical Sciences and Engineering Division at Argonne National Laboratory. He received his B.S. in the Department of Geological Sciences at Seoul National University (SNU), South Korea, in 1996, M.S. in the Department of Earth System Sciences at SNU in 1998, and Ph.D. in the Department of Earth and Environmental Sciences at University of Illinois at Chicago in 2007. His research in Argonne focuses on understanding the molecular-scale structure and energetics of solid-–water interfaces that are relevant to many natural phenomena, including heavy metal contamination and remediation, mineral and organic interactions, and chemical evolution of Earth materials via interaction with natural fluids, through the application of synchrotron-based X-ray scattering and imaging techniques. He has also been involved in various synergistic activities. He was the chair of the Chem/Bio/Environmental Panel for Advanced Photon Source in 2017–2019, associate Editors for the Journal of the Mineralogical Society of Korea and PLOS One. He was on the Council Committee for the Clay Minerals Society. He has been on the Executive Committee for the ACS-Geochemistry Division for which he currently serves as the Chair-elect.

Abstract

Charged solid–liquid interfaces are primary sites for a wide array of chemical reactions in various systems including ion adsorption/desorption in natural environments, heterogeneous catalysis, and energy storage. Probing the interfacial structure at the atomic scale can provide a direct insight into the reaction mechanisms. In this presentation, I show how ion charge and hydration influence the speciation and dynamics of metal pollutants adsorbed at mineral–water interfaces based on in-situ observations using synchrotron high-resolution X-ray reflectivity [1,2]. I also highlight how these structures can be modified with varying solution compositions that are relevant in natural environments [3]. These experimental observations are compared with computational simulations to provide a more detailed insight into molecular-scale behaviors in complex interfacial phenomena. Finally, I discuss new opportunities and challenges for studies of interfacial geochemistry using the high brilliance and coherence from the 4th generation source of synchrotron X-rays.

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2D Materials - Opportunities and Challenges

Mina Yoon

Senior R&D Staff & Group Leader, Microstructural Evolution Modeling Group, Oak Ridge National Laboratory

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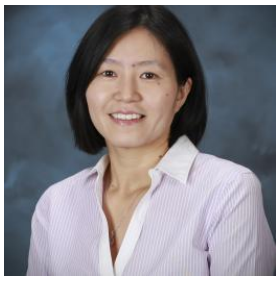
Bio



Dr. Mina Yoon is a senior R&D staff and the group leader of the Microstructural Evolution Modeling Group in the Materials Science and Technology Division (MSTD) at ORNL and is the joint Professor of the Department of Physics and Astronomy at the University of Tennessee (UTK), Knoxville. Her research focuses on the application of materials theory, advanced computational approaches, and data analysis/machine learning to understand fundamental physical phenomena and translate knowledge into the development of novel energy materials, including nanoscale materials and topological quantum materials. Prior to joining ORNL, Dr. Yoon spent three years as a Max Planck Fellow at the Fritz Haber Institute of the Max Planck Society in Germany. She is currently the secretary of the Electrical Division of the American Ceramics Society.

Abstract

The field of two-dimensional (2D) materials offers numerous opportunities, such as flexible and topological electronics that operate at room temperature and ambient conditions. Advances in theoretical, computational and experimental capabilities have enabled the manipulation of 2D materials at the atomic level, opening up a rich parameter space for novel applications. The synergy between theoretical and experimental approaches is crucial to exploit these opportunities. In this talk, I will discuss the integration of different computational approaches, enabled by the supercomputing capabilities at Oak Ridge National Laboratory, to explore the rich properties of 2D materials. We demonstrate the potential of these combined approaches using prototypical 2D quantum systems to improve theoretical predictability and guide experimental exploration of 2D materials. Significant challenges remain in accurately modeling 2D materials, particularly with first-principles approaches, including van der Waals interactions, level alignment problems, and topological inversion. By refining our theoretical and computational schemes, we aim to bridge the gap between theory and experiment, paving the way for robust quantum materials in practical applications.

Neutron Spectroscopy – Past, Present, and Future

Mark Lumsden

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Bio

Mark Lumsden received his PhD from McMaster University in Hamilton, Ontario Canada in 1999 and joined Oak Ridge National Laboratory (ORNL) as a Eugene P. Wigner Fellow. He then joined the neutron scattering group at the High Flux Isotope Reactor (HFIR) where he was an instrument scientist on the HB-3 triple-axis spectrometer and was part of a team that developed the SPICE data acquisition software. He moved from HFIR to SNS in 2011, serving as the Leader of the Time-of-Flight Spectroscopy Group until 2017. In 2017, he became the Group Leader for a larger Spectroscopy Group and in 2020, became the Spectroscopy Section Head within the Neutron Scattering Division. This section operates 10 neutron spectrometers at HFIR and SNS providing an unmatched set of capabilities to the US research community. Mark's research concentrates on using neutron scattering to study quantum materials and he is a fellow of the American Physical Society, the Neutron Scattering Society of America, and the American Association for the Advancement of Science.

Abstract

The development of nuclear reactors during the Manhattan Project enabled groundbreaking research using beams of neutrons. Ernest Wollan and Clifford Shull used the Oak Ridge Graphite Reactor to establish neutron diffraction as a technique for studying the structure of materials. Neutron spectroscopy, on the other hand, originated at the NRX reactor in Chalk River Canada. Bertram Brockhouse invented the triple-axis spectrometer and performed pioneering research studying dynamics of materials. Shull and Brockhouse won the 1994 Nobel Prize in Physics. Following his tenure in Chalk River, Brockhouse became a professor at McMaster University, my alma mater. In addition to their technical contributions, the legacy of both Brockhouse and Shull is also defined by the people they trained and attracted to the field. This legacy has influenced my career and, more broadly, neutron scattering at ORNL. While the triple-axis spectrometer remains an important tool in neutron spectroscopy today, time-of-flight spectrometers have, in recent years, transformed the technique. I will discuss the evolution of neutron spectroscopy over the last ~25 years with emphasis on the role ORNL has played in that development. Finally, I will provide a perspective on the future of inelastic neutron scattering including future sources and instruments and the expanded role computing will play in this technique.

Presentation Abstracts

Session: Materials Science in Separation and Energy Materials

Preorganized Ligands for Efficient Separation of Rare Earths

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Rare earth elements (REE) play a huge role in the US economy and national security spheres. These have wide applications in energy storage andSpacing 0 pt before/12 pt after advanced technologies. The separation of lanthanides is a massive task because of expensive methods and environmental challenges. The nation is highly depending other countries for trading in rare earths which creates a huge supply chain issue. My present work involves the design and synthesis of multidentate preorganized ligands for selective separation of lanthanides. A series of ligands on phenanthroline, bipyridine were designed and synthesized for efficient separation among adjacent lanthanides. Our main agenda is to regulate the cooperative interaction between "strong" interactions at the ligand-metal binding site; On other hand "weak" interactions in the surrounding coordination sphere. This regulation on selective separations; stimuli-responsive release of lanthanide will be triggered by these synthesized materials. Recently, we have been focusing on synthesizing a few redox-active ligands. These could lead to the development of new environmentally friendly separation strategy. This presentation will highlight our recent results in unraveling the synthesis and selective methods to separate rare earth metals.

Characterization of Complex Atomic Degrees of Freedom in Liquids and Glasses: Application to Heat Capacity

Jaeyun Moon

Materials Science and Technology Division, Oak Ridge National Laboratory

Developing microscopic understanding of the thermal properties of liquids is challenging due to their strong dynamic disorder, which prevents characterization of the atomic degrees of freedom. Following the success of normal mode analysis in solids, there have been significant research interests in the past few decades to extend the theoretical method to instantaneous structures of liquids. However, the nature of normal modes that arise from these unstable structures is still elusive. In this talk, I demonstrate novel, general frameworks to study heat capacity of liquids at the atomic scale via statistical approach to normal mode analysis. Our results show that heat capacity of liquids can be described by a combination of both solid-like and gas-like degrees of freedom, leading to a unified framework to describe heat capacity of all three phases of matter: solid, liquid, and gas. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Materials and Science and Engineering Division.

Efficient Cathode Recycling Process for Cobalt Recovery via Dual-function Green Solution

Lu Yu, Yaocai Bai, and Ilias Belharouak

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The growing usage of lithium-ion batteries in diverse fields, such as electric vehicles, grid energy storage, and electronic devices, has led to a steady accumulation of end-of-life batteries. The need for sustainable development and environmental protection has made efficient battery recycling methods imperative, aiming to reuse and maximize the recovery of valuable materials from spent batteries. Currently, considerable efforts are being made to develop and optimize lithium-ion battery recycling methods. Hydrometallurgy, a promising approach for commercial battery recycling, is known for its high leaching efficiency and adaptability to different metals. However, its extensive use of inorganic acids introduces impurities, leads to a complicated separation process, and generates hazardous waste, limiting its scalability. This study presents an updated hydrometallurgy method that is efficient, facile, and environmentally friendly. A dual-function solution consisting of green organic acid and solvent is employed for both cathode leaching and precipitation. The combination of solvents confers unique properties to the system and enables the leaching and precipitation process to occur in one-pot, without requiring a complicated separation and recovery process. This method addresses the challenges associated with conventional hydrometallurgy and holds the potential to advance battery recycling.

Thin Films of Ionic Polymers in Applied Electric Fields

Panagiotis Christakopoulos

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Ionic polymers are of great interest due to their vast amount of applications such as catalysis, gas separation and their use as polyelectrolytes in batteries and fuel cells. Recently, we have used scattering techniques such as X-ray Reflectivity (XRR) and neutron reflectometry (NR) to understand the effect of counteranion identity on the response of ionic polymers to external electric fields. The fitted reflectivity data indicated that the choice of counteranion leads to different changes in film thickness. Understanding responses of ionic polymers to annealing temperature can help us unravel the mechanisms, such as, alignment of chains and redistribution of counterions above the transition temperatures.

Single-Particle Inductively Coupled Plasma-Mass Spectrometry for Automated, Reproducible Elemental and Isotopic Analysis of Nanoparticles

Veronica Bradley

Chemical Sciences Division, Oak Ridge National Laboratory

Single particle-inductively coupled plasma-mass spectrometry (sp-ICP-MS) has recently emerged as a technique to characterize the chemical and isotopic composition of nanoparticles. Former elemental characterization with MS involved a bulk digestion, homogenizing the samples and obscuring any

compositional differences between particles. Most single-detector inductively coupled plasma-mass spectrometry (ICP-MS) instruments are too slow to measure more than one isotope for a single nanoparticle, except for time of flight (TOF) mass spectrometers. ICP-TOF-MS not only have fast acquisition times, but also measure all masses quasi-simultaneously, allowing for isotope ratio analysis of single particles. This technique can also be used to measure the capture of other elements on functionalized nanoparticles due to the capabilities of the TOF mass analyzer. A unique sample introduction system for automated analysis of nanoparticles was combined with an ICP-TOF-MS and evaluated for consistency of measurements and accuracy of size determinations and isotopic ratios. For 8-hour analysis times over the course of five days, this method demonstrated good in-run and day-to- day precision, and accurate size determinations. Finally, Fe nanoparticles coated with an enzyme that binds Pt was analyzed to determine the capability of the method to measure Pt uptake by the magnetic nanoparticles.

An Efficient Extraction of Rare Earth Elements by Using Versatile Diglycolamide-Based Ligands

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The rare earth elements (REE) have been playing crucial role in modern technologies ranging from permanent magnets, batteries, catalytic convertor to medical imaging agents. However, the separation and recovery of lanthanides into individual elements is a formidable challenge due to close resemblance in their physical and chemical properties. Moreover, the separation and purification steps produce a wide variety of waste products which requires expensive treatments and furthermore creates significant environmental challenges to improve the separation strategies. Even though there are numbers of extractants have been developed in past decade for separation of lanthanides, there is scarcity of efficiency and selectivity. Herein, we designed and synthesized a series of diglycolamides derivatives appended with variable lipophilic chains for effective Ln(III) extraction. The alkyl chain length not only improves the solubility but also influence the extraction strength and hence make them promising candidates for efficient extractions of lanthanides via liquid-liquid extraction. This presentation will highlight the role of DGAs substituted with tunable alkyl chain lengths towards efficient and effective separation of REE.

Session: Genetics and Structural Biology

Overexpression of a Member of the Cation/H+ Exchanger Gene Family CHX20 Confers Drought Tolerance in Arabidopsis thaliana and Hybrid poplar

Amith Devireddy

Biosciences Division, Oak Ridge National Laboratory

Drought is a primary limiting factor for plant growth and development impacting agricultural productivity worldwide. Water deficit conditions beyond the plant's physiological optimum can trigger significant physiological perturbations, reduce the rate of photosynthesis, and accelerate leaf senescence leading to a decrease in canopy size and yield. One way to enhance drought tolerance in plants is by delaying drought-induced leaf senescence, retaining photosynthetic activity, and maintaining leaf water potential. In this

study, genome-wide association studies (GWAS) in *Populus* identified a genetic locus that is highly associated with drought-induced leaf senescence. This genetic locus is predicted to encode a member of the putative Na^+/H^+ antiporter family CATION/H^+ EXCHANGER (CHX20). To validate the function of CHX20, we developed transgenic poplar lines with altered expression of CHX20 and tested these lines under water deficit conditions. The Populus CHX20 overexpression (OE) lines retained not only photosynthetic activity (albeit at a reduced level) but also maintained high water potential compared to wildtype (WT) or KO lines during the drought treatment without significant yield penalties. Furthermore, testing the role of CHX20 using *Arabidopsis thaliana* plants indicated that AtCHX20 transgenic overexpression (OE) plants had greater stomatal aperture size, enhanced photosynthetic activity, and higher osmolyte contents compared to WT or KO under water deficit conditions.

Visualizing Protonation States in Serine Hydroxymethyltransferase with Neutron Crystallography

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Serine hydroxymethyltransferase (SHMT) is a pyridoxal-5'-phosphate (PLP) dependent enzyme that catalyzes the tetrahydrofolate (THF)-dependent cleavage of L-Ser to form glycine and 5,10- methylene-THF, providing single carbon units to one-carbon metabolism. Human mitochondrial SHMT (hSHMT2) is overexpressed in a multitude of cancers and is acknowledged as a significant target for anti-cancer therapeutics. Here, we present two 2.3 Å joint X-ray/neutron (XN) structures of SHMT from homodimeric *Thermus thermophilus* (*Tth*SHMT), whose active site is conserved compared to that of hSHTM2, in the open conformation with PLP covalently bound to the catalytic lysine in the internal aldimine. In the second joint XN structure a pre-Michaelis complex is observed with substrate L-Ser at the entrance of the active site. We further tracked the substrate through the active site by obtaining an X-ray structure of a pseudo-Michaelis complex by soaking a *Tth*SHMT crystal with D-Ser, a non-reactive substrate enantiomer. By direct observation of the hydrogen atom positions by nuclear density maps, our study provides unique atomic-level understanding of the SHMT active site that sheds new light on the enzyme's catalytic mechanism and can be employed to advance the design of anticancer drugs targeting hSHMT2.

Plant Synthetic Biology to Enable Safe Biodesign of Novel Plant-Microbe Interactions

Yang Liu, Tomas Rush, Paul E. Abraham, and **Xiaohan Yang**

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Advancements made in plant engineering are necessary to address future challenges associated with climate change and food security. CRISPR/Css9-based genome engineering now provides novel methods for accelerating high precision engineering in non-model plants. Biocontainment of these advanced genome

engineering tools is important to mitigate risks of unwanted genome engineering. Therefore, we developed a biosensor for real-time detection of active CRISPR/Cas tools *in planta* and an anti-CRISPR (Acr) protein countermeasure to limit unwanted CRISPR/Cas9-based genome editing activity *in planta*. These advancements are important steps towards safe, high-throughput plant biodesign and genome engineering.

Targeted genome editing of plants alone may not facilitate the advancements necessary to achieve the Department of Energy's climate and economic competitiveness goals. Emerging research on plant holobiont theory and microbial invasion ecology emphasizes the importance of plant– microbe interactions. However, we currently lack the knowledge necessary to successfully introduce beneficial alterations, prevent undesired modifications, or assess the risks of proposed ecosystem engineering efforts. Therefore, we are making advancements to detect and control novel plant-microbe interactions for safe biodesign. We are currently developing plant-based biosensors to detect the establishment of fungi on poplar. Lastly, we are developing plant-delivered in situ engineering to control root-associated microbes through the delivery of small secreted proteins (SSPs). Preliminary result indicates these advancements have potential for engineering plants to detect and control associated microbes and thus facilitating new opportunities of safe ecosystem engineering.

Disordered Domain of Companion of Cellulose Synthase 1 Bundles Microtubules into Hexagonal Assemblies

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The production of cellulose for the cell walls of plants is a highly regulated process with several responses to cell stress evolved to maintain the integrity of the cell walls. The companion of cellulose synthase 1 (CC1) is upregulated during salt stress and restores plant cell growth upon addition of CC1 to CC1 knockout cells. CC1 is a transmembrane protein with a long disordered domain (CC1-NTD), a single transmembrane helix, and a periplasmic domain. This work focuses on the interaction of the CC1-NTD with microtubules, a key component of the cellulose production apparatus. CC1-NTD associates to microtubules, long hollow cylinders formed of α- and β-tubulin protein heterodimers, whereupon the microtubules form bundles. We have combined small angle scattering with hierarchical modeling and simulations to identify a structural ensemble of CC1-NTD bound to microtubules. We find the 2D packing structure of microtubules to be closest packed hexagonal with the CC1-NTD interacting at the surface of a microtubule. The CC1-NTD tends to associate in an extended conformation with specific interactions at the interface of the α- and β-tubulin. This structural study offers additional insights into the role of CC1-NTD in the response to salt stresses in plants.

Chelating Antimony(V) for Sb-119 Rargeted Auger Therapy

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Targeted Auger therapy utilizes Auger electron-emitting radioactive ions in combination with tumor-specific targeting vectors to precisely deliver cytotoxic radiation to cancer cells. Auger electrons are low-energy electrons emitted from core atomic orbitals following electron capture. Although Auger emitters have been largely overshadowed by the popularity of alpha- and beta- emitting radionuclides for targeted radiotherapy, the ultra-short penetration range and high linear energy transfer (LET) of Auger electrons offer unparalleled potential for targeting and destroying small tumor burdens such as micrometastases and single cancer cells, resulting in minimal damage to surrounding healthy tissue. Among the Auger electron-emitting radionuclides that are suitable for biomedical applications, antimony-119 (^{119}Sb, half-life = 38.2 h) has emerged as highly promising because it emits an average of 23.7 electrons with an average kinetic energy of 8.9 keV per decay, which is ideal for cellular and subcellular targeting applications, and only a single gamma photon of low energy (23.9 keV, 16%), which is highly desirable to minimize the radiation burden to patients arising from penetrating gamma rays. However, one outstanding challenge hindering the advancement of ^{119}Sb for targeted Auger therapy resides in the gap in knowledge of the coordination chemistry of this radionuclide, which is rendered complicated by its metalloid character, the existence of multiple stable oxidation states, and its tendency to form hydroxide species in aqueous solution. In this presentation, we report our efforts to develop chelators that stabilize the oxophilic Sb(V) ion and provide insight into the chemical and radiochemical challenges that arise from handling this metalloid. New methodology to assess the radiolabeling of chelators with radio-Sb(V) and the resulting stability of the complexes in human serum are also described. Finally, we share our results from in vivo studies of radio-Sb complexed by a catechol- rich chelator and our steps towards the development of a bifunctional targeted construct. Collectively, these studies aim to address the difficulties associated with Sb(V) chelation chemistry and guide the development of bifunctional chelators for ^{119}Sb in targeted radionuclide therapy.

Session: Earth and Environmental Science

Strontium Incorporation to Single Crystal Calcite Growth: In Situ Measurements Coupled with Multiscale Chemical Imaging

Si Athena Chen,[1] Juliane Weber,[1] Michael Zachman,[2] Jonathan Poplawsky,[2] Sabine Neumayer,[2] Anton Ievlev,[2] and Andrew Stack[1]

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Many environmental applications rely on accurate predictions of mineral growth rates, including CO_2 removal, contaminant sequestration, nuclear waste management, etc. Despite numerous observations that lattice strain affects reaction rates, the mechanisms remain unclear. Here we measured the kinetics of single-crystal calcite growth as a function of the Sr/Ca ratio (0-1.0) in calcite growth solution using *in-situ* flow-through atomic force microscopy (AFM). The chemical compositions of the growth hillocks were quantified by scanning transmission electron microscopy with energy-dispersive X-ray spectroscopy (STEM-EDS), AFM time-of-flight secondary ion mass spectrometry (AFM-Tof-SIMS), and atom probe tomography (APT). The strain caused by Sr incorporation was analyzed by contact resonance AFM (CR-AFM) and 4D-STEM. As observed by *in-situ* AFM, Sr inhibited the hillock growth and suppressed growth greater on the obtuse side than acute side. Using STEM-EDS, AFM-Tof-SIMS, and APT, the extent of Sr incorporation in calcite growth hillock showed a positive linear correlation. Moreover, 22% higher Sr concentration in obtuse than acute side caused ~6 GPa elastic modulus differences. Both 4D-STEM and CR-AFM analysis revealed that Sr substitution caused higher strain in the lattice compared to Sr-free calcite, which further suppressed the subsequent calcite growth by restricting the attachment of Ca.

Molecular Understanding of the Influence of Electrolyte Species on Boehmite Particle Aggregation Using Rare Event Simulations

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Nanoparticle aggregation is utilized beneficially for environmental remediation and in biomedical systems, but can be detrimental when it occurs during processing of nuclear waste slurry. The aggregation process is greatly affected by solution composition and concentration. We are motivated by a previous experimental study that shows how aggregation extent is strongly affected by different alkali cations and displays a complex concentration dependence that defies classical models at high concentrations.[1] Here, we examined the mechanisms for how sodium and potassium nitrates affect the aggregation process of boehmite nanoparticles at the molecular level. The energy landscape of aggregation was determined and showed that adsorbed electrolyte species in the interlayer facilitate aggregation by significantly reducing the magnitudes of the free energy barriers that particles experience as they aggregate. We found it likely that the addition of salts reduces the energy barriers for particle aggregation by disrupting and reconstructing the bonding network of water in the interlayer. We also found the aggregation by basal–basal surfaces is more favored than that by edge–edge. These results improve our understanding for why salt can drive aggregation of particles: by collapsing barriers through disrupting water structure and reducing barriers on multiple crystal faces.

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Evolving Phosphorus Biogeochemistry in an Emerging Coastal Delta

Matthew Behrens

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River management and flood control strategies are rapidly reshaping biogeochemical processes in coastal wetlands by altering freshwater and sediment inputs. These factors influence the formation or degradation of coastal deltas, potentially impacting the storage and processing of nutrients. The objective of this research is to evaluate how hydrologic gradients influence phosphorus dynamics in an emerging coastal delta. We established two contrasting study transects that are characterized by either old, organic- rich soils or recently deposited mineral soils, and each span a gradient of surface elevation and tidal influence. Porewater samples were collected from 0 to 50 cm below the soil surface and analyzed for geochemical parameters including dissolved and colloidal-phase nutrients, metals, and carbon. Environmental sensors were deployed to monitor concomitant variation in salinity, pH, and redox conditions at a high temporal resolution. Preliminary results show that porewater geochemistry varies with ground elevation relative to sea level and exhibits vertical gradients in the subsurface that are more pronounced in recently deposited (mineral-rich) soils than well-established (organic-rich) soils. We observed increased phosphate solubility in deeper porewater samples which indicates the potential release of phosphate from soil. Ongoing monitoring will improve mechanistic understanding nutrient dynamics in coastal wetlands subject to human intervention.

Water, Thermal, and Land Cover Factors Led to Contrasting Urban and Rural Vegetation Resilience to Heat Waves

Yaoping Wang

Environmental Sciences Division, Oak Ridge National Laboratory

With continuing global warming and urbanization, a better understanding of the resilience of urban vegetation to heat waves is valuable for urban ecosystem management and human well-being. We quantified and compared the urban and rural vegetation resilience to heat waves during 2001–2019 for 85 major cities across the contiguous U.S. In winter, the urban areas had more positive resilience than in rural areas. In the other seasons, the urban areas had more positive resilience than the rural areas in the western U.S., but less positive in the eastern U.S. The east-west pattern was because urban vegetation had considerably higher optimal growth temperatures and lower water stress than rural vegetation in the western U.S. The urban areas generally had smaller magnitudes of resilience metrics than rural areas, with the greatest difference compared to rural deciduous forests, and the least difference to rural evergreen forests. Further analysis at 1km pixel level showed that impervious fraction, fraction of the rural vegetation cover, local urban heat island intensity, and water stress were the key factors giving rise to the city-scale urban-rural differences. These findings advance the understanding of the effects of urbanization on vegetation growth and provide valuable insights for urban planners.

Wildfire Fuels Mitigation Biomass Estimates

Ryan Jacobson

Environmental Sciences Division, Oak Ridge National Laboratory

The Billion-ton Report 2023 has expanded its analysis to include materials removed from forests to reduce the risk and severity of wildfires. This new analysis was conducted using the BIOSUM model, developed at the Pacific Northwest Research Station of the United States Forest Service. The BIOSUM model estimates the costs and volumes of residues generated from forest management activities in the Four Forests Restoration Initiative (4FRI), a collaborative effort between federal and state agencies, local communities, and stakeholders to restore forest health and reduce the risk of catastrophic wildfires in Central and Northern Arizona.

Including materials removed from forests for wildfire risk reduction in the Billion-Ton Report 2023 is significant. It provides a more comprehensive analysis of forest biomass availability for bioenergy production and can identify synergistic pathways to more efficient usage of forest biomass. Using the BIOSUM model to estimate the potential volumes and costs of forest residues generated from this initiative will help inform decision-making and planning for sustainable forest management and bioenergy production. The study identifies the potential for significant amounts of biomass to be generated from removing forest residues, which can be used for energy generation and other applications.

Performance of Hemp Insulation as a Low Embodied Carbon Substitute for Fiber Glass in Building Envelope Systems

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In line with the Paris Agreement and to reach net zero by 2050, carbon dioxide emissions need to be reduced to combat climate change. Approximately 27% and 9% of global carbon dioxide emissions are attributed to building operations and materials, respectively. A promising solution to building decarbonization is to replace traditional building materials with energy efficient and low embodied carbon materials. Bio-based materials that have low embodied carbon such as hemp batt insulation have been developed for building envelope systems. It is essential to know the hygrothermal properties of hemp batt insulation and its energy and moisture performance in wall constructions before its wide application. We compared the performance of hemp batt insulation to its competitive traditional product – fiber glass batt insulation by performing large- scale laboratory tests in the Heat, Air, and Moisture (HAM) chamber at Oak Ridge National Laboratory's Building Technology Research and Integration Center (BTRIC). The thermal performance of two insulation materials was similar while hemp batt insulation led to a lower relative humidity at the sheathing panel surfaces. Hygrothermal simulations were conducted in WUFI® Pro to investigate the impact of different climate zones and wall constructions on the moisture durability of the hemp batt insulation.

Session: Computational Biology

Few-Shot Learning Enables Population-Scale Analysis of Leaf Traits in *Populus trichocarpa*

John Lagergren

Biosciences Division, Oak Ridge National Laboratory

In this work, we develop and apply few-shot learning methods to segment the body and vein architecture of *P. trichocarpa* leaves from high-resolution scans obtained in the UC Davis common garden. Leaf and vein segmentation are formulated as separate tasks, in which convolutional neural networks (CNNs) are used to iteratively expand partial segmentations until reaching stopping criteria. Our leaf and vein segmentation approaches use just 50 and 8 manually traced images for training, respectively, and are applied to more than 2,500 top and bottom leaf scans. We show that both methods achieve high segmentation accuracy, in some cases exceeding even human-level segmentation. The leaf and vein segmentations are subsequently used to extract more than 50 morphological and topological plant traits using traditional open-source image processing tools, which are validated using real-world physical measurements. For a biological perspective, we perform a genome-wide association study using the "vein density" trait to discover novel genetic architectures associated with multiple physiological processes relating to leaf development and function. The methods discussed here generalize to multiple image modalities with applications across scientific domains.

The Ecological Effects of Sub-Daily Flow Variability on Riverine Fishes: A Systematic Review

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The contribution of renewable energy to the global energy portfolio is increasing. Hydropower is a flexible form of renewable energy production capable of responding to grid demands for electricity on short timescales. Operating hydropower dams to respond to real-time energy market conditions can result in rapid and abnormal fluctuations in downstream flow, called hydropeaking. Hydropeaking alters the timing, magnitude, and rate of change of natural flow regimes by decoupling seasonal climate and flow patterns and rapidly changing river discharge via pulses of water from upstream reservoirs. Consequently, hydropeaking can affect wetted width, temperature, habitat quality and availability, and other biotic and abiotic river characteristics downstream of hydropower facilities. In this systematic review, we summarize and synthesize the growing body of literature on the ecological effects of sub-daily flow variability on riverine fishes associated with hydroelectric power production. Specifically, we characterize the magnitude and direction of reported impacts of hydropeaking on fish, the techniques and metrics used to assess these impacts, and identify research opportunities to address knowledge gaps and explore emergent dynamics. Findings from this review will help illuminate the generality of hydropeaking impacts on fish and inform hydropower operation strategies that balance flexible hydropower production with downstream ecosystem integrity.

A Computational Multiscale Framework for Simulated Radiotherapy of Multicellular Tumor Models

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The purpose of this study is to develop a multiscale dosimetric framework that models tumor growth and radiotherapy in digital twins from the cellular to whole body scales. In this pipeline body geometry, body composition, tumor growth parameters, radiation source, and tumor radiation response can be tailored to an individual patient.

In each *in silico* experiment, a multicellular tumor model developed in CompuCell3D is embedded in a 4D extended cardiac-torso (XCAT) human body phantom, and the models are collectively imported into Geant4 to simulate 50MeV proton beam single dose and multidose radiation protocols. In addition to tracking individual cell doses, the multicellular tumor is updated to reflect post-irradiation cell death.

CC3D, XCAT, and Geant4 were successfully interconnected to create a new framework for tumor growth and radiotherapy assessment. Simulations recorded cancer cell reduction post- irradiation: 4-Gy treatment caused reduction of 42.1±9.5%; 20-Gy treatment caused mean reduction of 97.5±1.5%; fractionated treatment caused mean reduction of 80.1±14.9%.

This framework provides a new tool for evaluating the effects of radiation on tumor models in silico. The modular nature of the platform allows the inclusion of additional clinically relevant models into the pipeline.

This work was supported by the Office of Biological and Environmental Research (BER), Biological Systems Science Division (BSSD) and Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy. This research used resources of the Compute and Data Environment for Science (CADES) at the Oak Ridge National Laboratory. This manuscript has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

Evaluating the Incentive for Soil Organic Carbon Sequestration from Carinata Production in the Southeast United States

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This study evaluated the incentives for farmers due to sequestrating SOC by adopting the bioenergy crop, carinata. Two agricultural management scenarios – business as usual (BaU) and a climate-smart (No-Till) practice – were applied under an agent-based modeling approach to account for farmers' carinata adoption rates within their context of traditional crop rotations, the associated profitability, influences of neighboring farmers, as well as their individual attitudes. The results show that, in a free market, farmers of Georgia in

the Southeast United States allocated 1443.4×103 acres (32.5%) of farmlands by 2050 at a contract price of $6bu-1 of carinata seeds under the BaU scenario. In contrast, with an incentive of $100 Mg-1 CO2e SOC sequestration, farmers allocated 1514.86×103 acres (34.1%) of land in the same year under the No-Till farming practices, keeping the contract price as low as $5.5 bu-1; while the SOC sequestration was 636.24×103 Mg CO2e, which is 5 and 3.7 times greater than the two BaU scenarios - with similar price and incentives and with higher price ($6) without incentive or in a free market. Thus, this study evaluated the optimal price and incentives that can encourage farmers for adopting carinata with climate-smart practices and attain higher SOC sequestration.

Session: Grids and Machines

Infomorphism: An Urban Planning Framework for Local Renewable Energy Integration

Fengqi Li

Biosciences Division, Oak Ridge National Laboratory

Infomorphism is a new hybrid urban planning framework that aims to prioritize the utilization of local renewable energy in cities. The framework is based on the harvest-store-exchange principles of Zero Energy Buildings (ZEBs), and it collectively optimizes urban form and local energy exchange networks. Infomorphism has three synergistic computational models: a parametric optimization model that maximizes renewable energy absorption based on the shape and orientation of urban planning envelopes; an energy quantification model that includes a simulation model of renewable energy supply, as well as an energy demand forecasting model; and an optimization model to maximize the renewable energy exchange efficiency and evaluate the energy performance of local energy networks. The framework also ensures equitable access to renewables across cities by complementing existing planning processes.

The efficacy of the framework has been evaluated using selected urban neighborhoods of Manhattan, New York, as a case study. The results show that Infomorphism can effectively derive energy-based zoning policies for cities that prioritize local renewable energy utilization. The framework can help cities absorb, store, and locally share produced renewable energy as well as reduce levelized renewable energy costs in the local energy exchange networks. The framework's capabilities and limitations have been discussed, and the results suggest that Infomorphism can provide policy-orientated approaches for decision-makers to address the challenge of renewable energy integration in cities.

Enhancing Efficiency and Stability in Multi-Port Autonomous Reconfigurable Solar Power Plants (MARS) through Advanced Control Methods

Qianxue Xia

Electrification and Energy Infrastructures Division, Oak Ridge National Laboratory

Today’s electric power systems are transitioning towards low-carbon grids with an increased penetration level of renewable energy resources. The multi-port autonomous reconfigurable solar power plant (MARS), which is an integration of photovoltaic and energy storage system to the transmission ac grid and

a high-voltage direct current (HVdc) link, is designed to provide frequency response and reject disturbances in the grid with continued operation and reduced transient instability. The inherent complexity of MARS and the intermittent nature of photovoltaic necessitate the development of simple, efficient, and generalizable control methods for MARS and similar systems integrating multiple power sources into submodules in each arm. An energy balancing control (EBC) method is introduced to balance the capacitor voltages of different types of SMs. Moreover, the system operation region is explored through data-driven method and a machine learning-based EBC criteria are proposed to improve the system efficiency and reduce the switching frequency. The proposed EBC criteria can disable/enable the EBC depending on the MARS input power dispatch commands with high accuracy according to the operation region. The advanced controls enable precise and efficient energy management for hybrid power generation within MARS, fully leveraging their potential while maintaining high efficiency over an extended operating region.

Voltage Source Inverter (VSI) with Enhanced Short-Circuit Fault Current Contribution to Enable Legacy Overcurrent Protection in Islanded Microgrids

Maximiliano Ferrari

Electrification and Energy Infrastructures Division, Oak Ridge National Laboratory

In microgrids, inverter-based resources (IBRs) control their short-circuit contribution close to their rated current, which is insufficient to reliably protect microgrids using legacy distribution overcurrent protection. Although numerous approaches for microgrid protection have been suggested, to date an economically, commercially available relay that effectively addresses the challenges of microgrid protection has not been developed. As a practical solution, this work addresses the root problem by increasing the short-circuit contribution of the inverter to leverage existing legacy protective devices for microgrid protection. Using experimental results and electrothermal simulations, this research contributes to the state of the art by demonstrating that only a few inverter components must be overrated to significantly increase the short-circuit current contribution during faults. The proposed and tested design provides sustained short-circuit current to achieve fuse-relay and relay-to-relay coordination. Additional contributions of this paper include the development of a novel inverter control that addresses challenges posed by saturable inductors during high-current operation. This paper demonstrates the feasibility of increasing the short-current from inverters, enabling the utilization of legacy overcurrent protective devices for inverter-based microgrids in islanded mode.

Identifying Travel Patterns of Low-Income Populations in New York State

Melrose Pan and Majbah Uddin

Buildings and Transportation Science Division, Oak Ridge National Laboratory

Low-income populations encounter barriers to mobility due to inadequate transportation options, limiting their ability to access employment, education, healthcare, and other essential services. Consequently, a comprehensive understanding of low-income travel behavior is necessary to inform transportation policy-making. This study utilized descriptive statistics to investigate the differences in mobility patterns and transportation service accessibility between low-income and non-low-income populations. By examining these disparities, this research aims to provide insight into the challenges faced by low-income populations in accessing transportation services. In particular, the study conducted a cross-referenced analysis of income status and individual travel and vehicle usage patterns, comparing trip purposes, modes of transportation

used, and travel time between low-income and non-low-income individuals. Based on the data from the 2017 National Household Travel Survey and a case study conducted in New York State, low-income residents traveled only one-third of the distance per trip as their non-low-income counterparts. Additionally, low-income households reported 20% fewer social or recreational trips compared to non-low-income households. These findings have significant implications for the development of transportation policies and emerging technologies, such as autonomous and electric vehicles, and policymakers should prioritize reducing these mobility gaps.

Implementing Low Global Warming Potential Refrigerants in the Next Generation of Condensers

Saad Ayub Jajja

Building and Transportation Science Division, Oak Ridge National Laboratory

The HVAC & R industry in the United States will transition to refrigerants with global warming potential (GWP) of less than one hundred and fifty. This is to satisfy the long term objectives of the Kigali amendment of the Montreal protocol. Accurate prediction of the thermal-hydraulic performance of these refrigerants in evaporators and condensers is critical for optimizing vapor compression systems for both efficiency and capacity. This work describes the experimental techniques developed to measure the condensation heat transfer and pressure drop for GWP < 150 refrigerants. Using these techniques, the thermal-hydraulic performance of these refrigerants was measured in a range of tube geometries. These include smooth, un-expanded enhanced, and expanded enhanced aluminum tubes. The experimentally determined heat transfer coefficients and frictional pressure drop values will compared against the existing correlations. If needed, the development of new correlations will be outlined.

Mechanical Stress, Vibration, and Rotodynamic Analysis of High-Speed Electric Motors

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High-speed electric motors are widely used because of their high power density. Outer rotor motors are axially shorter than inner rotor motors and can provide higher torque. For a given power, increasing the motor speed can reduce the volume and weight and increase the power density, but the rotating components encounter significant mechanical stress at high speeds. In this project, we designed a rotor structure and analyzed mechanical stress, modal vibrations, and response under external perturbations for the entire motor structure, including a rotating part (the rotor) and a stationary part (the stator). Testing was performed at an operating speed of 20,000 rpm. Two rotor configurations were proposed: a cantilever design in which the rotor was suspended at one end, supported by four bearings; and a simple design in which the rotor was supported by two bearings at each end. Static structural, modal, forced response, and rotodynamic analysis were performed via the finite element method to study the feasibility of both configurations. To prevent the magnets from scattering or failing at high speeds, we proposed a carbon fiber–based retaining sleeve design and interference fit between the magnet and laminates, which creates a compressive load to balance the centrifugal force.

Session: Functional and Advanced Materials

Metastable Access to Kitaev Quantum Spin Liquid Candidates: A Chemistry Approach

Lucas Pressley

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Since Alexei Kitaev proposed an exactly solvable model for spin ½ systems, there has been an influx of predicted and synthesized materials that would meet such requirements. These Kitaev quantum spin liquid (QSL) candidates are of particular interest for the realization of topological quantum computing due to their ability to host Majorana fermions in their QSL ground state. While many candidates have been investigated, no material has arrived as a clear winner for possessing a quantum spin liquid ground state. Here we will show through the chimie doucie approach the design of new metastable honeycomb compounds. We will show a mica-like cobaltate that undergoes irreversible structural phase transition at high temperatures, as well as stabilizing high valent Pt through means of oxidative deintercalation. The physical properties of the material are characterized showing metamagnetic behavior for the former, with no sign of magnetic ordering seen in the latter down to T=2 K. Future directions will be discussed in utilizing these chemical techniques for the design of Kitaev QSL candidates.

Energy landscape of $Li_xLa_{2/3-x/3}TiO_3$ (LLTO) synthesis explored *via* various precursors

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All-solid-state batteries (ASSBs) will play a crucial role in dealing with the energy crisis and removing dependence on fossil fuels. Solid-state electrolytes are a key component of ASSBs. Energy-efficient and convenient synthesis of solid-state electrolytes will be vital in the creation of ASSBs, yet different solid-state synthesis routes are rarely explored. We have probed various reaction pathways for Li-ion conductor $Li_xLa_{2/3-x}TiO_3$ (LLTO), which has a bulk ionic conductivity at 10^{-3} S cm^{-1} at room temperature, which has multiple polymorphs. To explore the energy landscape, we used two-step syntheses to investigate the effect of using different precursors in order to determine if we can find lower synthesis temperatures than the single-step route using Li_2CO_3, La_2O_3 and TiO_3. All of the syntheses at $T < 1300$ °C failed, but at $T = 1300$°C they all succeeded. This indicates that there is an energy barrier that needs to be overcome in order to form the perovskite structure. Furthermore, we have performed DFT calculations which elucidate the barriers that need to be overcome to form the target material. These results not only provide insight into the synthesis of LLTO, but into the solid-state synthesis technique as a whole.

Understanding Dynamics of Heterogeneous Ferroelectric Oxides at the Nanoscale Using Graph Neural Networks on Reactive Force-Field Simulations

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Ferroelectrics are a technologically important class of materials for next generation microelectronics platforms, such as ferroelectric memristors, which show spontaneous long-range ordering of electric polarization. Recent advances have even shown formation of novel nanoscale chiral polar structures, such as polar skyrmions in heterogeneous oxides, that open new possibilities for storing and manipulating information at the nanoscale. While formation of long-range polar order as well as polar skyrmions is understood to be a delicate balance between coupling between microscopic degrees of freedom, there is a critical need to understand dynamics of polarization switching in such heterogeneous materials under high fields. In this talk, we will present insights into the dynamics of polarization switching in defective $BaTiO_3$, obtained from combining large-scale atomistic reactive simulations with dynamical graph neural network approaches. Specifically, we will focus on how polar- structure and dynamics changes around point-defects, and how this interaction influences domain-wall dynamics.

Discovery of Two-Dimensional Weyl Semimetal

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A two-dimensional (2D) Weyl semimetal featuring a spin-polarized linear band dispersion and a nodal Fermi surface is a new topological phase of matter. It is a solid-state realization of Weyl fermions in an intrinsic 2D system. The nontrivial topology of 2D Weyl cones guarantees the existence of a new form of topologically protected boundary states, Fermi string edge states. In this work, we report the realization of a 2D Weyl semimetal in monolayer-thick epitaxial bismuthene grown on SnS(Se) substrate. The intrinsic band gap of bismuthene is eliminated by the space-inversion-symmetry-breaking substrate perturbations, resulting in a gapless spin-polarized Weyl band dispersion. The linear dispersion and spin polarization of the Weyl fermion states are observed in our spin and angle-resolved photoemission measurements. In addition, the scanning tunneling microscopy/spectroscopy reveals a pronounced local density of states at the edge, suggesting the existence of Fermi string edge states. These results open the door for the experimental exploration of the exotic properties of Weyl fermion states in reduced dimensions.

Pressure and Temperature: Tuning Knobs for a Practicing Solid-State Battery Researcher

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Development of thin, dense, defect-free solid electrolyte films is key for achieving practical and commercially viable solid-state batteries. In this work, we will showcase a facile processing pathway with pressure-temperature coupling for anti-perovskite (Li_2OHCl) solid electrolyte materials that can yield films/pellets with very high densities (~100%) and higher conductivities compared to conventional uniaxially pressed pellets. We identify the improvement mechanism by employing *in situ* neutron diffraction studies at VULCAN beamline. We have achieved close to 50% improvement in the critical current density of the material and an improved lithiophilicity due to the surface nitrogen enrichment of the processed pellets. Distribution of relaxation time analysis supports the contributions from "faster" transport mechanisms for the antiperovskite films/pellets developed using the new protocol. Overall, the results highlight the feasibility of our new processing pathway for engineering anti-perovskite solid electrolytes at the grain scale as a highly desirable approach for practical all-solid-state batteries.

References:

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Session: Building Energy and Efficiency Research

A Real-Time Evaluator to Enable Faster and More Affordable Building Envelope Retrofits

Nolan Hayes

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Abstract: More than 50% of US existing buildings were built before 1980 and lack modern technologies which enable high energy efficiency; however, less than 2% of buildings are retrofitted each year. The opaque building envelope affects 25% of building energy use, equal to 10% of total US primary energy use. Older buildings require retrofits to reduce energy use; however, technologies and construction practices have experienced little innovation in the past decade. At the current rate of retrofits, the US cannot meet decarbonization goals by 2035. Improvements to the construction processes must be made to increase the speed and accessibility of retrofits. A real-time evaluator is being developed to optimize and accelerate the installation of prefabricated overclad panel envelope retrofits while maintaining high installation quality and energy performance. The real-time evaluator uses advanced construction technologies and novel algorithms 1) to generate digital twins with minimal human input, 2) to track the position of prefabricated panels robotically and autonomously, and 3) to assist personnel in quickly and accurately installing prefabricated panels. The real-time evaluator aims to reduce installation time and cost of envelope retrofits

by at least 25%. A proof of concept was developed to demonstrate and evaluate the autonomous tracking of mock-up panel.

Coupling Thermal Energy Storage with Thermally Anisotropic Building Envelope for Demand Side Management of HVAC Loads

Zhenglai Shen

Buildings and Transportation Sciences Division, Oak Ridge National Laboratory

Buildings consume around 40% of U.S. primary energy and release a significant amount of greenhouse gas. Moreover, the unmatching between the electricity generation and demand sides during on-peak hours creates transmission constraints and congestion and raises the cost of electricity for end-users. To reduce building energy consumption and enable flexible demand side management (DSM), we study the coupling effects of thermal energy storage (TES) with thermally anisotropic building envelope (TABE) on peak load saving and utility cost reduction considering electricity tariff structures (time-of-use rates, or TOU rates). The coupling involves the co- simulation of TABE and TES systems with the whole building energy analysis and TES charging and discharging strategies. Case studies were conducted for a residential building under the climate conditions of Charleston, Los Angeles, and Denver. The results demonstrate the superior performance of coupling TES with TABE in DSM and AC load reduction. It reduces peak load by 26.1%, 73%, and 61.6% for Charleston, Los Angeles, and Denver respectively. Additionally, cooling energy costs in Los Angeles were reduced by 52.6%, 57.2%, and 61.4% for Low-TOU, Median-TOU, and High-TOU rates respectively.

Let's Use Buildings to Cool Down Our Cities

Jyothis Anand

Buildings and Transportation Science Division, Oak Ridge National Laboratory

Heat is added to the surroundings as a result of replacing natural landscapes with buildings. This includes waste heat from air conditioning systems and heat transferred into the environment from exterior surfaces. While numerous existing studies have focused on increasing building energy efficiency, they fail to recognize that building surfaces can heat the surrounding air significantly. Rather, most researchers consider heat rejected from the air conditioning system as the total anthropogenic heat released from the building. Therefore, they assume a reduction in energy consumption will have a proportional reduction in the urban warming effect. This is not correct in most cases. This presentation talks about the role of building energy efficiency measures in the urban heat island effect. The presentation further explores the potential for negative heat-releasing buildings through simulation studies in hot arid and humid cities—Phoenix, and Houston. Results show that it is possible to achieve net negative anthropogenic heat release from low-rise office buildings by certain existing technologies which are readily available to implement. This points to a compelling mechanism whereby buildings can be designed or retrofitted to have a beneficial impact on the local thermal environment.

Low-Cost Natural Fibers for Vacuum Insulation Panels Core Materials

Rui Zhang

Building Envelope Materials Research Division, Oak Ridge National Laboratory

Vacuum insulation panels (VIP) have a large potential to reduce energy consumption in buildings, but their high cost prevents their widespread use. This purpose of this study was to identify potential low-cost natural fibers as VIP core materials and lower core cost by 50 to 80%. It used a heat flow meter to assess the thermal performance of 13 natural fiber materials over a broad pressure range, from 6.33e-5 mbar (in a vacuum) to 1.3e3 mbar (at ambient). The micromorphology of each fiber was investigated by scanning electron microscopy (SEM). Thermal conductivity ranged from 2.16 mW/mK to 47.9 mW/mK, which improved R-value/in by 64.87 $h \cdot ft^2 \cdot °F/(Btu \cdot in)$. The average diameter range for these fibers was from 11.61 μm to 182.92 μm. The density ranged from 0.47 lb/ft^3 to 11.86 lb/ft^3. Recycled cotton, kapok, and bamboo fiber could be excellent options for VIPs core materials when taking thermal characteristics and cost into consideration.

Transformer Failure Probability Modeling under Geomagnetic Disturbances

Pratishtha Shukla and Jim Nutaro

Computational Sciences and Engineering Division, Oak Ridge National Laboratory

Severe disturbances of electrical power systems can be caused when an electrically charged mass is ejected from the Sun's corona in the direction of Earth. These coronal mass ejections (CMEs), also known as solar storms, can induce strong currents to flow through electrical transformers and transmission lines. These currents can damage or destroy electrical equipment. Of particular concern is damage to the very large transformers that connect generators and loads to the high-voltage transmission system. Damage to these transformers could produce long-lasting blackouts when spares are not readily available. This paper develops a probabilistic model to assess the cascading failure of transformers of an electric power grid under these high-impact geomagnetic disturbances caused by solar storms. We propose the probability of failure to be a function of the intensity of the solar storm, the physical properties of the transformer, the geographical location of the transformer, and the electrical power flow model. We perform a simulation case study on the IEEE prototype data set of the 14-bus system to observe the effect of a solar storm on the failure of the transformers which are the most vulnerable components of the grid to geomagnetically induced currents. This model easily computes the initial and cascading failure probabilities of the transformers in the system as a first step to risk projections and risk quantification for future imminent solar storms.

Quantifying the Economic Costs of Power Outages due to Natural Disasters: A Systematic Review

Archana Ghodeswar*, Mahabir Bhandari**, Bruce Hedman***

The economic cost of long-duration power outages is crucial to justify investments in resiliency and reliability improvement. However, these costs are imprecise, and it is confounding to identify the best approach to quantify these costs for an individual manufacturing facility.

Through a systematic review, our study aims to answer the economic costs of power outages due to natural disasters estimated by the current literature. We analyze 1) the best approaches for finding the cost of power outages at the individual industrial facility-level and economy-wide levels. 2) various empirical methods and data used to quantify the costs of power outages, and 3) the economic costs of power outages at the industrial, utility, and macroeconomic levels.

We reviewed 363 studies comparing the costs of power outages in natural disasters. Our systematic analysis offers recommendations for specific strategies for the macro and micro levels for future outage cost assessments. We conclude that using NREL's Customer Function Damage Calculator is the best option for individual-level assessments. However, for macroeconomic outcomes, the ICE calculator can estimate outage costs across industrial, commercial, and residential sectors. Finally, we discuss the relative strengths and potential future research directions.

Session: Magnetic Materials and Spintronics

Magnetism in a Disordered Co-Honeycomb

Colin Sarkis, Lucas Pressley, Alexander Kolesnikov, Matt Stone, Haidong Zhou, Craig Bridges, Alan Tennant, and Steve Nagler

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The search for magnetic materials displaying physics associated with Kitaev's exactly solvable S=1/2 honeycomb lattice model is a focal point of contemporary research due to the model's unique quantum spin liquid ground state and application towards fault tolerant quantum computing. Initial candidate materials focused on 4*d*/5*d* Mott insulators, but a more recent extension to 3*d* materials has led to a large body of work focused mostly on high-spin Co^{2+} systems realizing a Kramer's doublet jeff= 1/2 ground state. One promising candidate material is $Na_2Co_2TeO_6$. While the nature of the magnetism in $Na_2Co_2TeO_6$ remains an open topic, the onset of magnetic order below T_N = 27 K clearly indicates non- Kitaev terms present in the low-energy Hamiltonian. In the Kitaev candidate material α-$RuCl_3$, substituting nonmagnetic Ir^{3+} for Ru^{3+} suppressed conventional long-range magnetic order while keeping the signatures of fractionalized excitations, suggesting magnetic dilution as a promising route. Here we explore substitution of nonmagnetic ions for Co^{2+}. We present magnetometry and specific heat measurements on synthesized powders of disordered $Na_2Co_{2-x}R_xTeO_6$ (R = Mg, Zn) and discuss the effect of magnetic dilution on the complex magnetism found in the parent compound.

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Field-Induced Partial Disorder in a Shastry-Sutherland Lattice

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Geometrical frustration in magnetic systems can drive the stabilization of exotic phases such as spin-liquids. The Shastry-Sutherland lattice is one such geometrically frustrated lattice that consists of a two-dimensional orthogonal arrangement of spin dimers and results in rich phase diagrams. In this talk I will present the findings of the possible field-induced spin liquid state of S=1 spin dimers in the Shastry-Sutherland lattice material $BaNd_2ZnS_5$. A metamagnetic transition in the bulk magnetization measurement was observed under field along the *ab* plane below T_N =2.9K. We established the Ising behavior in the Nd spins by the local magnetic susceptibility method with polarized neutrons at the paramagnetic state. The zero-field 2-**Q** antiferromagnetic order of ferromagnetic dimers was determined by neutrons at 1.4 K. The constituting propagation vectors $\mathbf{q_1}$ = (½ ½ 0) and $\mathbf{q_2}$ = (-½ ½ 0) each exhibit a "stripe" order when viewing multiple layers and a Néel-type arrangement in a single layer. By applying field along [1 -1 0] the two sublattices respond differently. The $\mathbf{q_1}$ magnetic sublattice remains relatively intact up to 6 T while the stripe phase of the $\mathbf{q_2}$ magnetic sublattice order is suppressed at the critical field H_c = 1.7 T, indicating an emerging partial disorder, liquid state of ferromagnetic dimers, corresponding to the metamagnetic transition in the bulk measurement. With this information we constructed an *H-T* phase diagram from the bulk magnetization measurements that clearly defines the "stripe" state at lower field and a field polarized state at upper fields with a critical region emerging in between represented as a spin dimer liquid phase.

The research was supported by the U.S. Department of Energy (DOE), Early Career Research Program Award KC0402020 and used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by ORNL.

Magnetic Pair Distribution Function Analysis of 2D van der Waals Antiferromagnetic Material MnPSe3

Raju Baral

Neutron Scatttering Division, Oak Ridge National Laboratory

$MnPSe_3$ is a 2D layered antiferromagnetic material with Neel temperature of 74 K. The magnetic interaction within the ab-plane is much stronger than out of the plane. In our study we investigated the $MnPSe_3$, and its S-doped compositions to gain insight into the local magnetic structure and spin correlations in paramagnetic region as well as below the ordered temperature. The magnetic pair distribution function technique was adopted to analyze local spin correlations and how these local correlations change as we introduce the Sulphur disorder in the material.

Field-Induced Magnetic Disorder in the Kagome-Stripe-Lattice $Na_2Co_3(VO4)_2(OH)_2$

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Geometric frustration and quantum fluctuations are key ingredients to new types of complex quantum magnetic ground states. Here, we report the field-induced magnetic disorders in the newly synthesized kagome-strip-lattice (KSL) material, $Na_2Co_3(VO_4)_2(OH)_2$. KSL is a one-dimensional variety of kagome lattices consisting of alternating hexagonal and triangular motifs along one direction, the stripe direction. At zero field, the magnetic ground state is a non-collinear antiferromagnetic order with reduced ordered-magnetic moments on all Co sites. By increasing the magnetic field along the stripe direction, only 1/3 of the Co sites are flipped to the field direction, while 2/3 of the Co sites show suppressed ordered-magnetic moments despite the strong magnetic field. The field-induced magnetic disorders show intense magnetic frustration and strong quantum fluctuations in this KSL material. Furthermore, assisted with the local magnetic susceptibility method with polarized neutrons, I will discuss the mechanism of the field-induced magnetic disorder.

The research was supported by the U.S. Department of Energy (DOE), Early Career Research Program Award KC0402020 and used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by ORNL.

Doping Induced Magnetic Anisotropy in an Antiferromagnetic Semiconductor

George Yumnam

Material Science and Technology Division, Oak Ridge National Laboratory

The emergence of altermagnetism in MnTe has sparked recent interest in magnetism research due to its unconventional magnetic behavior. We report a recently discovered large spin- reorientation transition in MnTe via neutron scattering techniques. We studied MnTe doped with various concentrations of Li and probed the magnetic excitations and anisotropy. We demonstrate that Li doping induces a strong magnetic anisotropy and reorients the easy axis in MnTe. The magnetic excitation spectrum also exhibits a magnon gap opening at 5% Li-doping, which is attributed to the induced off-plane magnetic anisotropy that emerges due to doping. These findings highlight the potential of Li-doped MnTe in spintronic applications, including *thermo*-spintronics and magnon-based devices. Our results pave the path for developing functional devices that requires an easily controllable switching of magnetic states.

The Role of Electron Correlations in the Electronic Structure of Putative Chern Magnet TbMn6Sn6 Using Correlated Methods

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A member of the RMn_6Sn_6 rare-earth family materials, $TbMn_6Sn_6$, recently showed experimental signatures of the realization of a quantum-limit Chern magnet. Despite the promising experimental results, theoretical studies with accurate electron correlations which probe these observations have been lacking. In this work, we use quantum Monte Carlo (QMC) and density functional theory with Hubbard U (DFT+U) calculations to examine the electronic structure of $TbMn_6Sn_6$. To do so, we optimize accurate, correlation-consistent pseudopotentials for Tb and Sn using coupled-cluster and configuration-interaction (CI) methods. We find that DFT+U and single-reference QMC calculations suffer from the same overestimation of the magnetic moments as meta-GGA and hybrid density functional approximations. Our findings point to the need for improved orbitals/wavefunctions for this class of materials, such as natural orbitals from CI, or for the inclusion of multi-reference effects that capture the static correlations for an accurate prediction of magnetic properties. The necessity for multi-reference treatment is motivated by extrapolating the dynamic correlations to the exact limit. DFT+U with Mn magnetic moments adjusted to experiment predict the Dirac crossing in bulk to be close to the Fermi level, within ∼120 meV, in agreement with the experiments. Our nonstoichiometric slab calculations show that the Dirac crossing approaches even closer to the Fermi level, suggesting the possible realization of Chern magnetism in this limit.

Session: Mechanical Engineering and Metallurgy

Lightweight High-Temperature Aluminum Alloy Rotors for EV Regenerative Braking

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The next generation electric powertrain brakes require light weight, good resistance to wear, corrosion, creep, and heat, and high thermal conductivity. This study investigates the feasibility of using advanced aluminum alloys for electric vehicle (EV) braking rotors as an attempt to replace the traditional heavy cast iron material. ORNL recently invented high-temperature aluminum alloys with excellent microstructural and mechanical stability beyond 300 °C. Two alloys Al-Cu-Mn-Zr and Al-Ce-Ni-Mn-Zr were tested on a sub-scale brake tester against a commercial brake lining material and their performance was compared to cast iron. Analysis was done based on combination of frictional, wear, and temperature responses, which are among the key factors for candidate brake rotor materials.

This research was sponsored by the Powertrain Materials Core Program, under the Propulsion Materials Program (managed by Jerry Gibbs), Vehicle Technologies Office, US Department of Energy (DOE).

Development of a Lean Electrically Conductive Al-Zr Alloy through Sn Micro-Alloying

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With the rapid development and production of electric vehicles (EVs), the need for a lower density replacement for Cu components has become obvious. The high electrical conductivity and low density of lean Al-Zr alloys makes it a good candidate for replacing the existing Cu alloys that dominate conduction in EVs. The precipitation of the coarsening-resistant metastable Al_3Zr $L1_2$ phase provides age-hardening and reduces the detrimental effects of the Zr solute atoms on electrical conductivity. It has been observed in other aluminum alloy systems that micro-alloying additions of Sn can modify precipitation behavior to produce a stronger age hardening response. In this work, the influence of 0.09 wt% Sn (0.02 at%, 200 ppm) additions on the hardness and electrical conductivity is investigated via isochronal and isothermal aging of a lean Al-Zr alloy between 150 ˚C and 550 ˚C. Selected specimens were investigated with scanning transmission electron microscopy (STEM) and atom probe tomography (APT). A mechanism for heterogenous nucleation due to the formation of Zr-Sn-vacancy clusters is proposed based on advanced characterization and a density functional theory (DFT) model. It is demonstrated that Sn additions have a beneficial influence on the balance of mechanical and electrical properties in this lean Al-Zr alloy.

Processing Parameters Effect on Powder Bed Fusion Processed 316L

Selda Nayir and Peeyush Nandwana

Materials for Advanced Manufacturing, Materials Science and Technology Division, Oak Ridge National Laboratory

Powder Bed Fusion Processed 316L stainless steel microstructure can be tailored by controlling the processing parameters to achieve dense and high-strength material properties. This work investigates the mechanical and microstructural properties of 316L to establish a correlation between applied processing parameters, such as power, scan velocity, and hatch spacing, and examined materials properties of relative density, and tensile strength. The findings showed that defect type and formation in the structure directly correlated with applied energy density. The formation ranges of lack of fusion and keyhole defects on applied energy densities were identified by computing defect criteria which is a combined effect of meltpool depth and width. The processing parameters' impacts on material properties were investigated with the applied statistical methods and the results showed that applied energy and spot size were crucial while controlling the defects and producing high-performance builds. Additionally, 316L commercial powder chemical compositions were also analyzed to identify the solidification modes which can impact the fraction of delta ferrite, dendrite morphology, interdentritic segregation behavior of the material.

Grain Boundary Chemistries of an Additively Manufactured Ni-Based Superalloy: As Printed vs. After Hot Isostatic Pressing

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Grain boundary (GB) chemistries are of vital importance for the mechanical properties of structural alloys, and how it is influenced by the non-equilibrium solidification condition of additive manufacturing requires better understanding. In the current study, the GB chemistries of an additively manufactured Ni-based superalloys are investigated by comparing the non-equilibrium as-printed samples and the equilibrium ones after hot isostatic pressing (HIP). Some carbide- forming elements, such as Nb, Mo, and Ta, showed a clear non-symmetrical partitioning behavior among neighboring grains across the same GB, which disappeared in the after-HIP samples. In the meantime, the GB segregation contents of B showed decent variations only in the as-printed samples. The underlying mechanisms of these phenomena were understood through thermodynamic-based modelling. Results were also discussed with respect to the corresponding high temperature tensile test results.

Understanding Microstructure Evolution of Al-Alloys during Solidification through Meso-Scale Modeling

Indranil Roy,[1] John Coleman,[1] Matt Rolchigo,[1] Ying Yang,[1] Alex Plotkowski,[1] and Shaunglin Chen[2]

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The mechanical property of alloys is directly related to the solidified microstructure formed during solidification process. With the advancement of state-of-the-art manufacturing processes, drastically different microstructure is often observed compared to conventional casting, primarily due to difference in cooling condition. Having the ability to predict microstructure based on alloy properties and processing condition helps the researchers to design stronger material for vehicle technologies and other applications. Moreover, designing solidification of high impurity alloys will make useful recycling of scrap metallic alloys. We have developed technique to model dendrite, eutectic and a combination growth for binary alloys under different solidification conditions. The dendrite and eutectic model are validated against Lipton-Glicksman- Kurzand (LGK) and Jackson-Hunt (JH) analytical model respectively. Our model showed promise for simulating eutectic couple zone that is often observed experimentally for off-eutectic compositions.

Session: Computational and Statistical Methods

A Predictor-Corrector Strategy for Adaptivity in Dynamical Low-Rank Approximations

Stefan Schnake

Computer Science and Mathematics Division, Oak Ridge National Laboratory

In this talk, I present a predictor-corrector strategy for constructing rank- adaptive dynamical low-rank approximations (DLRAs) of matrix-valued ordinary differential equation systems. The strategy is a compromise between (i) low-rank step-truncation approaches that alternately evolve and compress solutions and (ii) strict DLRA approaches that augment the low-rank manifold using subspaces generated locally in time by the DLRA integrator. The strategy is based on an analysis of the error between a forward temporal update into the ambient full-rank space, which is typically computed in a step-truncation approach before re-compressing, and the standard DLRA update, which is forced to live in a low-rank manifold. This error is used, without requiring its full-rank representation, to correct the DLRA solution. A key ingredient for maintaining a low-rank representation of the error is a randomized singular value decomposition, which introduces some degree of stochastic variability into the imple- mentation. Numerical experiments comparing the predictor-corrector strategy to other methods demonstrate robustness to overcome shortcomings of step truncation or strict DLRA approaches: the former may require more memory than is strictly needed while the latter may miss transients solution features that cannot be recovered. The effect of randomization, tolerances, and other implementation parameters is also explored.

Can a Deep Learning Model Predict the Solution of a Partial Differential Equation Given the Boundary Values? An Initial Exploration

Aditya Kashi

National Center for Computational Sciences, Oak Ridge National Laboratory

For several reasons, it is beneficial to computationally model (simulate) the behavior of a physical system. Generally, many of these models may be described by partial differential equations (PDE). However, for complex real phenomena, the precise PDE terms or coefficients may not be known with certainty and solving the PDE by numerical methods may be very computationally expensive. Thus, it is of interest to model such systems by data-driven methods, such as neural networks. Current efforts in this direction usually fix the boundary conditions for the PDE boundary value problem; they train a network that accepts a spatial location as input and returns as output the solution value at that location. Here, we aim to accept the boundary values as input, and return the solution to the PDE as a (discretized) function. Thus, the model now represents an operator from one function space to another. We explore the ability of neural networks to adequately model such an operator for simple steady-state PDE problems such as Poisson (heat) and advection. In this preliminary study, we show that neural networks can be designed for such a task, at least in one spatial dimension.

How Many Unitaries Does It Take to Reach a Good Solution State?

Sarah Chehade

Computational Sciences and Engineering Division, Quantum Information Science Section, Quantum Computational Science Group, Oak Ridge National Laboratory

Variational quantum algorithms (VQA), which use classical optimization techniques to train a parameterized quantum circuit, are a great tool to help solve linear and non-linear systems, factoring, combinatorial optimization etc. Once a problem is encoded in a VQA, the question of how many layers in the circuit are required to guarantee existence of a good approximation to a solution has been partially answered through a concept of overparameterization. Overparameterization occurs whenever a quantum circuit has surpassed a critical number of layers that allows it to explore all relevant directions in state space. In this talk, I address how to mathematically characterize pre and post overparameterized algorithms and derive bounds for when a circuit becomes overparamertized. This is based on joint work with Phil Lotshaw and Ryan Bennink.

System Identification and Surrogate Modeling

Benjamin P. Russo

Computer Science and Mathematics Division, Oak Ridge National Laboratory

The goal of a system identification scheme is to use data from a measured but unknown dynamical system to identify equations that descibe the system. Related, the goal of surrogate modeling is to generate a simplified version of a dynamical system. In this talk, we will discuss the relationship between these two problems and some current data driven approaches.

A Short Software Demonstration for Symbolic Combinatorics

Elaine Wong

Computer Science and Mathematics Division, Oak Ridge National Laboratory

In this demo, we briefly highlight the use of two pieces of software: cylindrical algebraic decomposition in Mathematica and a newly developed SageMath package [sage_acsv]. Both can help with answering

questions related to symbolic computation, with applications in combinatorics. We will start the demo with two different, but easy to describe, combinatorial questions that we would like to answer (one in q-partition theory and the other in analytic combinatorics) and then show how the mentioned software can enable us to answer them. This is based on recent work of the presenter and external collaborators.

Session: Nuclear Energy

Distributed Strain Measurements in Additively Manufactured SS316 with Embedded Fiber-Optic Sensors

Holden C. Hyer and Christian M. Petrie

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Fiber-optic sensors are resistant to ionizing radiation and high temperatures (>1,000°C), making them promising candidates for measuring distributed strain in the harsh environments commonly found in energy applications. Site specific strain measurements require that the fiber be properly bonded to the matrix, necessitating embedding the fiber during component manufacturing. Laser powder bed fusion processing accommodates high geometric resolution (<200 μm) and location specific placement of sensors. Therefore, fiber-optic sensors were embedded in SS316, a relevant nuclear material, by carefully controlling the melt pool to properly bond the fiber to the matrix without causing fiber failure. The embedded fiber was interrogated using optical frequency domain reflectometry to determine light attenuation and fiber residual strain. Optical and electron microscopy was performed to confirm the fiber/matrix bonding. Distributed strains in the embedded fiber were accurately recorded during controlled heating to temperatures as high as 1,000°C as compared to thermal expansion modeling of the SS316 matrix.

SCALE Non-Light-Water Reactor (Non-LWR) Fuel Cycle Demonstration for a High- Temperature Gas-Cooled Reactor

R. Elzohery, D. Hartanto, F. Bostelmann, and W. Wieselquist

Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory

Non-Light Water Reactors (non-LWRs) are regaining interest in the nuclear community because of their enhanced safety, cost-effectiveness, and reduced proliferation risk. To assess and understand the behavior of these systems under different conditions, computational models are needed. Many existing modeling and simulation tools have been developed to focus on LWRs for which validation is possible based on extensive data from multiple decades of operation. For non-LWR applications, these tools must be validated and oftentimes extended to consider the different geometries/materials/temperatures and reactor physics behaviors of non-LWRs. The SCALE code, developed and maintained by ORNL, is one such tool that has been widely used by industry and regulators for reactor applications. Work at ORNL has been initiated to develop the code to include new features and capabilities that facilitate modeling non-LWR systems. The presented work focuses on the use of SCALE for the simulation of accident scenarios within the nuclear fuel cycle of one of these non-LWRs, namely, the High- Temperature Gas-Cooled Reactor (HTGR). The considered fuel cycle stages cover UF_6 transportation, fresh HTGR fuel pebble transportation, HTGR

operation, and spent HTGR fuel pebble storage onsite. The underlying analyses involved criticality calculations, fuel inventory and decay heat calculations, and radionuclide characterization.

Towards an MPEX Digital Twin: Validation Studies Using Proto-MPEX and SOLPS-ITER

Md Shahinul Islam, Jeremy Lore, Cornwall Lau, and Juergen Rapp

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The Material Plasma Exposure Experiment (MPEX) is being constructed at ORNL to investigate critical fusion reactor issues such as plasma-material interactions (PMI) under reactor-relevant conditions and time scales. The linear device Proto-MPEX was used as a test bed at ORNL to address research and development issues and develop the physics basis for MPEX. The state-of-the-art modeling code suite, SOLPS-ITER, has been recently applied to understand plasma and neutral transport in Proto-MPEX to increase confidence in predictive simulations for MPEX. Coupling between COMSOL and SOLPS is performed to implement a 2D electron heating profile of the helicon source. The simulations show reasonable agreement with the experimental data for plasma with helicon and auxiliary Electron Cyclotron Heating (ECH). The results indicate that ECH significantly enhances target heat flux, with ECH power of 50 kW increasing target heat flux from 0.4 to 17 MW/m^2. It is found that a small amount of gas puffing near the target plate can further increase the target heat fluxes at the higher ECH power cases, but the target heat flux is reduced at higher gas puffing conditions. ECH and gas puffing scenarios can generate higher target flux, which will address PMI issues in a reactor- relevant plasma condition.

Helium Flow Visualization Simulation for Fusion Reactor First Wall Cooling

Yuqiao (Joy) Fan

Fusion Energy Division, Oak Ridge National Laboratory

The first wall in fusion reactors is exposed to the high-temperature plasma where fusion reaction occurs, therefore the cooling of the first wall is a challenge due to its high heat flux. Helium, as the coolant, its gaseous state and nontransparency make investigations of local flow behavior difficult. Flow visualization is essential to understand helium cooling performance. Therefore, helium coolant flow is modeled in different test sections and heating conditions to utilize high- fidelity simulations to visualize the flow behavior. Firstly, simulations consider flow disturbances introduced by the inclusion of the viewing port (required by experiments). Such surface abnormality bifurcated the flow recirculation region into primary and secondary recirculation zones; greater disturbance and spanwise flow asymmetry were discovered as well. Secondly, heat flux was increased to the operational value at the channel bottom wall, mimicking the first wall. Heating changes the helium distribution dramatically and helium detached from the heated wall, which caused hotspot. Therefore, at last deflectors were added, which increased helium attachment significantly, enhanced the heat transfer coefficient (1.75x), and substantially reduced the hotspot area and temperature. This work serves as a first investigation of the helium flow visualization for the first wall cooling enhancement for fusion reactor design.

Session: Pattern Identification and Threat Detection

Securing Distributed Energy Resources (DERs) through Data and Device Verification

Raymond C. Borges Hink

Electrification and Energy Infrastructures Division, Oak Ridge National Laboratory

Distributed Energy Resources (DERs) proliferation presents new cybersecurity challenges to the electric grid. This presentation focuses on a study's outcomes to enhance DER security through verification techniques. The project conducted simulated cyber-attacks and electrical faults to test a previously developed system called Cyber Grid Guard system's resilience and extend its current capabilities.

A new anomaly detection algorithm was developed and deployed that uses new power quality metrics and validates them against industry standards while leveraging distributed ledger technology (DLT). Additionally, the project implemented an attestation that detects file changes more precisely, identifying the exact modified setting. The system can conduct random checks, manual checks, anomaly-triggered checks, and parallelized attestation checks for devices on the network.

These findings highlight the potential of anomaly detection and verification techniques in improving DER security. The advanced algorithm's application of power quality metrics could lead to more effective detection of anomalies, while the grid guard attestation enhances the accuracy of file change detection. The results provide insights into improving the security of DERs, which are increasingly critical electric grid components.

Cyber-Resilience of Blockchain for the Electric Grid

Aaron W. Werth

Cyber Resilience and Intelligence Division, Oak Ridge National Laboratory

Cybersecurity is essential to the power grid, especially considering recent attacks on the grid and critical infrastructure in general. These include the Ukrainian attack of 2015 and the ransomware attacks on the Colonial Pipeline in 2021. To combat these attacks, it is necessary to develop new technology with cyber-resilience. One such approach is the use of permissioned block chain to secure data associated with the grid. However, with this new technology, it is necessary to test to ensure that it is truly resilient. Therefore, we have created a framework for systematically launching DDoS attacks of varying intensities to thwart the communication between nodes of the blockchain and their functioning in general. Our findings indicate that the Cyber Grid Guard, a permissioned blockchain architecture, was resilient to DDoS attacks, which only delayed the communication. We found that the use of a permissioned blockchain architecture, which restricts access to authorized parties could effectively reduce the impact of the DDoS attacks. These findings have practical implications for governments and researchers that might develop and deploy blockchain technology in their infrastructure. The findings also show the importance of carefully designing and testing blockchain architectures to ensure their security and resilience.

Absorbed Doses from Accidental Extravasation of Radiotracers in PET Imaging

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This study aimed to determine the absorbed doses resulting from radiotracer extravasation and infiltration during PET imaging, both at the site of extravasation and in other organs in the body. To achieve this, a radiation dosimetry simulation was setup using whole-body XCAT phantoms embedded in the GATE Monte Carlo platform. The simulation used 10 mCi of ^{18}F-FDG to mimic a clinical PET scan scenario, with 10% of the injected activity being extravasated in the antecubital fossa of the right hand of the phantom. The dose contribution was calculated from the extravasation site and multiple organs of interest, and the energy deposition was estimated and converted to absorbed dose based on the mass of each (heart, gonad, liver, lung, spleen, kidney) organ. The results showed that the absorbed dose at the extravasation site was (0.29±0.01) Gy, while the absorbed doses in other organs were clinically insignificant. These findings suggest that PET imaging using radiotracers is generally safe, and measures to mitigate extravasation should be taken to reduce radiation exposure at the local site. Further studies will simulate the extravasated doses in a set of XCAT phantoms that represents a clinical population, and use multiple radionuclides: ^{18}F, ^{99m}Tc, ^{68}Ga, and ^{89}Zr.

Validating Monte Carlo Simulations Experimentally to Quantify DNA Damage in Breast Cancer Cells Following Exposure to ^{225}Ac

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In this study, we experimentally validated a multiscale Monte Carlo computational framework for estimating radiation-induced DNA damage in E0771 mouse breast cancer cells exposed to 225Ac. We exposed E0771 cells to 11.4±0.5 nCi of 225Ac for 24 hours and estimated the extent of DNA damage through γ-H2AX immunofluorescent staining. Subsequently, we replicated the experiment using the simulation framework, which used Geant4 and TOPAS-nBio Monte Carlo toolkits to simulate the phase space of particles entering the cellular volume and to estimate single- (SSBs) and double-strand breaks (DSBs). 100 cells from the simulation were selected randomly for DNA damage estimations and cell viability, and results were compared with experimental results. The simulations estimated an average of 5.83±3.13 DSBs per cell and predicted cell survivability of 88%, while the experimental observations showed an average of 6.2±1.3 foci per cell and cell survivability of 87%. The average dose to each cell with DSBs in the simulation was 0.19±0.03 Gy. We successfully demonstrated the validation of the simulation framework for estimating DNA damage in cells exposed to 225Ac. The results show a good agreement based on the direct correlation between DSBs and γ-H2AX foci per cell at the simulated dose.

Session: Computational Material Science

CrysFieldExplorer: A Software for Rapid Optimization of Crystal Field Hamiltonian

Qianli Ma

Neutron Scattering Division, Oak Ridge National Laboratory

We present a new lite python-based program, CrysFieldExplorer, for fast optimizing crystal electric field (CEF) parameters to fit experimental data. The main novelty of CrysFieldExplorer is the development of a unique loss function, referred to as the Spectrum-Characteristic Loss ($L_{Spectrum}$), which is defined based on the characteristic polynomial of the Hamiltonian matrix. Particle Swarm Optimization and Covariance matrix adaptation evolution strategy are used to find the minimum of the total loss function. We demonstrate that CrysFieldExplorer can performs direct fitting of CEF parameters to any experimental data such as neutron spectrum, susceptibility, magnetizations etc. CrysFieldExplorer can handle a large amount of none-zero CEF parameters and reveal multiple local and global minimum solutions. Detailed crystal field theory, description of the loss function, implementation and limit of the program are discussed within context of two examples.

A Bayesian Optimized Human Assessed Spectral Recommender System for Added Flexibility of Real-Time Decision Making in Automated Experiments

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Optimization for different tasks like material synthesis, characterization, and functional properties for desired applications over large parameter space need a rapid strategic search through active learning. However, in all cases prior to optimization, the target material properties are assumed known and fixed. However, in certain instances of material discoveries, the assumption is not true. In addition, the experimental data (eg. spectra), generated from microscope, are generally noisy and exact computation of multiple key features (such as spectral loop area, storage, peak width, height etc) to simplified numerical descriptors can be non-trivial. To address these challenges, we introduce a human-operator within the loop of the active learning based automated experiment framework. Here, the user iteratively provides visual structural assessment of spectra during real- time microscope measurements over the locations in the material image space, thereby sequentially learn/update the target spectral structure through a weighting system, with adaptive guidance for future sampling to maximize the custom target structural similarity-reward based acquisition function. We term this a Bayesian optimized spectral recommender system (BOSRS). The approach has been demonstrated to peizoresponse force spectroscopy of ferroelectric thin films (eg. $PbTiO_3$), exploring with different kernels functions. This approach is a new modality of human-driven automated experiment which adds flexibility to a standard automated experiment, where the human operator guides the active learning based rapid exploration with real-time decision making.

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Towards Meaningful Latent Space Learning via Variational Autoencoder with Physical Constraints

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Recent advances in scanning tunneling and transmission electron microscopies (STM and STEM) have provided a source for large experimental dataset, within which lies the key information (eg. lattice periodicities, order parameter distribution, repeating structural elements, or microstructures etc) towards discovery of physics. However, accurate and maximal extraction of patterns and features from such large and complex dataset are non-trivial and require an appropriate machine learning (ML) approach. While the advanced variational autoencoder (VAE) model (eg. shift invariance- VAE) can disentangle the complex experimental data with simplified learning than a vanilla VAE [1], however, such advanced VAE models do not possess any domain knowledge of a material system to guarantee a physically meaningful latent feature learning. To address this, we develop an approach of implementing VAE with physical constraints and demonstrate to improve the training process of sh-VAE. In this case study, as per the expected physical behavior of BiFeO3 and NiO-LSMO systems, we formulate a loss function to reduce the sharp edges in the latent variable maps, to maximize the smoothness on the length scale of atomic lattice. This physical constraint validation is transformed into a custom loss function, which is augmented with ELBO loss, and the hybrid total loss is minimized during model training process. This approach is implemented with various STEM 2D experimental data, and the results are compared with vanilla VAE and standard sh-VAE models. The results demonstrate the effectiveness of our approach in unsupervised extraction of meaningful information from large volumes of imaging data.

[1] Ziatdinov, M.; Wong, C. Y.; Kalinin, S. V. *Finding Simplicity: Unsupervised Discovery of Features, Patterns, and Order Parameters via Shift-Invariant Variational Autoencoders*; arXiv:2106.12472; arXiv, 2021. https://doi.org/10.48550/arXiv.2106.12472

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Inverse Design of Auxetic Materials with Prescribed Nonlinear Responses Using Deep Learning

Deepak Kumar Pokkalla,[1,] Raja Biswas,[2] Seokpum Kim,[1] and Vlastimil Kunc[1]

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Architected materials represent a category of deliberately designed structures that exhibit distinctive physical and mechanical traits that arise from their underlying geometry, rather than their composition. The application of such materials extends to controlling energy absorption, wave propagation, and shape morphing in a variety of engineering disciplines. Thanks to the emergence of additive manufacturing techniques, the rapid fabrication of such materials featuring complex microstructures in diverse materials and length scales has become feasible. However, identifying suitable microstructures capable of eliciting the desired mechanical response using existing design paradigms that rely on shape or topology optimization remains a formidable challenge. In this work, a deep learning framework for the inverse design of auxetic materials with target negative Poisson's ratios over large strains is proposed. The topological design space is explored through accurate and efficient isogeometric analysis for establishing structure-property relationships which serves as the training data. We demonstrate the application of deep neural networks based inverse design strategy to missing rib auxetics with controllable Poisson's ratios and specifically present biomimetic auxetic structure that reproduces the deformation behavior of cat's skin.

Synthesis of High-Performance Thermal Insulation Materials Guided by Multi-Scale Simulations

Bokyung Park

Buildings and Transportation Science Division, Oak Ridge National Laboratory

The massive energy usage and high energy cost in the heating and cooling of buildings call for improvements in the energy efficiency of buildings. Thus, there is a growing interest in developing cost-effective and high-thermal-performance insulation materials. Currently, a few high-thermal performance insulation materials are available in the market with an R-value greater than 10/inch, such as aerogels and vacuum-insulated panels. However, these are unsuitable for building applications due to high-cost, poor mechanical properties, low processibility, and vacuum requirements. Here, we propose developing economical but high-performance foam insulation material with an R-value exceeding 10/inch to increase energy efficiency in buildings. Also, this work aims to minimize modifying the current foam manufacturing and installation processes. First, use multi- scale simulations to understand the current limitations of state-of-art foam insulations for buildings. Then, simulation is further performed, providing detailed parameters as the function of solid conduction, gas conduction, and radiation to explore the lower thermal conductivity of foams to develop more efficient foam insulations. Finally, computationally obtained parameters are realized in experimental work by tailoring formulations. Then, fabricated foams' thermal performance, morphology, and mechanical properties are evaluated and collected results to develop/train further machine learning algorithms for designing high-performance insulation materials.

Reaction Pathways Search Using Adaptive-Learning Global Optimization Algorithm

Małgorzata Zofia Makoś and Vassiliki-Alexandra Glezakou

Chemical Sciences Division, Oak Ridge National Laboratory

The search for reaction pathways is a crucial aspect of chemistry, with numerous applications in drug design, materials science, and catalysis. It involves exploring the energy landscape of complex chemical reactions to identify the reactants, transition states, and products. However, this task is incredibly challenging, as it requires navigating a vast potential energy surface with multiple possible outcomes. Here, we propose the combination of a global optimizer combined with a machine learning algorithm that allow us to explore the potential energy surface to identify the reaction pathways. A recently developed global optimization algorithm (NWPEsSE) [1] is very useful in identifying low-energy minima for large systems (~102-103 atoms). Generative adversarial networks have been successfully used for the prediction of the transition states between a given set of reactants and products.[2] Here, we combine the two computational schemes connect a large set of possible reactants, transition states, and products, together with calculated energies at the DFT level. Our approach has been successfully used in identifying the mechanisms of various chemical reactions, including those involving heavy elements and surface reactions. This approach aid in the discovery of new reactions, optimization of existing reactions, the prediction of reaction outcomes and extraction of generalized system descriptors. Moreover, it can facilitate the development of more efficient and sustainable chemical processes, contributing to the advancement of the chemical industry.

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Session: Neutron Detection and Instrumentation

Improvement of Spatial Resolution and Gamma discrimination of Neutron Anger Cameras

Matthew Loyd

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Neutron scattering facilities provide important information about materials that cannot be determined via x-rays, such as magnetic properties and the structure of soft and biological samples. Neutron diffraction instruments require large-area, high efficiency detectors that can adequately discriminate against unwanted noise, such as gamma rays. Neutron sensitive Anger cameras satisfy these conditions and have the benefits of low operating voltage, uniformity, compactness, magnetic insensitivity, and low cost. In this talk I will discuss the experiments undertaken to optimize the optic configurations to improve the spatial resolution.

A novel composite scintillator geometry is tested to improve the gamma discrimination without sacrificing neutron efficiency. Additionally, a brighter scintillator material is being investigated for high-resolution applications.

High-Dimensional Phase Space Measurements for Halo-Level Hadron Beam Control

Austin Hoover

Research Accelerator Division, Oak Ridge National Laboratory

The beam intensity in modern hadron accelerators is limited by low-level *beam loss*: some particles collide with the accelerating structure, generating dangerous levels of radiation. Losses are partly due to electric interactions between particles in low-energy acceleration stages. These interactions result in complex dynamics including *halo formation*, where a small fraction of particles is driven to the edges of the available position-momentum space (phase space), far from a dense core. Halo is difficult to measure (due to its low density) and predict (due to its sensitivity to the initial six-dimensional phase space distribution and the applied electromagnetic fields, neither of which are known precisely in existing accelerators). These issues are being addressed at the Beam Test Facility (BTF), a replica of the front end of the Spallation Neutron Source (SNS) linear accelerator. Direct high-dimensional and high-dynamic range measurements have produced a detailed image of the initial phase space distribution. These measurements will be used to seed beam dynamics simulations for halo-level benchmarks at the end of the BTF. Here, I review the progress we have made on high-dimensional phase space measurements and data analysis.

Studying the Respirable Airborne Contamination from Spent Nuclear Fuel Fractures

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Spent Nuclear Fuel (SNF) assemblies, retrieved after its useful lifetime in a reactor, are stored in cooling ponds and then transferred into stainless steel canisters for further storage and disposal. An accidental cladding fracture during this timeline can result in the release of radioactive SNF dust, which is now available for contamination during potential canister failure events. My work focuses on understanding this source term of respirable aerosol fractions from fractured SNF rods under postulated accident scenarios. In this regard, an unpressurized 6-inch ZIRLO clad SNF rod segment with a local burnup of 63 GWd/MTU was fractured under 4-point bending and the radioactive aerosols released were collected and characterized.

The results show a total dust mass of ~4.6 mg was deposited on the collection apparatus (Figure 1), and ~0.5 mg of respirable aerosols collected in the cascade. The collected dust was analyzed separately using ICP-MS to obtain an isotopic distribution of the source term.

The test results will inform a number of studies including the amount of source term and particle size distribution available to a canister breach in storage. This work could also help in site boundary considerations and predictive models looking at respirable aerosol release from accident scenarios.

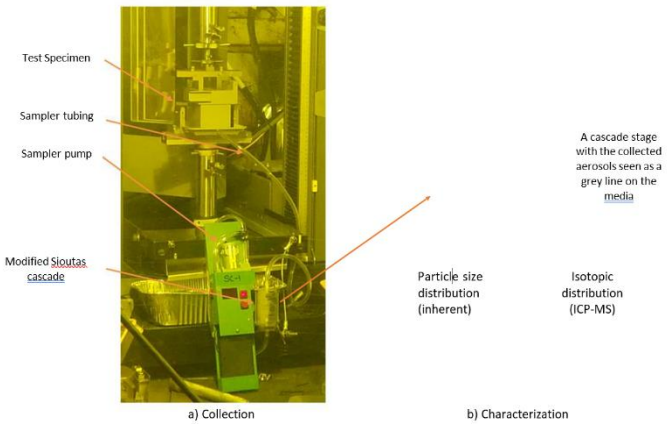

Figure 1. The two steps involved in this study: a) The 4-point bending test rig with the aerosol collection setup b) A cascade stage with the collected aerosol particles before characterization.

Low Temperature Liquid-Based Chlorination of Zirconium Alloys

Breanna King Vestal

Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory

Processing the zirconium alloy cladding found in used nuclear fuel would reduce the volume of high-level waste from commercial reactors by 25%. In the first stage of processing, high-temperature gas phase reactions have been the primary means to chlorinate the zirconium alloy. However, due to challenges associated with these reactions, two new liquid-based oxidative chlorination reactions have been discovered for zirconium. In both solvents, zirconium can be quantitatively chlorinated at temperatures less than 150°C. In sulfur monochloride, the reaction is completed in 2 – 4 hours via surface etching and exhibits 0^{th} order kinetic behavior. The elemental sulfur byproduct can be quantitatively rechlorinated to sulfur monochloride immediately following the zirconium alloy chlorination so that the only consumed material is chlorine. In thionyl chloride, the reaction is completed in 7 – 40 hours with a variable induction period. Both reactions may be feasible to chlorinate zirconium alloys, reducing the volume of high-level waste from commercial nuclear fuels.

Poster Abstracts

Session: Bioscience and Computer Science

Structure Determination of Moss Cellulose Synthase 5 (PpCesA5) Trimer

Lynnicia Massenburg

Biochemistry and Molecular Biology, Pennsylvania State University

Plant membrane proteins called cellulose synthases (CesAs) make cellulose, the most abundant plant polymer in the world found in plant cell walls. The cryo-EM structure of higher plant CesAs have revealed structural insights, but an evolutionary context of CesA structure in other plant species such as moss is needed. The aim of my research proposal is to understand the role of plant CesA trimer oligomerization in functional cellulose synthesis and assembly. To approach this aim, I seek to characterize the structure of an early plant moss PpCesA5 in nanodiscs using cryo-Electron Microscopy (cryo-EM), Small-Angle Neutron Scattering (SANS) and Small-Angle X-Ray Scattering (SAXS). These complementary structural techniques will provide insights on residue-level oligomer interactions from stable globular domains, as well as conformation ensembles from intrinsically disordered domains of moss PpCesA5 monomers and trimers. Preliminary results have shown PpCesA5 trimeric structure similarities with higher plant CesAs. Future work involves an evolutionary structure comparison with higher plant CesAs. This work reveals the importance of structura ltechniques to advance future work in biofuels and new biomaterials.

Unraveling Network Connections in a Constructed 3-Member Microbial Community

April Armes, Dale Pelletier, and Mitchel Doktycz

Biosciences Division, Oak Ridge National Laboratory

Microbial communities are highly complex in nature due to diverse metabolic abilities and varying abundances of microbial constituents. Interactions within microbial communities play important roles in various ecological processes. Constructed synthetic microbial communities offer insight into such interactions including competition, cooperation, and cross-feeding while reducing the complexity of natural communities. Previous work on 10-member synthetic communities consisting of bacteria isolated from Populus deltoides gave rise to three stable community members: Pseudomonas sp. GM17, Pantoea sp. YR343, and Sphingobium sp. AP49, likely as a result of competition and cross-feeding. However, recent work indicates these stable community members co-exist without depending on cross-feeding interactions. Here, we investigate network connections between GM17, YR343, and AP49 within this microbial community. We are performing drop-out experiments to evaluate the impact of individual community members on each other. Co-cultures in every possible combination will be monitored by optical density (OD 600nm) and viable plate counts. Microbial interactions will be analyzed using co- occurrence analysis to identify possible network connections and potential keystone species within the microbial community. Understanding microbial networks and interactions can aid in the engineering of synthetic microbial communities for ecological and agricultural importance, including enhancing host plant growth and tolerance to various stresses.

Effects of 3-Dehydroshikimate Dehydratase Expression Levels in the Organization of Cellulose Microfibrils in Poplar Mutants forEfficient Production of Sustainable Energy

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Lignocellulosic biomass, which is a complex polymer composite of cellulose hemicellulose and lignin, is important as a sustainable, carbon neutral, and non-competitive source of polysaccharides for the production of renewable fuels as well as advanced byproducts. The association of lignin with carbohydrate polymers hindered the access of water and enzymes to carbohydrate polymers, which is critical in the bioconversion process. Most of the thermochemical pretreatment approaches used for removing lignin to reduce the lignin recalcitrance to increase the efficiency of converting biomass to bioenergy are costly and energy-demanding. As an alternative approach, plants with lower lignin content were developed through the overexpression of the bacterial 3- dehydroshikimate dehydratase (QsuB) enzyme in poplar. Three different transgenic tree lines with reduced lignin content were produced and compared to the wild type (WT), and their level of QsuB expression varied as QsuB1>QsuB15>QsuB5>WT. The efficacy of biomass conversion into sugars follows the same trend. The compositional analysis determined 15% less lignin and 13% higher hemicellulose content in the QsuB1 and Qsub15 lines compared to QsuB5 and WT. To correlate plant cell wall structural features to higher efficacy for low lignin lines, small-angle neutron scattering (SANS) and wide-angle X-ray scattering (WAXS) were employed. SANS data were fit to a composite model of cylinders coupled with the Unified fit function. The cylinder modeled individual cellulose microfibrils and obtained the cross-sectional radius of the cellulose microfibrils. The fit results illustrated similar cross-sectional radii of the cellulose microfibrils for all mutants and the WT. However, the degree of order in the arrangement of the cellulose microfibrils progressively decreased with increasing QsuB expression levels, and the highest expression line QsuB1 showed no order. WAXS data also showed that the crystallinity of the individual microfibrils decreased with increasing QsuB overexpression, which can be attributed to the accumulation of protocatechuic acid (PCA) in the cell wall. The strong polar ends in PCA may result in penetration into the cellulose microfibrils and perturb intra-molecular H-bonding as well as Van der Wall forces.Together, comprehensive knowledge of the relationship between QsuB overexpression levels and cellulose microfibril size and order in poplar stems was achieved. This knowledge of the correlation between QsuB expression and structural changes at the molecular level in the plant cell wall will pave the way to develop a science-driven approach to tune poplar stems' characteristics from overcoming recalcitrance and enhancing biomass conversion efficiency to produce sustainable energy.

Using Hyperspectral Imaging to Predict Plant Resilience Traits

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We rapidly need solutions to scale the impacts of environmental stress across levels of biological organization. Technological advances have enabled the growing use of hyperspectral imaging to predict plant growth traits and function. This technology has benefits over traditional measurements as it can assess plant traits without destructive harvesting or labor-intensive measurements. Spectral wavelengths have been correlated with estimates of important physiological characteristics such as leaf pigments, leaf mass per area, plant nitrogen, and the rates of the biochemical reactions of photosynthesis. However, accuracy of such predictions across variable nutrient conditions is not well characterized. Therefore, we took hyperspectral images and measured a suite of plant anatomical, biochemical, and physiological traits of Populus trichocarpa grown across multiple nitrogen treatments. We found expected nutrient related results such as Rubisco carboxylation, photosynthetic electron transport, chlorophyll a/b, and protein content all increased with nitrogen. Ongoing analyses will correlate these plant traits with image analysis to assess how we can use hyperspectral technology to investigate plant responses to environmental stress. Ultimately, these data will be used to discover resilience genes and establish a gene-to-trait-to-spectra relationship methodology that can be expanded to other species and across levels of biological organization for resilience assessment.

Performance Portability at the NCCS

John Holmen

National Center for Computational Sciences, Oak Ridge National Laboratory

Diversity among supported architectures in high performance computing (HPC) systems makes performance portable codebases desirable. For example, current and emerging DOE systems will feature GPU accelerators from 3 different vendors, each targeting different programming models. Performance portability layers have emerged to help address this diversity. Examples include Kokkos, OCCA, RAJA, and SYCL/DPC++. This poster shares John Holmen's efforts relating to performance portability, which include organizing a collection of performance portable system tests for OLCF systems, helping to prepare the Uintah Computational Framework for exascale systems, examining scalability of AthenaPK across Frontier, and supporting ORNL's SYCL/DPC++ efforts.

MCHound: Wrapping Telemetry Collection in Userspace

Matthias Maiterth, Postdoctoral Research Associate - HPC and AI

National Center for Computational Sciences, Oak Ridge National Laboratory

Measuring and monitoring telemetry data has become a fundamental part of HPC operation and is done using continuously operating telemetry services. This is often not directly available to users. For users, tracing and profiling is traditionally used to understand application performance and to find bottlenecks and potentials for improvement. However, this may obstructs production runs and is therefore not used to understand performance of applications over larger sets of experiments.

We present MCHound, a tool for collecting telemetry data as a thin wrapper around the scheduler's job execution command. Each node participating in the job spawns a daemon querying the configured telemetry-collection tools in regular intervals, as configured for the system. The result is a structured directory of profiling data, per system, per job, for each participating node of the runs collected. These collections can then be analyzed using data analytics tools to identify patterns, outliers, performance regression and improvements.

The files are stored in a compressed long-format table as parquet-files.

The current implementation of MCHound runs on summit, crusher and frontier with telemetry collection using either nVidia's dcgmi, AMD's rdc or rocm-smi tools. For the user it is sufficient to 'module load mchound' and 'srun' or 'jsrun' their application.

Leveraging Multi-GPU Power for Large-Scale Graph Analytics on Frontier

Naw Safrin Sattar

National Center for Computational Sciences, Oak Ridge National Laboratory

Graph is a powerful abstraction to real-world scenarios. Large-scale graph analytics is particularly useful to solve many scientific problems across different domains such as medical science, environmental science, physics, chemistry and many more. However, the memory-boundedness of a single GPU makes it difficult for utilizing the full computing power of GPUs for large-scale graph analytics. Going beyond a single GPU, graph algorithms often have irregular memory access patterns, compounded by the challenge of load balancing, which can further complicate parallelization. In this work, we will discuss both the challenges in designing GPU-based parallel graph algorithms (namely, community detection and breadth first search) on multi-GPU systems and present strategies and solutions using algorithmic optimizations, specialized data structures, better partitioning techniques, communication patterns, and careful system-level design. This effort will enable the scientists and researchers applying graph algorithms for solving their problem more effectively and efficiently, by fully leveraging the compute power of the GPU- based system such as Summit and Frontier supercomputers.

Can Expert-Provided Lexicon Help Classify Pediatric Anxiety? A Random Forest-Based Approach

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Anxiety affects ~34% of children; untreated, it can affect long-term health. The aim of this study was to determine if a random forest model can classify patients with anxiety and without anxiety using clinical unstructured notes. We investigated the prevalence of expert- provided lexicon in notes within the pediatric electronic healthcare records (EHR) from Cincinnati Children's Hospital. Our dataset consisted of 104,625 anxiety patients with ~22 million notes and 793,060 non-anxiety patients with ~39 million notes. The expert lexicon (EL) was curated by interviewing 19 mental health providers for additional keywords used to indicate anxiety.

This preliminary study investigated two concepts: (1) how frequently EL appears in clinical notes, and (2) if a random forest model can classify an anxiety and non-anxiety patient using EL. The random forest features were created by finding the term frequencies for EL and creating embeddings based on these frequencies. We compared two datasets: undersampled and imbalanced. The undersampled dataset provided better results. It had an accuracy of 0.91 and an AUC score of 0.95.

The results demonstrate random forest-based classification can identify patients based on EL. These findings support the development of other algorithms for early detection of pediatric mental health conditions.

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Towards PBPK Informed Generative Modeling in Drug Design

Nolan English

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Generative modeling is an increasingly popular method for generating potential drug candidates for pharmaceutical applications. However, this high throughput generation approach faces a bottleneck: evaluating a candidate drug's efficacy relies on determining its kinetics (distribution through a host) and the dynamics (biological impact at target sites). Historically this was accomplished through lengthy in vitro experimentation, a practice unable to match the pace of high throughput generation. Therefore, we propose using mechanistic physiology based pharmacokinetic (PBPK) and dynamics (PBPD) models as a means of prioritizing and selecting candidate compounds for experimental study. However, implementing these models for this task is nontrivial due to two primary challenges: speed and sensitivity. Solving the extensive systems of equations that compose PBPK models is an order of magnitude slower than generative models. Additionally, as the input parameters for PBPK models are derived from predicted physiochemical properties instead of measured properties, the models are vulnerable to prediction error. To address these challenges, I present our implementation of a physiology-based pharmacokinetics (PBPK) model that lessens sensitivity to high error properties while being computationally efficient.

Faster Randomized Interior Point Methods for Tall/Wide Linear Programs

Agniva Chowdhury

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Linear programming (LP) is an extremely useful tool which has been successfully applied to solve various problems in a wide range of areas, including operations research, engineering, economics, or even more abstract mathematical areas such as combinatorics. It is also used in many machine learning applications, such as L1-regularized SVMs, basis pursuit, nonnegative matrix factorization, etc. Interior Point Methods (IPMs) are one of the most popular methods to solve LPs both in theory and in practice. Their underlying complexity is dominated by the cost of solving a system of linear equations at each iteration. In this paper, we consider both feasible and infeasible IPMs for the special case where the number of variables is much larger than the number of constraints. Using tools from Randomized Linear Algebra, we present a preconditioning technique that, when combined with the iterative solvers such as Conjugate Gradient or Chebyshev Iteration, provably guarantees that IPM algorithms (suitably modified to account for the error incurred by the approximate solver), converge to a feasible, approximately optimal solution, without increasing their iteration complexity. Our empirical evaluations verify our theoretical results on both real-world and synthetic data.

NdFeB and SmFeN Anisotropic Permanent Magnets in a Polyamide Matrix Made with Additive Manufacturing

James W. Kemp, Haobo Wang, and M. Parans Paranthaman

Chemical Sciences Division, Oak Ridge National Laboratory

The need for high-performance magnetic materials has drastically increased in recent years to meet the demands for modern electric devices for not only consumer electronics, but also clean energy technologies. The electrical requirements of power density and conversion efficiency on wind powertrains can only be met by new advanced materials. Exciting new materials that meet these requirements include Nd/DyFeB, SmCo, and SmFeN-based magnets. These materials are considered critical materials and there is a need to reduce the amount of waste used in producing permanent magnets (PMs) from them. Additive manufacturing (AM) via extrusion-based methods is considered one way to reduce waste because of its ability to produce components with near-net shape. This work shows AM, compression molded magnets. Two types of PMs were made via a mixture of $Nd_2Fe_{14}B$ (NdFeB) or $Sm_2Fe_{17}N_3$ (SmFeN) powder in a polyamide 12 (PA12) binder matrix. Their thermal properties and nano-hardness values are shown.

Interactive Distortion Compensation of Large-Size Component Fabricated by Wire-Arc Direct Energy Deposition

Shuvodeep De, Pei Zhang, Ramanan Sankaran, Yousub Lee

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Wire-directed energy deposition, owing to the high deposition rate and minimal material waste, enables the printing of large-scale parts with heights of 10 feet. However, varying printing conditions and complex geometry lead to undesirable inelastic deformation and internal stress buildup. Although the part deformation is known challenges in welding and powder bed fusion processes, it is even more dominant in large-scale AM because the deformation is magnified with part size. Therefore, advance ability to ensure geometrical conformity is required for large-scale parts. In this presentation, a computational framework will be first discussed to develop an effective distortion mitigation strategy. The framework involves thermo-mechanical simulation using finite element method and intelligent algorithm using graph neural network. The developed mitigation algorithm showed a distortion reduction by 97.8% and confirmed the effectiveness with an actual printed part. The optimization process was performed with a 2 ft tall, curved wall in a reasonable computation time of 178 min. for 29 iterations. In future the algorithm will be improved and implemented into more complex large-scale structures.

Session: Environmental Science, Energy Science, and Neutron and Nuclear Science

Improving Biogeochemical Modeling of Coastal Regions in a Land Surface Model by Representing Mangrove Hydrology and Ecosystem Functions

Shannon Jones

Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Coastal wetlands are vital landscape components that link terrestrial, aquatic, and ocean ecosystem processes. Incorporating these systems into process-based biogeochemical modeling is critical to improve model simulations and predictions of coastal biogeochemistry in response to climate extremes, sea level rise (SLR), and human landscape modifications. Yet, coastal wetlands are often excluded from both the terrestrial and oceanic components of land surface models. Furthermore, there is limited distinction in current models between different growth forms and functional traits of coastal wetland plants. Mangroves, which are major nutrient cyclers, are not currently represented in the Energy Exascale Earth System Model (E3SM) Land Model (ELM). Thus, this research aims to 1) define subtropical mangrove hydrology and plant functional types (PFTs) and 2) compare carbon & nitrogen cycling in Florida and Texas mangroves under extreme climate scenarios in ELM. Mangrove PFTs will be defined based on growth forms, biomass allocation, and abiotic factors (e.g., salinity and temperature) while hydrology will be defined using both field data and modeling. Three climate scenarios – a freeze event, short-term flooding, and long-term SLR – will be run to quantify mangrove biogeochemical responses in ELM with the future goal of scaling up to regional simulations of mangrove die-offs and expansion.

Precision Deconstruction of Mixed Plastics by a Tailored Organocatalyst

Md Arifuzzaman,[1] Bobby Sumpter,[2] Zoriana Demchuk,[1] Changwoo Do,[3] Mark A. Arnold, Md Anisur Rahman,[1] Pengfei Cao, Ilja Popovs,[1] Robert Davis, Sheng Dai,[1] and Tomonori Saito[1]

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Synthetic polymers have been widely used in our daily life, however their accumulation as plastic waste and associated environmental pollution present a significant challenge to be solved. Chemical deconstruction of commodity plastics is an emerging chemical path to convert discarded plastics to fuels, refinery feedstocks, monomers, chemicals, and upcycled materials. Organocatalysts provide promising "green" routes for polymer deconstruction, since the catalyzed depolymerization reactions yield highly pure small molecules that are adequate for subsequent polymerizations or other uses. However, most of the organocatalysts have been designed to depolymerize a specific type of polymer. Herein, we report a new organocatalyst and integrated process for depolymerization of mixed plastics to high-value chemicals. Our catalyst enabled glycolysis with more than 95% conversion within 2 hours using 1/10 of the catalyst and half of ethylene glycol compared to the conventional organocatalysts. Furthermore, this catalyst accomplished one pot, single batch selective glycolysis of diverse mixed plastic consumer products, which paves the way to increase commercial viability by eliminating costly mixed plastic sorting.

Assessment of 1D Channel Flow Models for Tritium Breeding Blanket Cooling

Monica Gehrig, Paul Humrickhouse

Fusion Energy Division, Oak Ridge National Laboratory

Reliable and rapid integrated simulations of heat transfer and fluid flow in fusion reactors are necessary to aid in the efficient design of fusion engineering systems. Computational Fluid Dynamic (CFD) simulations can be computationally expensive, and 1D "thermal hydraulic" models can reduce this expense; use of integrated modeling frameworks such as the Multiphysics Object-Oriented Simulation Environment (MOOSE) can facilitate coupling of these simplified fluid models to detailed 3D structures. This "hybrid fidelity" approach can accelerate the design process but requires suitable closures for friction and heat transfer in the 1D model. This work evaluates the accuracy of such closures in the MOOSE Thermal Hydraulics Module (THM) by comparing these directly to 3D CFD models built using the framework's Navier-Stokes Module. Channel geometries and conditions representative of the Fusion Nuclear Science Facility are considered, including those with radial/toroidal and poloidal orientations, and with bends. In both models, prototypic surface and volumetric heating conditions are applied to steady-state helium flows with ideal gas properties at 8 MPa. Quantities from the THM and Navier-Stokes simulations, such as Nusselt number, Darcy friction factor, and limiting temperatures, are compared to each other, existing correlations, and literature in assessing the validity of the 1D models.

A Novel Spectral Correlation Function Based Detection Method for Grid-Signal Distortions

Ozgur Alaca

Electrification and Energy Infrastructures Division, Oak Ridge National Laboratory

The smart grid refers to a burgeoning electric ecosystem created by integrating and automating many components of traditional power systems. Alongside this continually-evolving network of inter-working parts, new high-resolution monitoring tools and methods are being developed to increase observability and controllability further. However, these newer interconnected systems give rise to new classes of signatures in addition to existing known disturbances caused by natural events such as storms, improper vegetation management, and animals. Therefore, this study proposes a novel spectral correlation function (SCF)-based method for the detection and characterization of grid-signal distortions. In particular, the adaptive envelope detector-based phase fault detection method is developed for the identification and extraction of transient signals, and a novel SCF-based feature extraction method is proposed to obtain the characterization of grid-signal distortions. Our approach differs from existing treatments of signal distortion in its analysis of the varied spectral content of signals observed in real-world scenarios. The method we propose has state-of-the-art discriminative power that provides meaningful and understandable characterizations of various grid events and anomalies. To validate the approach, we use real-world data from the Grid Event Signature Library, which is maintained jointly by the DOE/Oak Ridge National Laboratory and Lawrence Livermore National Laboratory.

Comparison of Analysis Approaches for Time Series Sensor Data

Elizabeth Piersall

Electrification and Energy Infrastructures Division, Oak Ridge National Laboratory

The selection of sensors involves tradeoffs between aspects of functionality, such as between the price and quality of the equipment and the accuracy of the data collected. The choice of higher quality, more expensive sensors may limit how many can be purchased, resulting in less data available for analysis. By contrast, if more data is available, how well can that extra information compensate for some reduction in the quality of the individual measurements? The goal of this project is to take measurements of the same time-series signal with multiple, relatively low-quality sensors, and evaluate if the data can be combined for improved results. Approaches for data fusion include correlation and statistical comparison to discern consistent events measured across separate devices, and machine learning approaches for classification and prediction of events from the correlated data.

Lithium Morphology Evolution Through Crosslinked Poly(ethylene oxide) Solid Polymer Electrolyte

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Solid-state, lithium metal batteries are promising candidates for developing the safe, energy- dense devices needed to transition to an electrified economy. However, lithium is highly reactive, making it

thermodynamically unstable with many electrolyte materials. Achieving uniform Li plating and stripping during cycling is the key for enabling high energy Li metal batteries, however, the mechanism is not well understood in solid polymer electrolytes.

In this work, we investigate lithium morphology evolution through a solid polymer electrolyte at different stages of battery cycling. Crosslinked poly(ethylene oxide) (xPEO) solid polymer electrolyte is used as a model electrolyte and full cells using single crystal LiNi0.6Mn0.2Co0.2O2 (NMC622) cathode, dry xPEO electrolyte, and lithium from two commercial sources are assembled. Our results show that different lithium sources lead to different Coulombic efficiencies and capacity fade rate of the full cells assembled. The lithium morphology evolution at different stages of cycling is examined using scanning electron microscopy and the lithium plating/stripping mechanism are compared between the two anodes. Furthermore, the lithium morphology is compared to a gel polymer composite electrolyte with the same host polymer (xPEO). A better understanding of the roles of each of these components is essential to control for uniform lithium stripping and plating.

Analysis of Power and Momentum Transport and Removal in Spherical Tokamaks Using SOLPS-ITER

I. Paradela Perez,[1,*] J. D. Lore,[1] MAST-U team,[2] ST-40 team[3]

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In this work, SOLPS-ITER simulations of MAST-U with three different mag- netic geometries (Conventional, Elongated, and Super X configurations) and of ST-40 have been used to study the underlying physics of power and momentum transport and removal in spherical tokamaks. An extensive understanding of power and momentum transport and removal within the Scrape-Off Layer is fundamental for the successful operation of future fusion devices. Spherical tokamaks present unique challenges and opportunities in this area. The ex- haust problem is exacerbated due to their more compact sizes, while devices such as MAST-U provide access to advanced divertor configurations such as the super-X.

The simulations have been carried out using the standard version of SOLPS- ITER (3.0.8), as well as the new numerical schemes: 9-point stencil (3.1.0) and the unstructured, Wide Grid (3.2.0). These new versions incorporate improved numerical schemes and enable additional physics studies. Specifically, the 9- point stencil has been shown to improve the performance of the fluid neutral model in SOLPS and, in some cases, result in a modified plasma solution in the divertor region. The wide grid version of the code allows for calculation of the power and particle deposition distribution onto the different plasma facing com- ponents of the divertors and the main chamber walls and eliminates boundary conditions that are difficult to constrain.

A set of simulations consisting of density and power scans, high field side vs low field side gas puff locations, and multiple plasma currents and toroidal fields will be presented. Comparisons to upstream and downstream experimental measurements will be shown.

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Design of Future Batteries: Insights from Molecular Simulations

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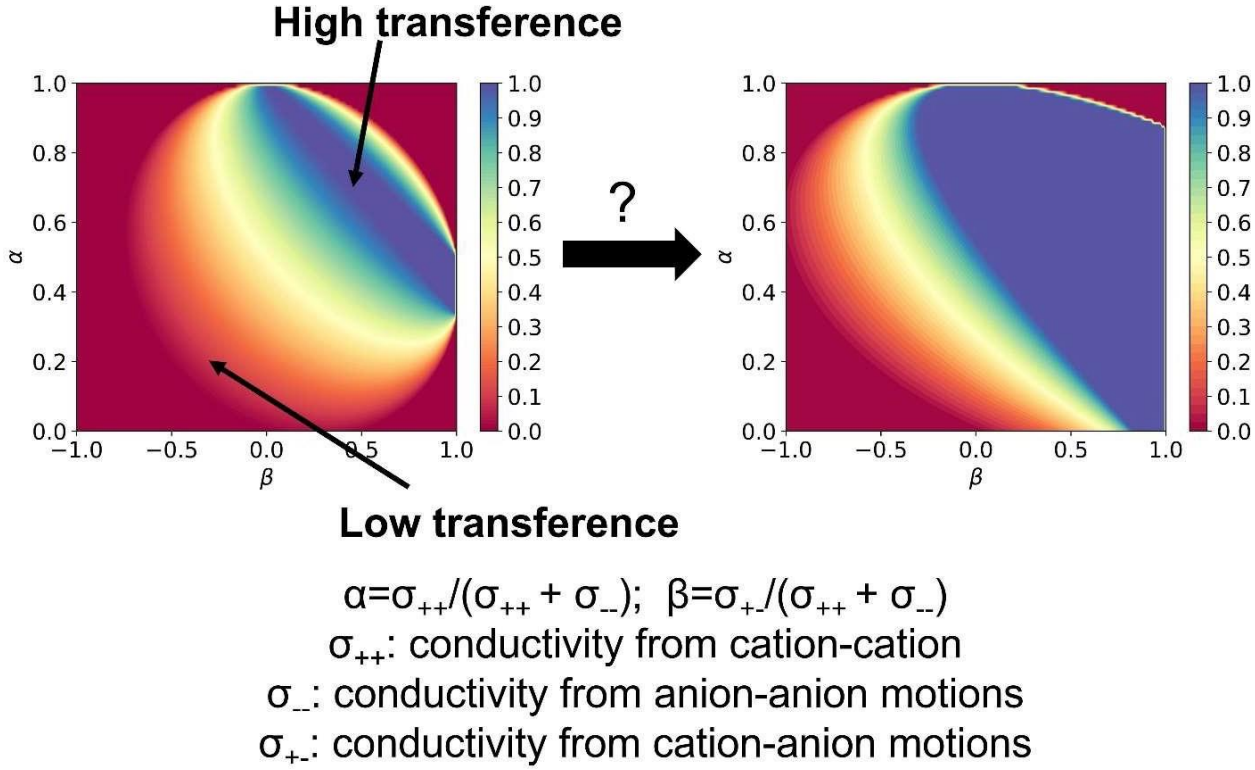
Design of next-generation lithium-ion, lithium-metal and multi-valent batteries have become one of the most widespread research interests among the scientific communities. The reliance of molecular- level insights, either from high-throughput experiments or high-resolution simulation models, has become more significant and critical. In this study, the simulations of battery materials using polarizable force field have been conducted for the research of ionic transport, local self-assembly and electrochemical reactions under the conditions of constant electric potentials. The influence of the constraints due to realistic battery operation conditions is also studied and compared with multi-valent counterpart, i.e. Mg2+ and Zn2+. New definitions for ion transference have been proposed and compared for verifications.



$\alpha=\sigma_{++}/(\sigma_{++}+\sigma_{--})$; $\beta=\sigma_{+-}/(\sigma_{++}+\sigma_{--})$

σ_{++}: conductivity from cation-cation

σ_{--}: conductivity from anion-anion motions

σ_{+-}: conductivity from cation-anion motions

Microchannel Plates with Quad Timepix3 Readout (MCP/TPX3) Detector for High Spatial-Resolution Neutron Imaging with Time-of-Flight Capability

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Microchannel plates (MCPs) coupled to quad Timepix3 readout have emerged as a promising neutron imaging camera for neutron imaging with time-of-flight (ToF) capability. A microchannel plate consists of millions of ultra-thin conductive glass capillaries that act as independent secondary electron multipliers. To make it neutron sensitive, the glass mixture of an MCP is doped with neutron absorbers with very high neutron capture cross-section such as ^{10}B and ^{157}Gd. The signal multiplication of a neutron interaction is spatially constrained to a single MCP pore (several pores in case of several MCPs stacked for higher gain), allowing event encoding with high spatial resolution. The Timepix3 readout is triggerless event-by-event data driven and zero-suppressed readout. The readout chip has 256×256 pixels, and each pixel size is 55×55 μm^2. It can record the time-of-arrival (ToA) and time-over-threshold (ToT) information of every hit in a pixel simultaneously, up to 80Mhits/s per chip. The timestamping of each hit enables the detector to do ToF measurements, suitable for ToF experiments in a pulse source. In this work, we present a neutron imaging camera capable of ToF imaging with a sub-55 μm spatial resolution.

Raman Spectroscopic Investigations of Uranyl Phosphates and Arsenates

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Uranyl phosphates and uranyl arsenates constitute about 32% of known uranyl minerals and are of particular interest because of their low solubility in the environment. These materials have implications for the fate and transport of hexavalent uranium and the overall understanding of mobility of uranium in contaminated sites. Uranyl phosphates and arsenates have not been sufficiently studied using vibrational spectroscopy, especially Raman spectroscopy, as only a fraction of each class has an easily accessible spectrum. We report additional Raman spectra for uranyl phosphates and uranyl arsenates, as well as an improved average spectra for each class.

This work investigates and relates discernable spectroscopic features to structural motifs, topology, and charge-balancing cations to gain a better fingerprint for these materials.

Session: Material Science and Physical Science

Eco-Friendly and Anti-Wear Ionic Liquids Additives in Marine Turbomachinery Lubricants

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Tidal energy, capable of generating clean and sustainable electricity through specially designed generators (e.g., turbomachinery), is a promising source of the renewable energy portfolio. The conventional lubricants currently used in marine turbomachinery are toxic and exhibit low biodegradability, potentially resulting in a serious threat to marine ecosystems in the case of a leak or spill. Therefore, it is crucial to develop an environmentally acceptable lubricants (EALs) with high performance in wear protection. Recently, eco-friendly, high-lubricity ionic liquids (ILs) have been successfully invented at Oak Ridge National Laboratory and being further developed for tidal turbine gearbox lubrication. In this work, tribology behaviors of a series of candidate lubricants with and without ILs were evaluated using a rolling-sliding test through simulating the actual operating conditions in marine turbomachinery. Compared with the commercial baselines, the IL-additized lubricants performed more effectively in mitigating the friction, rolling contact fatigue and wear loss. The wear modes and ILs' surface protection mechanisms were discussed with the assistance of surface and tribofilm characterization. In addition to the excellent lubricating performance, aquatic toxicity and biodegradability testing results suggest that the IL-additized lubricants can be classified as 'not toxic' and 'readily biodegradable'.

Nanoscale Interrogation of Metallic Nuclear Materials: Atomic Force Microscopy and Magnetic Force Microscopy

Jenn Neu

Nuclear Nonproliferation Division, Oak Ridge National Laboratory

Relationships linking chemical and physical material properties with formation conditions is the scientific basis for nuclear nonproliferation materials analysis. Metallic nuclear materials present unique challenges for physical property measurement, specifically their unsuitability for optical spectroscopy. In this work, we deploy a new measurement modality, atomic force microscopy/magnetic force microscopy (AFM/MFM), for the analysis of uranium steel alloys. We show that surface topography, relative hardness, and magnetic properties of the constituent phases can be separated using AFM/MFM. In addition to finding two novel uranium-transition metal (M=Fe, Cr, Ni) intermetallic phases, differences in surface oxide topography for four distinct UMx phases are characterized, and changes in ferromagnetic-steel fraction as a function of uranium content is described. These physical properties could be used to discern material formation history, cooling rates, or other pertinent nonproliferation process parameters.

Investigation of Nanoparticle Degradation in Hydrogen Fuel Cell Systems through Automated Electron Microscopy

Lynda Amichi

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Proton exchange membrane fuel cells (PEMFC) are promising devices for the deployment of hydrogen-powered heavy-duty vehicles, providing a higher efficiency and similar driving range and fueling time compared to internal combustion engine vehicles. However, PEMFCs still encounter durability challenges, mainly due to catalyst degradation in the cathode. Mitigating these performance losses requires a better understanding of the degradation mechanisms under heavy- duty accelerated stress tests. Scanning transmission electron microscopy (STEM) combined with energy dispersive X-ray spectroscopy (EDS) is a key tool for analysis of catalysts nanoparticle size, spatial distribution, and composition. In addition, electron tomography can be used to determine the rate of catalyst nanoparticle degradation as a function of position on the carbon support.

We have used electron tomography to distinguish between nanoparticles residing on the carbon support surface (exterior) and within the pore structure (interior) to determine their relative stability. We compared the catalyst particle size distribution at the beginning of test and end of test. This shows the importance of the electron tomography workflow, i.e., acquisition, reconstruction, and visualization, to increase sampling and determine the standard deviation of measurements. Utilizing low-dose cryo-tomography for limiting damage to the catalyst, support, and especially proton-conducting ionomer will be investigated.

Multiscale Computational Modeling for Predicting Mechanical Behavior of Binder Jet 3D-Printed Structures

Yawei Gao

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Binder jet 3D printing (BJ3DP) is a rapid and cost-effective additive manufacturing technique involving both inorganic metals and organic polymers/molecules. Despite its vast applicability, achieving a high density in the 3D-printed structure via BJ3DP remains elusive due to various challenges (e.g., incomplete binder penetration, its quality, and improper post-processing, among many). Low density in the 3D-printed structures could affect their integrity and durability, resulting in premature failure. To prevent such failures, the use of a computational framework for predicting the mechanical behavior of 3D-printed binder jet structures could be beneficial. The continuum-based finite element analysis has been utilized, requiring input material properties obtained from experiments that can be arduous, time-consuming, and expensive. This work aims to bridge this gap via multiscale computational modeling. We have developed and implemented a molecular-level reactive molecular dynamics (MD) model to estimate the material property evolution by studying the underlying physical and chemical mechanism involved in BJ3DP. Furthermore, the derived material properties are used in the finite element modeling for the binder jet-printed structures failure analysis. Moreover, the collaboration with material characterization techniques such as X-ray photoelectron spectroscopy and scanning electron microscopy imaging will be discussed. Such collaborations can validate the reliability of our proposed multiscale modeling framework and quantify the propagation of uncertainties from the nanoscale to the macroscale. Our proposed framework has the potential to revolutionize the design and manufacturing of high-density binder jet-printed structures,

offering an efficient and cost-effective alternative to traditional experimental methods while improving the durability and reliability of the additively manufactured structures.

Magnetothermal transport in the kagome van der Waals compound Pd3P2S8

Eleanor Clements, Heda Zhang, Andrew May, Michael McGuire

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In crystalline materials with certain characteristic lattice geometries (such as the kagome, Lieb, and bipartite lattices) interference of electronic wavefunctions can lead to a quenching of kinetic energy, resulting in dispersionless bands with a high density of states. These flat topological electronic bands can lead to strong electron-electron interactions and have the potential to drive emergent magnetic and electronic states, such as unconventional superconductivity observed in twisted bilayer graphene, particularly if the bands are close to the Fermi level (E_F).

$Pd_3P_2S_8$ is a layered van der Waals compound with an ideal Kagome net of Pd^{2+} ions, where interference effects lead to a flat band just below E_F, a concomitant peak in the density of states, and a Dirac like dispersion in the Brillouin zone. Because of its semiconducting nature, the flat bands are relatively isolated and band mixing is avoided. Here, we present recent single crystal growth, magnetic and thermodynamic characterization, and transport results in $Pd_3P_2S_8$. We have performed thermal transport measurements on cleaved samples in the presence of a magnetic field. Our results reveal an intriguing thermal magnetoresistance and thermal Hall effect. As the compound does not order magnetically and has a relatively large band gap, this effect is rather surprising. We will discuss these results considering possible mechanisms, including a phonon thermal Hall effect observed in a short list of materials.

Session: Other

Innovative Family of Guanidium-Based Aqueous Complexants for Technetium Management

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Technetium (Tc) is one of the harmful fission products developed during the reprocessing of spent nuclear fuel. Due to the long-term radiotoxicity of ^{99}Tc ($t_{1/2} = 2.1 \times 10^5$ years), and high solubility of TcO_4^- in water, it poses harm to the environment and human health. To mitigate this problem, Tc must be isolated from spent nuclear fuel. The proposed Tc management strategies utilize exchange resins and/or lipophilic host molecules. Hereby, we have designing novel aqueous complexants that are simple yet functional and show extraordinarily high affinity for TcO_4^- even in the presence of excess NO_3^-, offering simple solution to Tc management in aqueous environments. This talk will cover various fascinating findings from research conducted on guanidium-based complexants, including the development of more advanced structures that offer improved solubility and greater affinity.

Audio-Based Lossy Compression of Power Line Signals

Layla Marshall

Enrichment Science and Engineering Division, Oak Ridge National Laboratory

The Multi-Informatics for Nuclear Operations Scenarios (MINOS) project collects data from a variety of sources including infrared, electromagnetic, and acoustic sensors to characterize a research nuclear reactor located at the Oak Ridge National Laboratory (ORNL). Currently, electromagnetic data are sampled and collected using a low-cost audio analog-to-digital converter at 96 kHz with 24-bit resolution, which produces approximately 4 terabytes of data per month per system.

This poster will explore the benefits and shortcomings of using standard audio compression algorithms to reduce the storage size of the raw data. Certain frequency bands and features are of particular interest to the project, including power line harmonics and transients potentially associated with reactor events. The intent is to determine whether standard lossy audio compression methods will preserve the data of interest by analyzing two standard lossy audio compression methods, identifying metrics for determining their usability for this application, and applying the compression methods to previously collected raw electromagnetic data.

This work satisfied the capstone paper requirement for the author's Master of Engineering in Acoustics degree from the Pennsylvania State University, completed in May 2022.

From Local Chemistry to the Macrostructure: Characterization of Emerging Materials for the Separation and Extraction of Rare Earth Elements

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The need for high-purity rare earth elements (REEs) has been an emerging trend, vital for a variety of energy and nation security applications and typically difficult to separate efficiently. We have developed a series of 2,9-bis-lactam-1,10-phenanthroline (BLPhen) ligands that exhibit high selectivity for the extraction of adjacent, light lanthanides by exploiting a unique binding pocket that allows the larger ionic size of the light lanthanides to easily bind relative to heavier lanthanides. We combine element-specific X-ray absorption spectroscopy, X-ray and light scattering with electron microscopy to describe the extraction environment ranging from the atomic structure to the macroscale as we develop a more complete picture of these Ln^{3+}–ligand aggregates. Finally, we have developed trends in solvation and binding across the full Ln series, including Pm, to describe the coordination environment and the first shell bond contraction.

Understanding CO_2 Release and Regenera0on Mechanism of Methyl-glyoxal-bis- imminoguanidine (MGBIG) Linkers

Debmalya Ray, Jeffrey Einkauf, Bryantsev Vyacheslav, Radu Custelcean

Chemical Sciences Division, Oak Ridge National Laboratory

Direct air capture (DAC) of CO2 is of extreme importance. It is important to understand the energy needed for the CO2 capture as well as the regenera0on of the linkers used when CO2 is released for the crystal structure. In this work, we explored different phases of MGBIG linkers and showed how the protona0on state as well as presence of crystalline water affects the energy needed for the CO2 release and regenera0on of the MGBIG linker. Our study shows, removal of crystalline waters plays a crucial role in the process of MGBIG regenera0on. We believe this study will motivate future studies of designing new BIG linkers that can be crystallized with less water.

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