13TH ANNUAL
OAK RIDGE POSTDOCTORAL ASSOCIATION
RESEARCH SYMPOSIUM

JULY 17–18, 2025

TENNESSEE ROOMS

OAK RIDGE National Laboratory

U.S. DEPARTMENT of ENERGY | Office of Science

Foreword by the Laboratory Director

Welcome to the 13th Annual Oak Ridge Postdoctoral Association (ORPA) Research Symposium! Each year, ORPA brings together the ORNL community to showcase the transformative research happening at the lab, which is enriched by the innovative ideas and energetic contributions of our postdocs.

Regardless of whether our postdocs continue a career with the national labs or pursue paths in academia or industry, I value the research contributions they bring to ORNL during their time with us. Our goal is to not only set our postdocs on a successful career trajectory but to help them identify the research questions that will fuel long and fulfilling careers.

I'm pleased to announce that this year's first keynote address will be delivered by Dr. Troy Carter, Fusion Energy Division Director. Fusion energy has been a cornerstone of ORNL's mission for almost 70 years, and the technology holds great potential for powering humanity's increasing energy demands as well as our own future scientific endeavors.

I'm also excited to see the full docket of keynote speakers includes Environmental Sciences Division Director Eric Pierce, AI Programs Director Prasanna Balaprakash, and nuclear physicist Kelly Chipps. Their insights into ORNL research in environmental sciences, artificial intelligence for science, and nuclear astrophysics will be highly beneficial to the discussions taking place during this year's Research Symposium.

I envision our postdocs making lasting contributions in various disciplines on the cusp of technological revolutions, including AI, quantum science and technology, advanced manufacturing, biotechnology, and beyond.

Thank you to our contributors for sharing your invaluable research and to our staff and attendees for fostering a vibrant research environment where we can share insights, make connections, and pursue bold ideas. I look forward to an illuminating experience!

Dr. Stephen Streiffer
Laboratory Director

Foreword by the Office of Research Director

I'm pleased to welcome you to ORNL's 13th annual Oak Ridge Postdoctoral Association (ORPA) Research Symposium! The ORPA Executive Committee (ORPEX) has curated an exceptional program that provides a platform for sharing groundbreaking research and engaging with the work of your peers. It's inspiring to see such a diverse array of presentations and posters featured this year—a testament to both ORPEX's commitment to delivering a dynamic scientific agenda and your dedication to advancing discovery.

This year, we are honored to welcome four distinguished keynote speakers who will share their insights and experiences, offering valuable perspectives across a range of research topics. These speakers are all senior research staff and lab leaders. Please take the time to attend their talks to hear about their research career paths and how they have contributed to ORNL science over the course of their careers.

I extend my heartfelt gratitude to ORPA's Research Committee chairs, Parul Raghuvanshi and Nikki Zou, and to Laurie Varma from the Office of Research Education (ORE) for their meticulous organizing efforts. I also thank all our postdoc and postdoc ally volunteers who have worked diligently to bring this program to life, as well as the ORNL staff members who are generously serving as judges.

ORPA and ORPEX play a pivotal role in nurturing a vibrant scientific community at ORNL. Their efforts include welcoming new postdocs, providing essential resources, fostering community through social events, promoting volunteer opportunities, and supporting career development through programs like the annual ORPA Research Symposium. Highlights this year include *R U Feeling OK?*, the *Your Science in a Nutshell* competition, and *Postdoc Appreciation Week*. ORE and ORPA also continue to collaborate to bring industry to ORNL events—connecting postdocs with career opportunities and showcasing their talents to external partners.

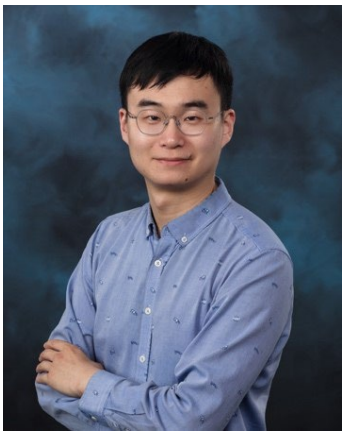
This year, ORPEX is further strengthening connections with postdoc associations at other national laboratories and at ORNL's Core Universities. These efforts will expand collaboration and programmatic success across institutions. ORPA's sustained leadership helps maintain ORNL's reputation as a premier destination for postdoctoral research—where emerging leaders thrive and forge professional relationships that transcend disciplinary boundaries. The excellence of ORNL's postdoc experience is a key contributor to our standing as a global research leader.

I look forward to the insights and discoveries you will share at this year's symposium and to the new connections you will form as we celebrate postdoctoral research at ORNL.

Best wishes,

Moody Altamimi

Foreword by the 2025 ORPA President



On behalf of the Oak Ridge Postdoctoral Association (ORPA), I feel honored to welcome you to the 13th Annual ORPA Research Symposium. As our postdoctoral community grows, ORPA becomes more important in facilitating career development, improving well-being, and enhancing the research experience for postdocs.

The Research Symposium, being one of the major events organized by ORPA, provides a great opportunity for postdocs and early career researchers to showcase impactful research, learn from field experts, discuss with knowledgeable peers, and explore potential collaborations.

This collaborative spirit is at the heart of ORPA's mission. We actively partner with ORNL leadership to champion our postdoctoral researchers' professional and social development. With the addition of the Sponsorship Chair to the FY25 Executive Committee (ORPEX), the symposium continues ORPA's efforts to actively engage with industry partners. Further tightening of the relationship with our potential sponsors allows the postdocs to gain valuable insights into the industry and academia landscapes.

This year's symposium aligns perfectly with the priorities of DOE Office of Science, featuring keynote speakers from artificial intelligence and fusion energy. Through this abundant two-day symposium with oral and poster presentations, lunch-and-learn and networking opportunities, we believe the energetic research environment here at ORNL can be further extended.

The success of this symposium would not be possible without the guidance and support of Dr. Moody Altamimi, Office of Research Education (ORE) director, and Laurie Varma, Early Career Programs Specialist in ORE. Their dedication to ORPA and commitment to our postdoctoral researchers' professional development are invaluable. Last but not least, ORPEX wishes to thank all the postdoc volunteers for their time and effort in helping us organize this event.

Thank you for your participation in the 13th Annual ORPA Research Symposium, and we truly appreciate your attendance and support.

Sincerely,
Yuchen Jiang
President, ORPA

Foreword by the 2025 ORPA Research Committee Chairs and Sponsorship Chair

Dear Attendees,

As Research Co-Chairs of the Oak Ridge Postdoctoral Association (ORPA), we are excited to welcome you to the **13th Annual ORPA Research Symposium**!

Now in its 13th year, this symposium continues ORPA's tradition of supporting the professional growth, collaboration, and visibility of postdoctoral researchers at ORNL. Each year, we aim to provide a dynamic platform for postdocs and early-career researchers, and students to share their work, exchange ideas, and build lasting connections — and this year, we're taking things up a notch.

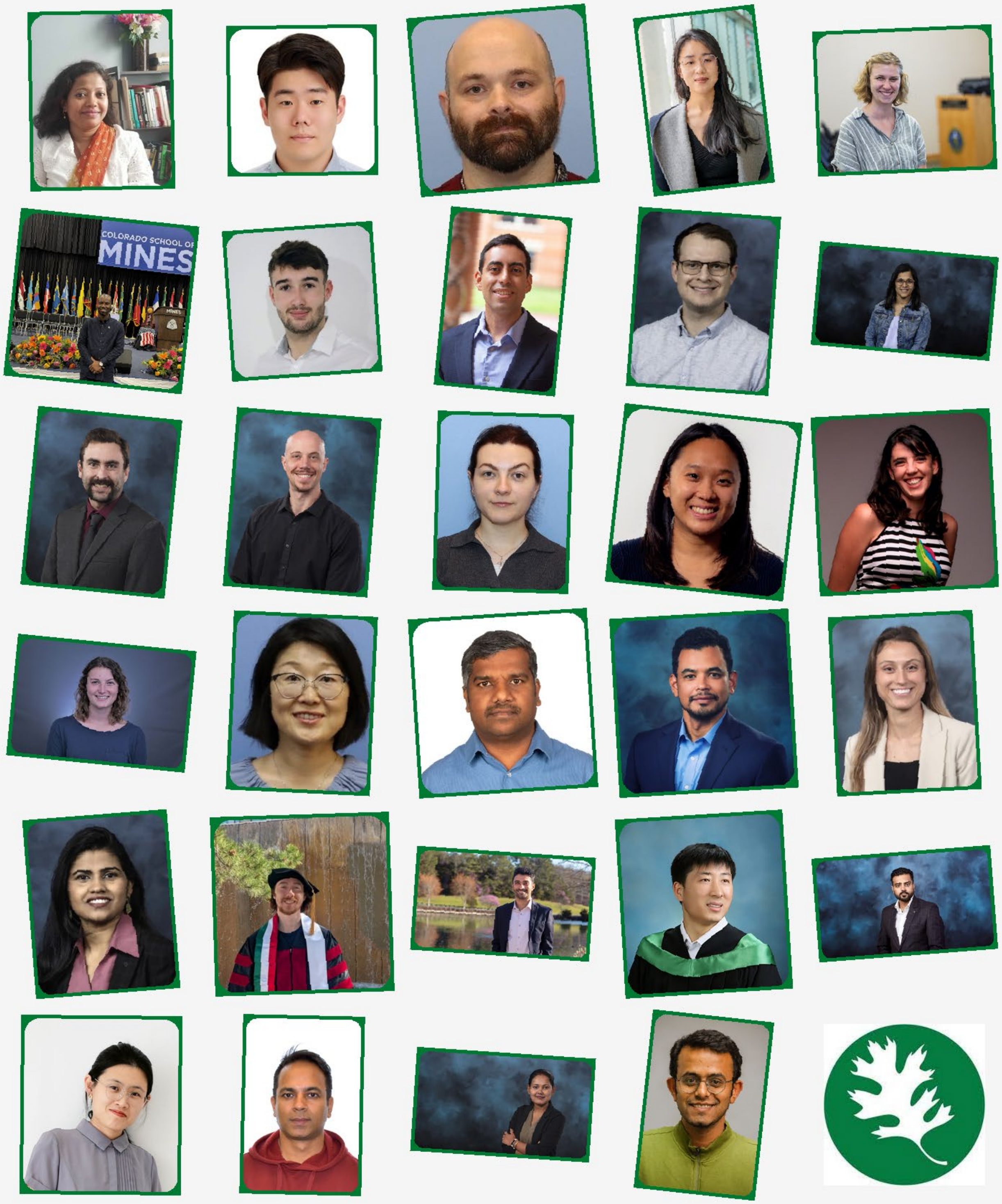
Our goal for this year's symposium is to make it more **lively, interactive, and engaging**. In addition to our traditional oral and poster presentations, we've included new and enhanced opportunities for networking, collaboration, and creative exchange. We're pleased to have Endeavor Composites with us for a presentation on Thursday. They'll be with us both days so be sure to stop by their table in the TN Rooms lobby. We want this to be more than just a scientific gathering — we want it to feel like a celebration of the talent, energy, and potential within our postdoc community.

We'd like to extend our sincere thanks to our keynote speakers and Dr. William Jenks, Dr. Moody Altamimi, Director of the Office of Research Education (ORE), and Laurie Varma, Early Career Programs Specialist, for their ongoing support and dedication to the postdoc community.

Thank you for being part of this year's event. We can't wait to see the ideas, conversations, and energy that come out of the 13th ORPA Research Symposium!

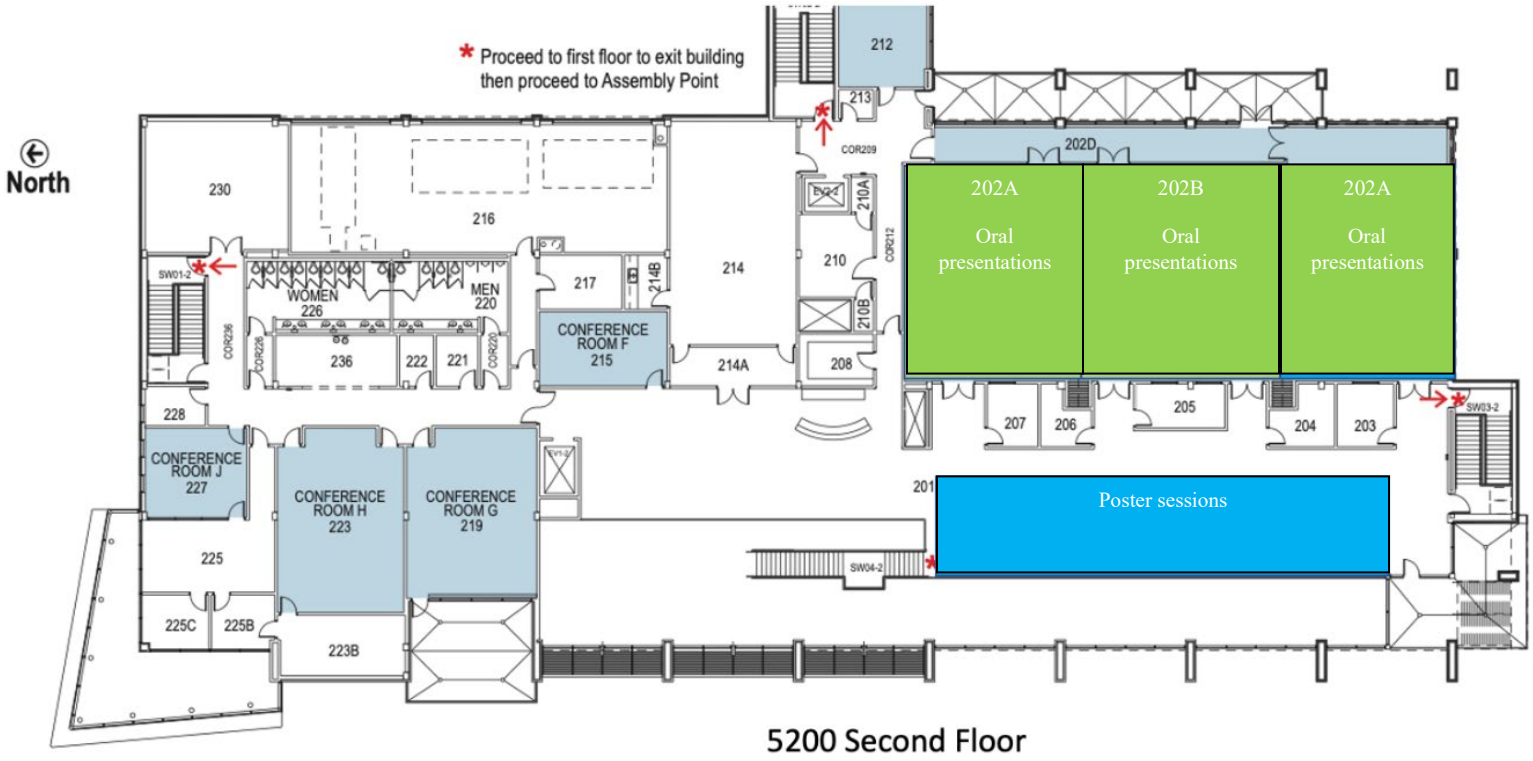
Warmest regards,
Rongge Zou & Parul Raghuvanshi
Research Co-Chairs, ORPA

Thank You, Volunteers!



Oak Ridge Postdoctoral Association 12th Annual Research Symposium Agenda

ORNL Conference Center, Building 5200, Tennessee Rooms (A, B, and C) and 2nd Floor Lobby



Thanks to our sponsors!

ENDEAVOR COMPOSITES

13th Annual ORPA Research Symposium

July 17, 2025 (Day – 1)			
09:00 – 09:10	Rooms 202ABC Tennessee Rooms Conference Center Building: 5200	**Paul Langan** Associate Laboratory Director, Biological and Environmental Systems Science Directorate ALD	Welcome Remarks
09:10 – 09:30	Rooms 202ABC	**Parul Raghuvanshi** and **Rongge/Nikki Zou**	Research Symposium Announcements
09:30 – 10:15	Rooms 202ABC	**Troy Carter** Division Director, Fusion Energy Division	*Keynote 1:* Overview of a career in plasma and fusion science
10:15 – 10:30	Break		
	Oral Session 1 (Materials Science - 1 Room 202A	**Oral Session 2 (Building & Transportation) Room 202B**	**Oral Session 3 (Chemistry - 1) Room 202C**
10:30 – 10:45	**Bogdan Dryzhakov** *Direct-write ferroelectricity in AlN*	**Ajibola Lawal** *Catalytic Conversion of Captured Monoterpenes to Sustainable Aviation Fuel*	**Charini Maladeniya** *Light-induced crosslinking of ultrathin polyzwitterionic coatings for anti-fouling performance*
10:45 – 11:00	**Shaofei Wang** *Investigation of Phonon Density of States in ZrN via DFT and Inelastic Neutron Scattering*	**Md Masudur Rahman** *Impact of H2 and alcohol on N2O formation on commercial emissions control catalysts*	**Surya Mitra Ayalasomayajula** *Physics-based modeling of current imbalance and aging in lithium-ion battery modules*
11:00 – 11:15	**Simon Kim** *Measuring Depth Scaled Magnetism in Helium-Implanted PdCoO2 using Muon Spin Resonance Spectroscopy.*	**Deepika Patel** *State-of-the-art microgrid protection: An imbalance squared factor based fault detection, classification and relay coordination scheme*	**Hunter Jacobs** *Role of binder selection during formulation of dealuminated beta zeolite extruded catalysts for ethanol upgrading to olefins*
11:15 – 11:30	**Parul Raghuvanshi** *Stability, magnetism, and vibrations in MnTexSbyBi1-x-y alloys*	No speaker	**Abishek Kasturi** *CO2 Capture from Flue Gas Using Aqueous Amino Acid Salts and Mineralization into Cementitious Materials*

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11:30 – 11:45	No speaker	No speaker	**Yifan Liu** *Data-Driven Discovery of Non-Aqueous Proton Conductors for Polymer Electrolytes with Small Dataset*
11:45 – 12:05	Rooms 202ABC	Endeavor Composites Company Overview Hicham Ghossein, CEO, Endeavor Composites; Matthew Sausen and Peter Shpik	
12:05 – 12:30	Rooms 202ABC	**Working lunch:** **ORPA Board Introduction and Outlook** **(short presentation, panel with Q&A)**	

	Oral Session 4 **(Biology Science -1)** **Room 202A**	**Oral Session 5** **(AI / ML - 1)** **Room 202B**	**Oral Session 6** **(Nuclear Science - 1)** **Room 202C**
12:30 - 12:45	**He Liyuan** *Applying a genomics-informed carbon cycling model to long-term soil warming*	**Sahil Tyagi** *Enabling Large-Batch AI Training via Learned Gradient Mapping*	**Harisree Krishnamoorthy** *Results from LEGEND-200 experiment in search for neutrinoless double beta decay*
12:45 – 13:00	**Elise Phillips** *Multilayered regulation by RNA thermometers enables precise control of Cas9 expression*	**Debvrat Varshney** *Generative AI for Landcover Forecasting*	**Yuchen Jiang** *Integrated modeling of MHD flow, heat transfer, and solid mechanics for fusion reactor applications*
13:00 – 13:15	**Andrew Deas** *An Agent-Based Approach for Modeling Air Pollution Exposure at the Individual Level*	**Luis Caicedo Torres** *On Synthetic Data Generation for AI Video Instance Segmentation*	**Jordan Stanberry** *Advanced Applications of MicroExtraction - Single Particle - Inductively Coupled Plasma - Mass Spectrometry*
13:15 – 13:30	**Jinping Xue** *Mercury removal from aqueous solutions by novel sorbents: Influencing factors and potential implications*	**Anna Vlot** *The MENTOR interpretation agent: From network embeddings to mechanistic narratives via retrieval-augmented LLMs*	**Jayasai Rajagopal** *Time-resolved dosimetry for alpha- and beta-emitters in radiopharmaceutical therapy: an in silico comparison*
13:30 – 13:45	**Celestin Bourgery** *Discovery, characterization and engineering of substrate- and product-selective nylon hydrolases for nylon recycling*	**Chao Lu** *Practical Scalability of LuGo: Benchmarking the HHL Algorithm Using an Enhanced QPE Algorithm*	**Samuel Fagbemi** *Pore-resolved Simulations of Electro-Thermal Processes for Alkane Dehydrogenation in Graphite Reactors*

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13:45 – 14:00	No speaker	No speaker	**Daniel Suarez** *A natural circulation breeding blanket*

14:00 – 16:00	Lobby	Poster Session - 1	
16:00 – 16:15	Break		
16:15 – 17:00	Rooms 202 ABC	**Eric Pierce** Division Director, Environmental Sciences Division	*Keynote 2:* Navigating a Career in Environmental Science: A Path to Leadership at ORNL
17:00	Closing Remarks/ADJOURN **Moody Altamimi,** Director, Office of Research Education		

July 18, 2025 (Day – 2)			
09:00 – 09:10	Rooms 202ABC	**Peter Thornton,** Corporate Fellow, Earth Systems Science Section Head, and Postdoctoral Engagement Committee co-chair	Welcome Remarks
09:10 – 09:30	Rooms 202ABC	**Parul Raghuvanshi** and **Rongge/Nikki Zou**	Research Symposium Announcements
09:30 – 10:15	Rooms 202ABC	**Prasanna Balaprakash** Director of AI Programs and Data and AI Systems Section Head	*Keynote 3*: AI for Science: A Tectonic Shift Underway—Are We Ready for What's Next?
10:15 – 10:30	Break		

	Oral Session 7 (Chemistry - 2) Room 202A	**Oral Session 8 (Material Sciences - 2) Room 202B**	**Oral Session 9 (Biology Sciences - 2) Room 202C**
10:30 – 10:45	**Jane Agwara** *Functionalized porous polymer-based catalysts for CO2 conversion to formic acid*	**Ryan (Jeongkeun) Song** *Strain-engineering in correlated oxide quantum heterostructures*	**Stephen Zambrzycki** *Enhancing Single-Cell Mass Spectrometry: Comparing Liquid Vortex Capture and the Rapid Droplet Sampling Interface*

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10:45 – 11:00	**Arvind Ganesan** *Aqueous Porous Liquids for Gas Separations, Transport and Conversion*	**Deb Mallick** *Focused Si++ ion irradiated nanometer sculpting and vortex pinning in a topological superconductor heterostructure FeTe0.75Se0.25/Bi2Te3*	**Shane Franklin** *Controlling Matric Potential In Microfluidics To Examine Microbial Dynamics In Unsaturated Porous Media*
11:00 – 11:15	**Nicholas Gregorich** *Utilizing Mining and Battery Recycling Waste for Marine Carbon Dioxide Capture via Ocean Alkalinity Enhancement*	**Ciril Samuel Prasad** *Nanofabrication and integration of Quantum Spin Liquid materials into test structures and devices.*	**Dileep Kishore** *Improving the prediction and interpretability of microbial nutrient utilization phenotypes*
11:15 – 11:30	**Noor Md Shahriar Khan** *Catalytic Role of Methanol in Anodic Coupling Reactions Involving Alcohol Trapping of Cation Radicals*	**Gyan Shankar NLN** *Effect of precipitates formation and oxide particle on the grain boundary mobility assisted recrystallization in SS 316H alloy processed by L-PBF*	**John Vant** *Predicting membrane permeability using realistic mammalian bilayers and LipidLure: a steered molecular dynamics pipeline*
11:30 – 11:45	**Xin Wang** *Uncovering the phase transition mechanism in upcycling of spent NMC cathodes with in-situ neutron diffraction*	No speaker	**Yu Ma** *Cost efficiency of US hydropower plants: A Stochastic Frontier Analysis*
11:45 – 12:00	**Alexander Wiechert** *Biphasic Solvents for Energy Efficient CO2 Capture from Natural Gas and Coal Flue Gas Streams*	No speaker	No speaker

12:00 – 12:30	Rooms 202ABC	**Working lunch:** **Academic Career Path** Speaker: William Jenks, Core University Student Programs Lead, Office of Research Education	
12:30 – 13:15	Rooms 202ABC	**Kelly Chipps** Nuclear physicist, Physics Division	*Keynote 4:* Nuclear Astrophysics in the Next Decade

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	Oral Session 10 (AI / ML - 2) Room 202A	Oral Session 11 (Manufacturing) Room 202B	Oral Session 12 (Nuclear Science - 2) Room 202C
13:15 - 13:30	**Viktoriia Baibakova** *Optimization of rare earth elements recovery with large language models*	**Pavan Ajjarapu** *Macro- and Micro-scale Evolution of SS 316L Powders Hot Isostatically Pressed (HIPed) at Intermittent Temperatures and Pressures*	**Soyoung Kang** *Characterization of irradiated Inconel 718 using in-situ SEM-EBSD analysis*
13:30 – 13:45	**Emily Herron** *HARMONY: Evolutionary Design of Efficient Hybrid Transformer-Mamba-MoE Language Models Through Large-Scale Architecture Search*	**Subhabrata Saha** *Development of vinyl ester resin for unsupported direct-ink-write horizontal printing*	**Shaileyee Bhattacharya** *Understanding hydrogen retention behavior through revealing local phase fraction variations in YH2*
13:45 - 14:00	**Nasik Muhammad Nafi** *Generalizing Time-series Modeling of Stably Stratified Turbulence using Parameterized Neural ODE*	**Geeta Kumari** *Microscale Mechanical Insights into AM 316 Stainless Steel Using Nanoindentation*	**Jopaul Mathew** *Maximizing Uranium recovery using monoamide extractants*
14:00 - 14:15	**Ankit Shrivastava** *DIALED into Discovery: Autonomous Active Learning for Nanoscale-Ordered Materials Diffractometer Experiments*	**Ajay Jayswal** *Finite element analysis of additively manufactured textile-inspired braided metamaterials for high specific energy absorption and shape recovery*	**Daniel Felton** *Processing Signatures of Uranium Ore Concentrates*
14:15 - 14:30	**Qixing Wang** *Credit-Based Coordination for Resolving the Tragedy of the Commons in Autonomous Agent Networks*	**Abdul Sayeed Khan** *Additive Manufacturing of Functionally Graded Materials*	**Ryan Chesser** *Molten Salt Thermophysical Properties Measurements and Database*

14:30 – 16:30	Lobby	Poster Session- 2
16:30 – 16:55	Rooms 202 ABC	**Closing Ceremony** Parul Raghuvanshi and Rongge/Nikki Zou
16:55 – 17:00	Rooms 202 ABC	**Closing Remarks** **Moody Altamimi,** Director, Office of Research Education
17:00	ADJOURN	

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POSTER PRESENTATION LISTS

Sl. No.	Presenter	Poster Title
Day 1		
1	Kristyn Ardrey	Examining EBC coating systems on SiC substrates in varying high temperature steam oxidizing environments
2	Delaney Ryan	Investigating size limitations of single particle inductively coupled plasma mass spectrometry in nano and microparticle research
3	Chathurika Kosgallana	Structural Characterization of Chitosan-Immobilized Carbonic Anhydrase with Contrast Variation SANS
4	Christine Cummings	Using process monitoring to identify voids and heat accumulation in laser powder bed fusion additive manufacturing
5	Louis Dagobert	Flow through a U-Bend: Comparing four Turbulence Models with Experimental Results
6	Chandra Sekhar Somayajula	Systems analysis for the development of cost competitive technologies
7	Preeti Sar	A machine learning model for predicting nonlinear 1D saturated potentials from linear gyrokinetic simulation data
8	Pyeongjae Park	Leveraging thermal fluctuations to investigate the spin dynamics of quantum magnets
9	Komal Sharma	One-pot bioconversion of PET plastic using a thermophilic microbe
10	Sarah Szakas	Ablate and Illuminate: High-Resolution Bioimaging with LA-ICP-TOFMS

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Sl. No.	Presenter	Poster Title
		Day 2
11	Wenqi Li	Understanding Wetting Behavior of Graphite by Water Contact Angle Measurement
12	Wenbo Wang	Discrepant impact of CNTs as Additive on Lubricant Tribological Performance
13	Ajay Jayswal	Factors governing thermal transport in carbon fibers reinforced nylon 6 composites for thermal management applications
14	Emily Kurfman	Liquid extraction surface sampling mass spectrometry for detection of adsorbed microbial metabolites across polymer-modified surfaces
15	Matthias Maiterth	Extending ExaDigiT's Resource Allocator and Power Simulator (RAPS) for Scheduling and Synthetic Workload generation
16	Bharath Raghavan	Leveraging Exascale Computing for Scalable Drug Discovery: Integrating Multiscale Simulations and AI-Driven Molecular Design
17	Zachary Windom	Hybrid quantum/classical algorithms for exotic quantum chemistry
18	Mohit Chandra	Temperature-dependent Neutron Diffraction Study of a New Piezoelectric
19	Mallory Morgan	Constitutive and Inducible Oleoresin Defenses Share Genetic Architectures and Mechanisms in Pinus taeda
20	Nabarupa Bhattacharjee	Extraction and stimuli-driven release of superhydrophilic oxyanions using amphiphilic iminoguanidine ligand
21	Latif Patwary	Travel Patterns and Characteristics of Millennial Population in New York State

Oral Session 1: Materials Science 1

1.1 Direct-write ferroelectricity in AlN

Bogdan Dryzhakov[1*], Kyle Kelley[1]

[1] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: dryzhakovb@ornl.gov

Wurtzite Aluminum nitride (w-AlN) has long been established for microelectronic and photonic applications, yet ferroelectricity in any III-V material has only been possible through conventional doping. Here, we demonstrate the ability to induce, localize, and tune this ferroelectric functionality in the w-AlN platform through using direct-write ion-beam processing. This post-growth strategy leverages ion-induced defect engineering as a transformative alternative to conventional doping, achieving defect-driven tunability of ferroelectric, optical, and thermal properties on demand and enabling nanoscale-precision patterning. The evolving signatures of defect states are shown to be predictable with cross-correlative spectroscopic imaging, and structural analysis revealing that defects behave in a highly localized manner within an otherwise crystalline w-AlN framework. The high thermal and mechanical tolerance, robust reprogrammable polar states, and optical transparency open possibilities for extreme-environment memory storage and photonic circuits.

Keywords: ferroelectrics, ion-beam, photonics, aluminum nitride

https://www.linkedin.com/in/bogdan-dryzhakov/

1.2 Investigation of Phonon Density of States in ZrN via DFT and Inelastic Neutron Scattering

Shaofei Wang,[1] Mark A. Mathis,[2] Chris A. Marianetti,[3] J. Matthew Mann,[4] David B. Turner,[5] Douglas L. Abernathy,[6] Raphaël P. Hermann,[1] and Michael E. Manley[1]

[1]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
[2]Computational Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
[3]Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York 10027, USA
[4]Air Force Research Laboratory, Sensors Directorate, Dayton, Ohio 45433, USA
[5]Azimuth Corporation, Fairborn, Ohio 45324, USA
[6]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

*Corresponding author: wangs1@ornl.gov

Zirconium nitride (ZrN) is a promising candidate for applications in extreme environments, such as in advanced nuclear power plants and in ultra-high temperature ceramics, where its phonon thermal conductivity plays a critical role. Understanding the lattice dynamics of ZrN is essential for these applications. In this work, we employ inelastic neutron scattering experiments and density functional theory calculations to investigate the phonon density of states in polycrystalline ZrN. Our results confirm that the maximum phonon energy aligns with previous theoretical predictions (65 meV) while being significantly lower than the value reported in earlier experimental studies (75 meV) by Christensen et al. [1] Our findings address existing controversies and provide a solid benchmark for future theoretical and experimental research. Neutron work supported by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division. This research used resources at the Spallation Neutron Source and High Flux Isotope Reactor, facilities supported by DOE, BES, Scientific User Facilities Division.

[1] A. Christensen, O. Dietrich, W. Kress, and W. Teuchert, Physical Review B 19, 5699 (1979).
[2] S. Wang, M. A. Mathis, C. A. Marianetti, J. M. Mann, D. B. Turner, D. L. Abernathy, R. P. Hermann, and M. E. Manley, Physical Review B, 2025.

Keywords: ZrN, inelastic neutron scattering, DFT, phonon density of states

http://www.linkedin.com/in/shaofei-wang-a3a0802b7/

1.3 Measuring Depth Scaled Magnetism in Helium-Implanted $PdCoO_2$ using Muon Spin Resonance Spectroscopy.

Simon Kim[1]* and Matthew Brahlek[1]

[1] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: kims6@ornl.gov

In spintronics, the study of combining of magnetic excitations to electronics, the field is constantly searching for novel materials to use in next generation devices. As a pristine crystal, the delafossite $PdCoO_2$ is a non-magnetic material consisting of alternating layers of highly conductive palladium and Mott insulating octahedral cobalt oxides. However, both Co and Pd layers are magnetically metastable, meaning a low dose of helium implantation can induce a ferromagnetic transition [1]. Such a material could have exciting new applications in printable spintronics when combined with traditional implantation techniques or helium microscopy techniques [2]. In this presentation, I examine data from muon spectroscopy measurements [3] alongside simulated depth profiles from TRIM [4] calculations, correlating the helium implantation depth profile with the muon magnetic volume fraction. My analysis reveals magnetic regions that follows the simulated distributions for vacancies and interstitials, which are shifted closer to surface than the implanted helium. This suggests defects are the primary contribution to the induced magnetism and that the use of $PdCoO_2$ for spintronics will require a careful control of defects generated during helium implantation.

[1] Brahlek, M. *et al.* Emergent Magnetism with Continuous Control in the Ultrahigh-Conductivity Layered Oxide PdCoO2. *Nano Letters* **23**, 7279–7287 (2023).
[2] Toulouse, C. et al. Patterning enhanced tetragonality in BiFeO3 thin films with effective negative pressure by helium implantation. *Physical Review Materials* **5**, 024404 (2021).
[3] Morenzoni, E. *et al.* Implantation Studies of keV Positive Muons in Thin Metallic Layers. Nuclear Instruments and Methods in Physics Research B **192** (2002). 254-266
[4] Ziegler, J. F., Ziegler, M. D., & Biersack, J. P. Srim – the stopping and range of ions in matter. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* ***268*** **(11–12)**, 1818–1823 (2010).

Keywords: Spintronics, Ion Implantation, Muon Spectroscopy.

http://www.linkedin.com/in/sangkim8

1.4 Stability, magnetism, and vibrations in $MnTe_xSb_yBi_{1-x-y}$ alloys

P. R. Raghuvanshi[1], X. Li[2], T. Berlijn[1], A. Ghosh[1], D. S. Parker[1], V. R. Cooper[1], and L. Lindsay[1*]

[1]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
[2]Walker Department of Mechanical Engineering and Texas Materials Institute, The University of Texas at Austin, Austin, TX 78712, USA

*Corresponding author: lindsaylr@ornl.gov

Alloy design typically targets structural improvements or functional enhancements, often studied independently. Here, we simultaneously investigate stability, magnetism, and vibrations in ternary and quaternary $MnTe_xSb_yBi_{1-x-y}$ alloys ($x + y \leq 1$). The end-members MnTe, MnSb, and MnBi share a common hexagonal nickeline structure yet exhibit distinct electronic, magnetic, and vibrational behaviors. Using density functional theory calculations, we generate comprehensive compositional phase diagrams revealing the interplay between static energetics, magnetic ordering, and vibrational entropy. Our results highlight alloy-induced magnetic transitions, particularly the antiferromagnetic-to-ferromagnetic transformation, and identify conditions for metastable states enabling magnetic field switching. Additionally, we quantify the influence of compositional disorder on phonon properties, comparing explicitly with virtual crystal approximation methods. Vibrational entropy contributions are analyzed relative to configurational entropy and other energetic terms, providing insights into alloy stability across the composition space. By bridging structural stability with functional properties, this integrated theoretical framework supports targeted alloy development for spintronics, magneto-optics, and thermal management applications.

Keywords: Mn-based alloys, density functional calculations, phase stability, magnetic ordering, lattice vibrations

http://www.linkedin.com/in/parul-raghuvanshi-194828219/

Oral Session 2: Building and Transportation

2.1 Catalytic conversion of captured monoterpenes to sustainable aviation fuel

Ajibola Lawal[1*], Kim T. Tutin[2], and Andrew D. Sutton[1*]

[1] Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA
[2] Captis Aire LLC, 1612 Cleveland Ave, Ste 1, East Point, GA, 30344, USA

[*] Corresponding authors: lawala@ornl.gov, suttonad@ornl.gov

Consistent effort has been made to reduce emissions in the aviation sector, as demand is consistently expected to rise, due to the utility of aviation travel. Present state of the art sustainable aviation fuel (SAF) contains mostly (~95 %) synthetic paraffinic kerosene (SPK) comprising mostly linear and branched alkanes.[1] However, there is still a need to research low-cost renewable route to meet the cycloalkane, and aromatic (~20%) hydrocarbon demand in jet fuel. [2] Cyclic monoterpenes, as a starting feedstock, enables the production of cycloalkanes and aromatics, that sufficiently position renewable SAF to replace all hydrocarbon components in traditional aviation fuel. Robust conversion of captured monoterpenes from wood drying to sustainable aviation fuel was established using a combination of metal Pd catalyst and Zeolite. We established that our catalytic system could convert multiple monoterpenes with complete conversion to aromatics, and cycloalkanes suitable for blending with Jet-A. Mechanistic studies highlighted the role of the zeolite Brønsted acid sites to facilitate isomerization of pinene and camphene to limonene, limonene undergoes subsequent dehydro-aromatization to p-Cymene. This provides a renewable source for aviation fuel aromatics and enables the potential for a fully renewable SAF that meets the criteria for direct petroleum replacement.

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Keywords: Sustainable Aviation Fuel (SAF), Scale-up, Catalysis, Reaction Engineering

http://www.linkedin.com/in/lawal-ajibola-5b7295139/

2.2 Impact of H_2 and alcohol on N_2O formation on commercial emissions control catalysts

Md Masudur Rahman[1], Sreshtha Sinha Majumdar[1*], and Josh A. Pihl[1]

[1]National Transportation Research Center, Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA

*Corresponding author: sinhamajumds@ornl.gov

U.S. engine and vehicle manufacturers are developing new technologies that will allow the diesel engines that power many segments of the American economy to run on alternative fuels such as methanol, ethanol, ammonia, and hydrogen. ORNL is partnering with these companies to increase fuel choice, improve energy security, and support competitiveness of U.S. manufacturers in the global market. While much of the research in this area is focused on maintaining diesel engine performance and efficiency while running on alternative fuels, these engines must still meet emissions regulations to achieve commercialization.

This study investigates the effects of hydrogen and alcohol fuels on N_2O formation over commercial oxidation catalysts using a synthetic exhaust flow reactor system. Under the relevant conditions of hydrogen fueled internal combustion engine (ICE), two commercial diesel oxidation catalysts (DOCs), Pt DOC and Pd+Pt DOC produced notable N_2O levels when NO concentrations exceeded 100 ppm. N_2O formation during methanol and ethanol oxidation over the DOCs and a high PGM Pt oxidation catalyst (OC) was also explored. While alcohol oxidation resulted in minimal N_2O emissions, toxic aldehyde intermediates were detected. These findings underscore the requirements to optimize emission control strategies tailored to alternative fuels to ensure compliance with emissions regulations.

Keywords: N_2O formation, diesel oxidation catalyst, emissions control.

http://www.linkedin.com/in/md-masudur-rahman-306321bb/

2.3 State-of-the-art microgrid protection: An imbalance squared factor-based fault detection, classification and relay coordination scheme

Deepika Patel* and Maximiliano Ferrari
Energy Science and Technology Division, Oak Ridge National Laboratory, Knoxville, TN, 37932, USA
*Corresponding author: pateldh@ornl.gov

Higher penetration of inverter interfaced distributed generators (IIDGs) at distribution level improves the reliability and efficiency of the power supply. This has resulted in the system operators recognizing the need for the distribution system to move from the usual passive unidirectional flow to a bidirectional active distribution network (ADN). ADNs are designed to break up into small power system network (dominant with IIDGs) and are expected to function like an independent grid, known as islanded microgrids/power islands. However, the low fault current magnitude and control dependent fault behavior of IIDGs make the conventional overcurrent protection schemes mal operate. In this regard, a communication-less imbalance squared factor (ISF) based protection scheme is proposed, which can be implemented in cost effective existing relays with embedded mathematical operations. The scheme is tested on a modified IEEE 13 bus unbalanced distribution network with battery energy source, a single and a three-phase inverter having grid forming and grid following control structures. Various faults and no-fault scenarios are investigated with varying parameters to improve the efficacy of the method. The proposed scheme is validated in the real time hardware in the loop with Typhoon HIL 604 and SEL 751 relays for fault detection, fault classification and relay coordination.

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https://www.linkedin.com/in/deepika-chhetija-phd-94b400232/

Oral Session 3: Chemistry 1

3.1 Light-induced crosslinking of ultrathin polyzwitterionic coatings for anti-fouling performance

Charini Maladeniya[1*], Spencer Cox[2], Panagiotis Christakopoulos[1], Liam Collins[1], Ruben Millan Solsona[1], Jong K Keum[1], Marti Checa[1], Marea Blake[3], Benjamin Doughty[3], Jennifer L Morrell-Falvey[2], Ilia N. Ivanov[1], Retterer Scott[1], Rajeev Kumar[1] and Advincula Rigoberto[1]

[1]Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN37831, USA

[2]Biosiences Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831, USA

[3]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831, USA

*Corresponding author: cmalade@ornl.gov

Antifouling refers to the process of preventing the attachment and growth of unwanted organisms, such as bacteria, algae, and other microorganisms, on surfaces. Polyzwitterions, a distinctive class of polyampholytes, have emerged as highly effective materials for antifouling applications. Characterized by both positive and negative charges on individual monomers, polyzwitterions demonstrate exceptional resistance to fouling due to their ability to create strong hydration and high surface energy, forming a physical and energetic barrier that prevents the adsorption of proteins and other biomolecules. In this study, we investigate the use of polyzwitterions as ultrathin coatings to combat biofouling, exploring their synthesis, properties, and performance on solid surfaces. We synthesized a sulfobetaine polyzwitterion, poly (2-vinylpyridine propanesulfonate) (P2VPPS), via free-radical polymerization. A photoreactive benzophenone derivative was covalently anchored to a SiO_2 substrate using a silane group. Ultrathin P2VPPS films were then fabricated by spin-coating and drop-casting onto the benzophenone-modified substrate, enabling comparisons of thickness and antifouling performance across various film thicknesses. Different degrees of crosslinking were introduced by exposure to 365 nm UV light, resulting in a series of films with varying crosslinking densities.

The films were characterized using X-ray photoelectron spectroscopy, X-ray reflectometry, contact angle measurements, atomic force microscopy, and sum frequency generation methods. To evaluate the antifouling properties, neutron experiments, quartz crystal microbalance with dissipation, and amphiphilic β-casein protein were used. Antifouling properties were further determined by multi-scale imaging of *Pantoea sp.*, to assess the effectiveness of the coatings in preventing microbial attachment. Our results show that light-induced crosslinking significantly impacts both the structure and properties of the films, with increases in both film thickness and protein retention as the degree of crosslinking rises.

https://www.linkedin.com/in/charini-maladeniya-42559924a/

3.2 Physics-based modeling of current imbalance and aging in lithium-ion battery modules

A. Surya Mitra[1]*, Yuliya Preger[2], Jacob Mueller[2], Srikanth Allu[1]*

[1]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830
[2]Sandia National Laboratories, Albuquerque, NM, 87185

*Corresponding authors: ayalasomayas@ornl.gov , allus@ornl.gov

Lithium-ion battery (LIB) packs are a key solution for grid-scale energy storage, enabling the integration of intermittent renewable energy sources. LIB modules and packs experience current imbalances and uneven cell aging due to various design and operational factors and require a battery management system (BMS) to continuously monitor and control. In this context, a physics-based modeling framework for LIB modules and packs (liionpack) was enhanced to identify design and control strategies that minimize current imbalance and improve module/pack operation. Simulations of an 8-cell parallel-connected module demonstrate that reducing current imbalance leads to more uniform cell aging and improved module/pack-level degradation predictions. The analysis shows that current imbalance are affected by the electrical resistances. Terminal location significantly affects imbalance, with opposite-end terminal connections at intermediate branches minimizing the imbalance, and the pack circuit construction influences the accuracy of physics-based analysis at the pack scale. This framework enables design optimization of modules and packs through a fast and easy evaluation of pack performance and aging, and supports the development of aging-informed balancing strategies compatible with BMS implementation. Thereby, offers practical pathways to improve reliability and cycle life predictions in large-scale battery energy storage systems.

Keywords: lithium-ion battery packs, current imbalance, module/pack aging, physics-based modeling

https://www.linkedin.com/in/surya-mitra-ayalasomayajula/

3.3 CO_2 Capture from Flue Gas Using Aqueous Amino Acid Salts and Mineralization into Cementitious Materials

Abishek Kasturi,[1*] Gyoung Gug Jang,[1] Diana Stamberga,[2] Denise A. da Silva,[3] Greeshma Gadikota,[4] Radu Custelcean,[2] Costas Tsouris[1]

[1]Oak Ridge National Laboratory, Manufacturing Sciences Division

[2]Oak Ridge National Laboratory, Chemical Sciences Division

[3]Oak Ridge National Laboratory, Buildings and Transportation Science Division

[4]Cornell University, School of Civil and Environmental Engineering

[*]Corresponding author: kasturias@ornl.gov

The global cement industry contributes ~8% of total CO_2 emissions. This study explores a sustainable approach to mitigate these emissions by capturing CO_2 using amino acid salts and mineralizing it with electric arc furnace (EAF) slags. Amino acid salts offer rapid CO_2 uptake and low volatility, making them attractive for flue gas treatment (15% CO_2). Unlike conventional methods, this process eliminates the need for energy-intensive thermal regeneration by coupling capture with mineralization.

We evaluate eight amino acid salts based on carbamate formation, CO_2 flux, mineralization efficiency, and cyclic capacity. Regeneration efficiencies exceed 90%, while over 75% of uncarbonated slag is converted into carbonates. CO_2 fluxes range from 2.3 to 4.9 × 10^{-3} mol/m²/s, with potassium arginate (K-Arg) and potassium glycinate (K-Gly) showing the highest performance. Calorimetry reveals favorable absorption enthalpies for several salts. At 50°C, sarcosine, glycine, and arginine demonstrate high regeneration and mineralization efficiencies.

These findings establish a promising pathway for scalable carbon capture and utilization in cement production. By identifying effective amino acids, this project will enable CO_2 sequestration and will generate valuable carbonate materials, advancing sustainable practices in the cement industry.

Keywords: Point-source CO_2 capture, CO_2 sequestration, carbon mineralization, amino-acid carbonates.

3.4 Data-driven discovery of non-aqueous proton conductors for polymer electrolytes with small dataset

Yifan Liu[1]*, Wesley F. Reinhart[2] and Valentino R. Cooper[1]

[1] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

[2] Department of Materials Science and Engineering, The Pennsylvania State University, University Park, State College, PA 16802

*Corresponding author: liuy6@ornl.gov

Polymer electrolytes are vital for energy storage and conversion devices such as fuel cells and lithium-ion batteries. Compared to liquid or ceramic alternatives, they offer superior electrochemical stability, mechanical flexibility, and interface compatibility. However, their reliance on water as a proton conductor limits operating temperatures to below 100 °C, restricting the performance of polymer electrolyte membrane fuel cells. In this study, we explore amphoteric molecules—capable of both proton donation and acceptance—as potential non-aqueous proton conductors using density functional theory (DFT). We assess proton affinity and proton transfer barriers as proxies for conductivity and examine how molecular features such as electron donating/withdrawing groups, dipole moments, and structural characteristics influence proton mobility. Our analysis identifies structure–property relationships and highlights candidates with water-like proton affinities. These insights lay the foundation for data-driven discovery of high temperature, water-free polymer electrolytes from limited datasets. This work is supported by the Fast and Cooperative Ion Transport in Polymer-Based Materials (FaCT) EFRC, funded by the U.S. DOE Office of Science, Basic Energy Sciences, at ORNL.

http://www.linkedin.com/in/yifan-liu-588089179

3.5 Uncovering the phase transition mechanism in upcycling of spent NMC cathodes with in-situ neutron diffraction

Xin Wang[1], Tao Wang[1*], Huimin Luo[2], Si Chen[3], Qingju Wang[4], and Sheng Dai[1,4*],

[1]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[2]Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[3]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[4]Department of Chemistry, Institute for Advanced Materials and Manufacturing, University of Tennessee, Knoxville, TN, 37996, USA

*Corresponding author: wangt@ornl.gov, dais@ornl.gov

The effective management of end-of-life (EoL) lithium-ion batteries (LIBs) is increasingly vital to their widespread adoption. To maximize the value of spent cathodes, direct recycling and upcycling have emerged as promising strategies by restoring cathodes to their pristine states through the revitalization of degraded structure and compositions. Notably, nickel-manganese-cobalt-oxide (NMC) cathodes are anticipated to dominate the market soon, underscoring the necessity for efficient direct recycling and upcycling methods for spent NMCs. Our group has previously developed the "reciprocal ternary molten salts" (RTMS) system specifically for these processes. This system consists of molten salts incorporating two cation species and two anion species (Li+, Na+ || Cl-, NO3-), offering a wide working temperature range and an oxygen-rich environment conducive to the lithiation of EoL-NMC batteries. Despite significant advancements using this method, further improvements are still necessary. In this study, we employed ball milling to refine particle size and promote the integration of lithium or nickel into the NMC structure, resulting in a well-defined layered configuration. The duration of ball milling and the initial material amount play crucial roles in influencing the performance of the recycled materials. This approach not only enhances electrochemical performance but also provides insights into the growth and phase transition mechanisms, ultimately leading to improved efficiency in upcycling practices for EoL LIBs.

Keywords: end-of-life (EoL), lithium-ion batteries (LIBs), spent cathode, direct upcycling, phase transition, lithium integration

www.linkedin.com/in/xin-wang-83494932

Oral Session 4: Biology Sciences 1

4.1 Applying a genomics-informed carbon cycling model to long-term soil warming

Liyuan He[1*], Qiuming Yao[2], Kristen M. DeAngelis[3], Luiz A. Domeignoz Horta[4], Yang Song[5], Melanie Mayes[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
[2]School of Computing, University of Nebraska-Lincoln, Lincoln, Nebraska, USA
[3]Department of Microbiology, University of Massachusetts Amherst, Amherst, Massachusetts, USA
[4]Université Paris-Saclay, INRAE, AgroParisTech, UMR EcoSys, 91120 Palaiseau, France
[5]Department of Hydrology and Atmospheric Science, the University of Arizona, Tucson, AZ 85721-0011 USA

*Corresponding author: hel4@ornl.gov

Warming has dramatic influences on soil microbial respiration. However, the underlying mechanisms are not yet well understood. Here, we integrated metagenomic data with the Continuum Microbial-ENzyme Decomposition (CoMEND) model, representing the mediating role of 22 enzyme functional groups in decomposition cascades, to investigate the impacts of 5°C warming on soil microbial respiration at Harvard Forest during 2006-2021. We first evaluated and observed good model performance in reproducing the seasonal variations of microbial respiration (MR) and soil microbial biomass and soil carbon pools in both control and warming plots. We found that warming, on average, increased MR by 12.6% during 2006-2021. The increase in MR under warming resulted from the enhanced microbial carbon uptake. However, warming impacts on MR varied with experimental period. We observed increases in MR of 51.2% during 2006-2010 (short-term) and of 14.4% during 2017-2021 (long-term). Warming-induced increase in MR in short-term was attributed more to growth, while that in long-term was more dominated by maintenance. The increases in proportion of active soil microbes can explain the higher increases of MR as well as the higher contribution of growth to MR in short-term. This study demonstrated the feasibility of integrating metagenomics data with model.

Keywords: Warming, Microbial respiration, Microbial metagenomics, CoMEND model, Data-model integration

http://www.linkedin.com/in/liyuan-he-b2010910b/

4.2 Multilayered regulation by RNA thermometers enables precise control of Cas9 expression

Elise K. Phillips[1,2], Dawn M. Klingeman[1,2], Adam M. Guss[1,2], Carrie A. Eckert[1,2], and William G. Alexander[1,2*]

[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830; [2]Center for Bioenergy Innovation, Oak Ridge National Laboratory, Oak Ridge, TN, 37830

*Corresponding author: alexanderwg@ornl.gov

Many organisms used in microbial engineering are intolerant to certain genes when inducible promoters have background expression, also known as promoter leak. Widespread cell death can occur from low expression of toxic genes, like *cas9*. In Cas9- based mutational methods that assess the fitness impact of a large pool of mutations, like CRISPR-enabled trackable genome engineering (CREATE), this cell death can alter the composition of the gRNA library before the experiment begins, preventing a full assessment of how mutations impact host fitness. To reduce the effect of leaky inducible promoters, we added a layer of post-transcriptional regulation to *cas9* expression. Specifically, we demonstrate the use of temperature sensitive RNA secondary structures, RNA thermometers (RNATs), to prevent undesired *cas9* expression in repressive conditions. We demonstrate that RNATs improve survival with uninduced *cas9* and prevent gRNA library skew during a two-day time course. This expands the functional genomics toolkit as we can now maintain active gRNA libraries for population- level multiplex mutations without worrying about skew due to promoter leakage. Because RNAT secondary structure is largely context independent, this regulatory strategy is likely to be adaptable to a wide diversity of other microbial systems.

Keywords: Synthetic biology, Cas9, RNA thermometer

4.3 An Agent-Based Approach for Modeling Air Pollution Exposure at the Individual Level

Andrew Deas[1, *], Adam Spannaus[1], Dakotah Maguire[1], Joe Tuccillo[2], Heidi Hanson[1]

[1]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2] Geospatial Science and Human Security Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[*]Corresponding author: deasaj@ornl.gov

Fine particulate matter (PM2.5) is a hazardous air pollutant linked to numerous adverse health outcomes and poses serious public health risks. As part of a broader effort to enhance preparedness for future public health crises at the national scale, we have developed an agent-based model that leverages a synthetic population in Utah to estimate individual-level exposure to PM2.5. As agents transition between daily activities, such as commuting from home to work or school, their exposure is calculated using geospatial PM2.5 concentration data mapped at the H3 hexagonal spatial level. The model outputs hourly exposure distributions over a representative week, which can be disaggregated by agent role and day of week. These outputs enable the analysis of exposure patterns by agent type, activity, and time of day, and support direct comparisons across demographic or occupational groups. This work provides a computational foundation for investigating how environmental factors contribute to health disparities and offers a pathway toward more personalized exposure modeling.

Keywords: Agent-based modeling, exposure modeling, PM2.5, air pollution

4.4 Mercury removal from aqueous solutions by novel sorbents: Influencing factors and potential implications

Jinping Xue, Peijia Ku, and Scott C. Brooks*

Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States

*Corresponding author: brookssc@ornl.gov

Mercury (Hg) is a global contaminant that poses a significant threat to human life and the environment. Mercury-contaminated freshwaters are sensitive ecosystems due to the substantial release of legacy Hg and its highly toxic methylation product (e.g., methylmercury). *In-situ* sorbent amendments have been shown to be a relatively low-cost, low-impact approach for the remediation of Hg-contaminated sediments by limiting Hg mobility and bioavailability. Despite this, their large-scale *in-situ* application is still limited. Here, we report our ongoing efforts to study Hg adsorption by a novel brominated powdered activated carbon (MercLok^{TM} P-640). Our initial results showed that MercLok concentrations greater than 0.1 g L^{-1} consistently removed > 99% of Hg from phosphate-buffered solutions with Hg levels up to 1 mg L^{-1}. This removal efficiency suggests its potential as a promising adsorbent for Hg remediation in contaminated sites, such as the East Fork Poplar Creek (EFPC), which has been historically influenced by the Y-12 National Security Complex. We hope that the gradual efforts to incorporate the complex water and sediment matrices under laboratory conditions will enable us to assess the actual performance of this novel sorbent in eliminating Hg risks in complex water-sediment ecosystems.

Keywords: Mercury remediation, functionalized activated carbon, water-sediment ecosystems

http://www.linkedin.com/in/jinpingx

4.5 Discovery, characterization and engineering of substrate- and product-selective nylon hydrolases for nylon recycling

Celestin Bourgery*, Erin Drufva, Patricia Saint-Vincent, John Cahill, Vilmos Kertesz, Jerry Parks, Omar Demerdash, Alexis Williams, Nikolas Capra, Flora Meilleur, Dana L. Carper, Vera Bocharova, Isaiah T. Dishner, Jeffrey C. Foster, Muchu Zhou, Delyana Vasileva, Serena Chen, Joshua Michener*

Oak Ridge National Laboratory

*Corresponding authors: bourgerycl@ornl.gov and michenerjk@ornl.gov

Plastic waste is a major environmental and societal concern because it can affect human health, environment, and economy by breaking down into microplastics or because of their chemical additives. Plastic pollution can also be expensive. An average cost of $2.2 billion per year has been estimated, including damage to infrastructure, oceans, and greenhouse gases. In 2022, approximately 400 million tons of plastic have been generated worldwide. Unfortunately, while efforts are being made, recycling is not obvious, involving expensive mechanical methods and a difficult route to achieve as it usually involves complex composites and is not therefore adapted to a sustainable economy.
Enzymatic recycling of these plastics has a bright future due to the intrinsic properties of these enzymes, such as selectivity, promiscuity, ability to operate under mild pressure and temperature conditions, and scalability. Enzymatic recycling of polyethylene terephthalate (PET) has been well studied and proven on an industrial scale in recent years. However, it remains a challenge for polyamide (PA) thermoplastic polymers, commonly known as nylons, which are produced on a scale of about million tons per year.
In our work, we identified and tested a diversity panel of 95 Ntm hydrolases with 25 to 40% amino acid homology, based on the first Nylon hydrolase, NylC. Surprisingly, about 1/3 of these variants showed hydrolytic activity on PA6 or PA6,6 powder [1]. However, some of these enzymes possessed interesting properties of activity and substrate selectivity that had never been demonstrated before. The best variants identified are currently being engineered using different approaches including site-saturation mutagenesis to improve their ability to specifically degrade PA6 or P6,6 from a mixed feedstock. Efforts are also being made to combine pretreatment methods and process optimization with the engineering of these enzymes to make them compatible with more realistic conditions for degrading more complex materials such as commodity plastics. This diversity panel and engineering approach could be used to recycle a variety of polyamides, allowing them to be converted into defined oligomers and incorporated as amide linker groups for the synthesis of new circular-by-design polymers.

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Keywords: Enzyme engineering, Nylon, Plastic recycling, Enzyme discovery

http://www.linkedin.com/in/célestin-bourgery-0885521b9

Oral Session 5: AI-ML 1

5.1 Enabling Large-Batch AI Training via Learned Gradient Mapping

Sahil Tyagi*, Feiyi Wang

Computing and Computational Sciences Directorate (CCSD), Oak Ridge National Laboratory (ORNL), Tennessee, USA

*Corresponding author: tyagis@ornl.gov

Distributed deep learning enables fast training of deep neural networks (DNNs) over multiple nodes or devices in a concurrent and collaborative manner. Different data-parallel algorithms usually trade-off between parallel and statistical efficiency, where the former pertains to training speedup and latter to convergence quality. Training execution can be accelerated via vertical scaling where nodes frequently exchange updates over large clusters, or horizontal scaling by incurring additional compute overhead and using larger batch-sizes. However, the latter faces loss of test accuracy with large-batch training. This is because unlike small batch-size that saturate to flatter minima, large batches converge to sharper minima that is associated with generalization gap. To address these issues, this work presents principled, low-overhead techniques to balance the parallel and statistical challenges in large-batch training. First, we develop a resource and performance modeling technique to estimate memory requirements and the largest, intra-node batch-size supported by a device, followed by estimating the iteration/training time for different batch-size. To improve generalization performance, we develop a low-overhead, profiling-based approach to map small-batch updates to larger batches; essentially adding noise to large-batch gradients and perform SGD update as if computed over smaller-batches. By combining the parallel scaling concepts in distributed training with learned gradient mapping, we outperform vanilla training as well as other large-batch optimization techniques in many cases. In our evaluation, we were able to estimate memory requirements within 1-19% error-rate, and predict iteration time within 10.3% error on average. Compared to vanilla large-batch training, parameter-wise gradient mapping achieves 6.67-18.6% higher accuracy, thus significantly mitigating generalization gap.

Keywords: Distributed deep learning, large-batch training, federated learning, generalization gap, performance modeling, resource modeling, gradient mapping, knowledge distillation, noise modeling

http://www.linkedin.com/in/sahiltyagi4/

5.2 Generative AI for Landcover Forecasting

Debvrat Varshney[1*#], Vibhas Vats[2#], Bhartendu Pandey[1],
Christa Brelsford[3], Philipe Dias[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA
[2]Indiana University Bloomington, Bloomington, IN, 47405, USA
[3]Los Alamos National Laboratory, Los Alamos, NM, 87545, USA
[#]Equal contribution

[*]Corresponding author: varshneyd@ornl.gov

Recent advances in remote sensing and artificial intelligence (AI) have greatly enhanced our ability to characterize land use and land cover (LULC) at both regional and global scales. High-resolution historical LULC datasets are now widely available, providing detailed spatial and temporal insights. The next critical step is to develop reliable methods for forecasting LULC at fine spatial resolutions, which is essential for supporting policy decisions related to equity, climate resilience, and land use planning. Generative AI (GenAI) has emerged as a promising tool for this purpose, offering new ways to model and synthesize complex spatiotemporal data. It can model intricate patterns of spatiotemporal change, surpassing simpler methods that rely on Markovian assumptions. Further, diffusion-based GenAI models can generate multiple plausible future scenarios, enabling probabilistic forecasting. In this context, we propose leveraging GenAI for LULC forecasting by treating it as a conditional data synthesis problem, utilizing both historical and auxiliary datasets such as soil characteristics, topography, population trends etc. We explore mechanisms for integrating domain knowledge into such a data-driven approach, such as LULC change expectations from urban theories. Our proposed framework is able to leverage large datasets, improve forecasting accuracy, and generalize across diverse regions, compared to conventional region-specific models.

Keywords: Diffusion models, land cover change forecasting, urban heterogeneity

http://www.linkedin.com/in/debvrat

5.3 On Synthetic Data Generation for AI Video Instance Segmentation

Luis Caicedo Torres[1]*, Noel Nelson[1], and Scott Greenwood[1]

[1] Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: caicedotorla@ornl.gov

The next generation of effective radioisotope process and workflow development tools call for realistic and interactive 3D environments—but manual annotation of video data inside controlled environments is expensive, slow, and raises security concerns. We leverage existing XR simulations to automatically generate pixel-perfect video instance segmentation (VIS) labels for the training of AI object identification and tracking. This approach not only reduces the cost and time associated with data collection but also addresses security concerns by eliminating the need for real-world data acquisition. These synthetic annotations are then used to refine and evaluate the performance of object segmentation, object tracking, and end-to-end VIS models. We present a friendly survey of VIS model approaches trained on synthetic data, demonstrating the potential to reduce manual data collection efforts while maintaining robust model performance. Our pipeline paves the way for secure, scalable, and cost-effective XR solutions in nuclear science and beyond.

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Keywords: computer vision, object tracking, instance segmentation, video

http://www.linkedin.com/in/luiscaicedotorres/

5.4 The MENTOR interpretation agent: From network embeddings to mechanistic narratives via retrieval-augmented LLMs

Anna H. C. Vlot[1,*], Matthew Lane[1,2], Kyle Sullivan[1], Peter Kruse[1,2], John Dandy[1], Selin Kaplanoglu[1], Alice Townsend[1,2], Jean Merlet[1,2], Daniel A. Jacobson[1]

[1] Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA
[2] Bredesen Center for Interdisciplinary Graduate Research and Education, University of Tennessee-Knoxville, Knoxville, TN, USA

*Corresponding author: vlothc@ornl.gov

Despite the growing availability of complex omics datasets, extracting comprehensive mechanistic insights from these data remains challenging. To address this, we developed the MENTOR Interpretation Agent (MENTOR-IA), a human-in-the-loop agentic pipeline that uses retrieval augmentation and large language models (LLMs) to identify novel relationships among multi-omic gene sets. We applied MENTOR-IA to interpret a previously characterized set of 211 opioid addiction-related genes. We first partitioned these genes into clades using hierarchical clustering of random walk with restart (RWR)-based graph embeddings presented in a dendrogram using our previously described MENTOR algorithm. MENTOR-IA identified Akt, ERK, and BDNF signaling pathways known to be critical to synaptic plasticity, previously reported to be associated with the 211-opioid addiction-related genes. In addition, our pipeline identified novel biological processes, such as extracellular matrix remodeling and neuroinflammation, which were not identified through prior manual review. These results illustrate that our integrative pipeline facilitates scalable interpretation of multi-omic datasets, accelerating our capability to comprehend complex biological traits. Ultimately, these innovations will enhance our ability to derive actionable insights for disease biology and therapeutic development from multi-omic data.

Keywords: Systems biology, human-in-the-loop, LLM-assisted data interpretation, data-driven discovery, opioid addiction

http://www.linkedin.com/in/annahcvlot/

5.5 Practical Scalability of LuGo: Benchmarking the HHL Algorithm Using an Enhanced QPE Algorithm

†Chao Lu, †Muralikrishnan Gopalakrishnan Meena, †Antigoni Georgiadou, †Kalyana Chakravarthi Gottiparthi, †Michael Sandoval, †Eduardo Antonio Coello P´erez, ‡Paul Lin, †In-Saeng Suh, †Seongmin Kim

†National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, USA, ‡National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Corresponding author: luc1@ornl.gov

Harrow-Hassidim-Llyod (HHL) algorithm is a prominent quantum algorithm that offers exponential speedup over its classical counterparts by solving linear systems of equations with logarithmic complexity. However, synthesizing and executing HHL circuits demand significant computational resources from both classical and quantum systems. In this work, we benchmark the HHL algorithm using the optimized Quantum Phase Estimation (QPE) generation algorithm, LuGo, to enhance its scalability and efficiency. We leveraged Frontier and Perlmutter supercomputers to evaluate the scalability of generating HHL circuits and to measure the simulation time of the generated circuits. Additionally, we provide a comprehensive analysis of quantum hardware performance, including studies on qubit connectivity, fidelity comparisons, and average execution times. Our results offer preliminary insights into potential applications of the HHL algorithm enhanced by the LuGo framework and the performance on quantum hardware.

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Key words: Quantum algorithms, quantum linear solver, quantum phase estimation.

Oral Session 6: Nuclear Science 1

6.1 Results from the LEGEND-200 experiment in the search for neutrinoless double beta decay

Harisree Krishnamoorthy[1]
[1] Oak Ridge National Laboratory, Oak Ridge, TN, USA
krishnamoorh@ornl.gov

The discovery of Neutrinoless double beta decay (0νββ) would provide unambiguous evidence for the Majorana nature of neutrinos, lepton number nonconservation and a measurement of the absolute neutrino mass scale. The Large Enriched Germanium Experiment for Neutrinoless ββ decay (LEGEND) is a phased search for 0νββ in the 76Ge isotope with enriched high-purity germanium (HPGe) detectors. The LEGEND experiment brings together the innovation and expertise from its very successful, 76Ge-based predecessors, GERDA and MAJORANA DEMONSTRATOR. The Oirst phase, LEGEND-200, located at LNGS, Italy, is presently acquiring physics data with close to 100 kg of HPGe detectors. With an exposure of 1 ton-year and a background index in the region of interest of less than 2 ´ 10-4 cts/ (keV kg yr), LEGEND-200 will reach a discovery sensitivity of a half-life of 1027 years. This talk will provide an overview of the LEGEND experiment, including the latest results from the

6.2 Integrated modeling of MHD flow, heat transfer, and solid mechanics for fusion reactor applications

Yuchen Jiang[1]*, Sunday Aduloju[1], Joy Fan[1], Daniel Suarez[1], Sergey Smolentsev[1]
[1] Fusion Energy Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
Corresponding author: jiangy@ornl.gov

For the ongoing research and development of the blanket and divertor components of a fusion reactor, an integrated multi-material model involving liquid metal (LM) Magnetohydrodynamics (MHD), conjugate heat transfer and solid mechanics was built, tested and applied to different design studies. The model adopts the Boussinesq approximation as well as the inductionless approximation and thus, it is applicable to the analysis of mixed-convection MHD flows in both experimental conditions and real fusion applications. The heat transfer and solid mechanics are coupled using the thermal expansion and fluid structure interaction. The velocity and temperature fields as well as stresses, displacements and pressure distributions have been computed and analyzed for various scenarios. The proposed integrated model will be coupled with a corrosion model for candidate steels in the future studies for pre- and post-experimental analyses for an experimental loop.

Keywords: Nuclear fusion, fusion blanket, liquid metal, magnetohydrodynamics

www.linkedin.com/in/ycjiang

6.3 Advanced Applications of MicroExtraction - Single Particle - Inductively Coupled Plasma - Mass Spectrometry

Jordan Stanberry*[1], Dehlia Lang, Sarah Szakas[1], Hunter Andrews[1], Brian Ticknor[1], Cyril Thompson[1], Benjamin Manard[1]

[1] Oak Ridge National Laboratory, Oak Ridge, TN, USA
[2] Clemson University, Clemson, SC, USA

*Corresponding author: stanberryjs@ornl.gov

The ubiquitous use of nanoparticles in industry and research has led to a large demand for innovative analytical approaches for their characterization and quantification. Microextraction -single particle - inductively coupled plasma - mass spectrometry (ME-SP-ICP-MS) has been pioneered in our laboratory and can be used to directly analyze particles from sample surfaces. We previously demonstrated that the technique is capable of extracting and characterizing Au and Fe nanoparticles loaded on a polytetrafluoroethylene (PTFE) surface. Here we present our progress on expanding the application space of this technique to include isotopic analysis of particles, detection of challenging elements (e.g., F), and use on a variety of surfaces (e.g. silicon wafers, carbon planchettes etc.). This presentation will include addressing the improvements in the extraction design and the coupling of microextraction to various ICP-MS platforms for respective applications.

Key words: ICP-MS, microextraction, nanoparticles

6.4 Time-resolved dosimetry for alpha- and beta-emitters in radiopharmaceutical therapy: an *in silico* comparison

Abstract author(s): Jayasai Rajagopal, Zakaria Aboulbanine, Anuj Kapadia

Author affiliation(s): Multiscale Biomedical Systems Group, Computing and Computational Sciences Directorate, Oak Ridge National Laboratory

Corresponding author: rajagopaljr@ornl.gov

Radiopharmaceutical therapy (RPT) delivers high intensity radiation to treat tumors. While beta-emitters, including ^{177}Lu, are commonly used, there is interest in alpha-emitters, including ^{225}Ac, due to their higher linear energy transfer and shorter range. In this study, we used a computational workflow to compare time-resolved dose between beta- and alpha-emitters. An adult male virtual patient (BMI 28) was treated using either beta-emitting (3 GBq ^{177}Lu-PSMA-617) or alpha-emitting (8 MBq ^{225}Ac-PSMA-617) sources. A physiologically based pharmacokinetic (PBPK) model was used to generate time-activity curves for organs-at-risk. Time-activity curves and patient anatomy were imported into a Monte Carlo code (GEANT4) to calculate time-relative and cumulative dose. The highest organ activity for the beta-emitting source (^{177}Lu) was found in the liver at a value of 85.3 MBq at 18.9 hours while the highest organ activity for the alpha-emitting source (^{225}Ac) was in the salivary glands at 0.3 MBq at 15.2 hours. Compared to ^{177}Lu, ^{225}Ac had lower cumulative dose for liver (0.19 vs 0.38 Gy) and kidneys (0.97 vs 1.52 Gy) and a higher cumulative dose in the salivary glands (2.69 vs 1.87 Gy). This work demonstrates a virtual approach to estimate organ dose for alpha- and beta-emitting radionuclides.

Keywords: radiopharmaceutical therapy, isotopes, simulation

www.linkedin.com/in/jayasai-rajagopal/

6.5 Pore-resolved Simulations of Electro-Thermal Processes for Alkane Dehydrogenation in Graphite Reactors

Samuel Fagbemi[1], Vimal Ramanuj[1], Mohammed H. Saffarini[1], Philip C. Roth[2], Ramanan Sankaran[1]

[1]Multiscale Materials Group, Oak Ridge National Laboratory
[2]Algorithms and Performance Analysis Group, Oak Ridge National Laboratory

Joule heating has been regarded as an energy-efficient and sustainable method for heating materials and gases at large scales. The modeling of local temperature effects at pore-resolved scales for such systems, however, has been difficult to achieve due to challenges in coupling thermo-chemical processes in complex porous media and in large representative volume elements (RVEs). To this end, we developed an electro-thermal model at the pore scale to study Joule heating effects in large heterogeneous systems with different microstructures. This was achieved using the level set method to implicitly delineate distinct regions within the domain, and an embedded boundary method to facilitate heat exchange across the fluid-solid interface. Moreover, we applied this method to investigate unsteady non-linear electro-thermal effects in non-woven fibrous graphite conductors for RVEs with characteristic lengths of 2 mm, with different fiber orientations, porosity (80% – 90%) and fiber diameters (10 – 20 μm). The coupled equations were solved numerically and they produced peak temperatures greater than 2000 K resulting in heating rates as high as 80,000 K/s. The microstructure had an impact on electrical and thermal behavior. Fiber networks displaying higher temperatures had higher current densities, with the strength of the current density depending on the fiber orientation and the connectivity of the fibers. High-performance computing (HPC) was applied for modeling the coupled equations within the representative volumes. The model is being expanded upon for modeling catalysis of organic substances, such as for alkane dehydration.

6.6 A natural circulation breeding blanket

Daniel Suarez[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

Corresponding author: suarezcambrd@ornl.gov

The successful design of tritium (T) breeding blankets is a necessary step towards fusion energy deployment. The main research lines for designing liquid breeding blankets can be divided into (1) fast flow breeders and (2) slow flow breeders. While the first category uses the breeder fluid as a coolant, the second relies on an auxiliary system for cooling. The concentration of bred T in fast flow breeders is low and makes its recovery expensive, regardless of the type of extraction systems. Although the concentration of bred T in slow flow breeders is higher, the flow suffers from natural convection and T accumulation in undesired locations, increasing the risk of T leakages. Recent investigations suggest that by controlling the cooling rate of the blanket walls we can create customized recirculation eddies that can accumulate T at specific locations of the blanket. The novelty of our design is to leverage such T accumulation to increase the efficiency of the extraction process. Where slow-flow breeder blankets see a problem, we see an opportunity.

Keywords: Breeding Blankets, Heat Pipes, Electrochemical Tritium Extraction.

linkedin.com/in/daniel-suarez-cambra-b8592615

Oral Session 7: Chemistry 2

7.1 Functionalized porous polymer-based catalysts for CO2 conversion to formic acid

Jane N. Agwara,[1] Luke Daemen,[1] Shannon Mark Mahurin,[2] Harry Meyer III,[2] and Michelle Kidder[1]*

[1]Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: kidderm@ornl.gov

The catalytic conversion of CO2 from flue gas into formic acid offers a sustainable route for producing chemicals and fuels. However, the reaction is thermodynamically unfavorable (ΔG = 32.9 kJ/mol at 298 K), requiring efficient catalytic systems to operate under mild conditions.1 While heterogeneous catalysts suffer from poor product selectivity and homogeneous systems face challenges in catalyst stability and recovery, functionalized polymers with intrinsic microporosity (PIMs) present a promising hybrid solution.2, 3 We have developed a PIM-based catalyst functionalized with ruthenium (Ru) for selective CO2 hydrogenation to formic acid under mild temperatures (30-50 °C). The PIM demonstrated high BET surface area (629.7 m^2/g) and thermal stability (>400 °C), with slight reductions after Ru incorporation (568.2 m^2/g; >300 °C). Characterization (ATR-FTIR, ICP, N2 physisorption, SEM/EDX, XPS, TGA, etc.) confirmed successful PIM synthesis, Ru integration, and preserved structural integrity. Under mild conditions, CO2 uptake was high and temperature dependent. NMR analysis after CO2 hydrogenation batch reactions (1:1 CO2/H2, 100 bar) confirmed exclusive formic acid production, with high turnover numbers (TON) of 2372, 2415, and 468 at 30 °C, 40 °C, 50 °C respectively. These findings demonstrate that PIM-Ru catalysts combine the selectivity of homogeneous catalysts with the robustness of heterogeneous catalysts, offering a scalable and stable catalyst for CO2 utilization.

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Keywords: CO2 utilization, Polymers of intrinsic microporosity, Formic acid synthesis

http://www.linkedin.com/in/janengoziagwara/

7.2 Aqueous Porous Liquids for Gas Separations, Transport and Conversion

Arvind Ganesan,[1] Debrata Moitra,[2] Zhenzhen Yang,[1] Shannon M. Mahurin,[1] Tao Wang,[1] and Sheng Dai[1,2]

[1]Chemical Sciences Dvision, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]Department of Chemistry, University of Tenneessee Knoxville, Knoxville, TN, 37916, USA

*Corresponding author: ganesana@ornl.gov

Porous liquids, fluids with permanent porosity have been explored over the past decade as transformative functional materials for several sustainable chemical processes. Liquids are generally associated with no porosity or microscopic transient porosity characterized by extrinsic free volumes. On the other hand, the paradoxical permanent porosity within porous liquids is of great interest to both fundamental sciences and industrial applications. The introduction of intrinsic porosities within liquids enables the synthesis of transformational materials that synergistically combine the significant advantages of solids (tailored nanoscale interactions, increased selectivity and capacity, reduced regeneration energy, etc.), and liquids (continuous operations, accelerated kinetics, efficient heat, and mass transfer). Porous liquids have been traditionally designed with sterically hindered solvents. Alternatively, recent efforts rely on dispersing microporous frameworks in simpler solvents like water. Here we report a unique strategy to construct macroporous water by selectively incorporating hydrophilicity on the surfaces of hydrophobic hollow carbon spheres (HCS). Specifically, we show that the stable dispersion surface ionized HCS in water while retaining the inherent porosity. The electrocatalytic conversion of small gas molecules in aqueous electrolytes is limited by the concentration and diffusion rate of gas molecules in water. In this case, macroporous water exhibited 6 times gas uptake to nonporous (pure) water. By leveraging the high gas capacity and enhanced diffusion kinetics, the limiting diffusion current of oxygen reduction reaction (ORR) in macroporous water is 2 times that in nonporous water, offering promising prospects for sustainable energy conversion technologies.

7.3 Utilizing Mining and Battery Recycling Waste for Marine Carbon Dioxide Capture via Ocean Alkalinity Enhancement

Nicholas Gregorich,[1]* Joseph Kalla,[2] Stephanie Cho,[2] Shailesh Dangwal,[1] Zachary Coin,[1] Mary Irwin,[2] Ramesh Bhave,[1] Syed Z. Islam[1]

[1]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]University of Tennessee-Knoxville, Knoxville, TN 37996

*Corresponding author: gregorichne@ornl.gov

Reversing the global warming crisis remains at the forefront of modern research as human activities continue to release more greenhouse gases than natural processes can remove. The ocean behaves as a natural sink for carbon dioxide (CO2) and has absorbed ~30% of all emissions since the industrial revolution. This absorption has decreased the pH of the ocean by 0.1, a 26% increase in acidity that is detrimental to marine wildlife. The ocean's ability to sequester CO2 from the atmosphere can be enhanced by increasing the ocean's alkalinity, a process known as Ocean Alkalinity Enhancement (OAE). Traditionally, critical materials mining facilities release waste in the form of mining tailings that contain alkaline materials such as calcium and magnesium oxide (CaO, MgO). These tailings are a significant environmental concern for local communities and could serve as a major source of alkaline materials for OAE that are otherwise considered waste. Alkaline wastewater from a lithium battery recycling process can also be used to effectively implement OAE in seawater and reverse ocean acidification. Results from this study underscore the importance of identifying and utilizing cost-effective sources of alkaline waste materials to perform OAE and provide a pathway for achieving net-negative carbon emissions.

Keywords: Carbon capture, sustainability, critical materials

http://www.linkedin.com/in/nicholas-gregorich-38358911a

7.4 Catalytic Role of Methanol in Anodic Coupling Reactions Involving Alcohol Trapping of Cation Radicals

Shahriar N. Khan,[1,2*] John H. Hymel,[2] John P. Pederson,[2] and Jesse G. McDaniel[2]

[1]Computing and Computational Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]School of Chemistry and biochemistry, Georgia Institute of Technology, Atlanta, GA, 30332, USA

*Corresponding author: khann@ornl.gov

In anodic electrosynthesis, cation radicals are often key intermediates that can be highly susceptible to nucleophilic attack and/or deprotonation, with the selectivity of competing pathways dictating product yield. In this work, we computationally investigate the role of methanol in alcohol trapping of enol ether cation radicals for which substantial modulation of the reaction yield by the solvent environment was previously observed. Reaction free energies computed for intramolecular coupling unequivocally demonstrate that the key intramolecular alcohol attack on the oxidized enol ether group is catalyzed by methanol, proceeding through overall second-order kinetics. Methanol complexation with the formed oxonium ion group gives rise to a "Zundel-like", shared proton conformation, providing a critical driving force for the intramolecular alcohol attack. Free energies computed for methanol solvent attack of enol ether cation radicals demonstrate an analogous mechanism and overall third-order kinetics, due to similar complexation from a secondary methanol molecule to form the "Zundel-like", shared proton conformation. As catalyzed by methanol, both intramolecular alcohol attack and methanol attack on the oxidized enol ether group are barrierless or low-barrier reactions, with kinetic competition dictated by the conformational free energy profile of the cation radical substrate and the difference in reaction rate orders.

http://www.linkedin.com/in/noor-md-shahriar-khan-a2968466/

7.5 Uncovering the phase transition mechanism in upcycling of spent NMC cathodes with in-situ neutron diffraction

Xin Wang,[1] Tao Wang,[1,*] Huimin Luo,[2] Si Chen,[3] Qingju Wang,[4] and Sheng Dai[1,4,*]

[1]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[3]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[4]Department of Chemistry, Institute for Advanced Materials and Manufacturing, University of Tennessee, Knoxville, TN, 37996, USA

*Corresponding author: wangt@ornl.gov, dais@ornl.gov

The effective management of end-of-life (EoL) lithium-ion batteries (LIBs) is increasingly vital to their widespread adoption. To maximize the value of spent cathodes, direct recycling and upcycling have emerged as promising strategies by restoring cathodes to their pristine states through the revitalization of degraded structure and compositions. Notably, nickel-manganese-cobalt-oxide (NMC) cathodes are anticipated to dominate the market soon, underscoring the necessity for efficient direct recycling and upcycling methods for spent NMCs. Our group has previously developed the "reciprocal ternary molten salts" (RTMS) system specifically for these processes. This system consists of molten salts incorporating two cation species and two anion species (Li+, Na+ || Cl-, NO3-), offering a wide working temperature range and an oxygen-rich environment conducive to the lithiation of EoL-NMC batteries. Despite significant advancements using this method, further improvements are still necessary. In this study, we employed ball milling to refine particle size and promote the integration of lithium or nickel into the NMC structure, resulting in a well-defined layered configuration. The duration of ball milling and the initial material amount play crucial roles in influencing the performance of the recycled materials. This approach not only enhances electrochemical performance but also provides insights into the growth and phase transition mechanisms, ultimately leading to improved efficiency in upcycling practices for EoL LIBs.

Keywords: end-of-life (EoL), lithium-ion batteries (LIBs), spent cathode, direct upcycling, phase transition, lithium integration

http://www.linkedin.com/in/xin-wang-83494932

7.6 Biphasic Solvents for Energy Efficient CO2 Capture from Natural Gas and Coal Flue Gas Streams

Alexander Wiechert,[1*] Gyoung Jang,[1] Diāna Stamberga,[2] Gang Seob Jung,[3] Aye Meyer,[1] Michael Cordon,[1] Radu Custelcean,[2] Costas Tsouris[1]

[1]Oak Ridge National Laboratory, Manufacturing Sciences Division
[2]Oak Ridge National Laboratory, Chemical Sciences Division
[3]Oak Ridge National Laboratory, Computational Sciences and Engineering Division

[*]Corresponding author: wiechertai@ornl.gov

Biphasic solvents have been identified as an energy efficient alternative to the benchmark monoethanolamine (MEA) solution for CO2 capture. These solvents undergo a process of phase separation when loaded with CO2 that splits the solvent into immiscible CO2-rich and CO2-lean liquid phases. This characteristic dramatically reduces the total volume of solvent that requires regeneration. Nevertheless, significant energy savings may also be obtained by regenerating these solvents in the presence of catalytic materials (e.g., tertiary amines, TiO2, ZrO2, etc.). For this work, a novel diethylenetriamine (DETA) biphasic blend was developed, and catalytic regeneration was studied using simulated natural gas (5 % CO2) and coal (13 % CO2) flue gas loaded samples. When regenerating the DETA solvent with heterogeneous catalysts, the total volume regenerated and energy cost of regeneration per mol CO2 recovered were reduced by 50 % and 37 %, respectively, vs the benchmark MEA solution in natural gas flue-gas loaded samples. Additional energy savings, up to 46 % per mol CO2 vs the MEA solution, were observed when using homogenous catalysts during regeneration but this came at the cost of slightly increasing the total volume regenerated. Further investigation of the DETA solvent's performance under coal flue gas conditions is underway.

Keywords: Biphasic solvents, Post Combustion CO2 capture, Amine Absorbents

Oral Session 8: Materials Science 2

8.1 Strain-engineering in correlated oxide quantum heterostructures

Ryan (Jeongkeun) Song[1†] and Ho Nyung Lee[1]

[1] Materials Science and Technology, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Corresponding author: songj1@ornl.gov

Over the past decades, the demand for stable, energy-efficient, and high-performance materials has driven the discovery of novel quantum materials. Realizing these materials depends on advancing our understanding of fundamental physics of solid-state systems and their entangled quantum phenomena. In this talk, we present our recent research on discovery of novel topological states in correlated oxide thin films and heterostructures composed of ANbO3 (A = Ca and Sr) and their strain engineering that leads exceptional quantum transport properties, including ultra-high carrier mobility and unconventional magnetotransport responses. By strain-engineering, the carrier mobility (m) is dramatically enhanced from 103 to 105 cm2/Vs, surpassing traditional limits in typical oxide materials. Furthermore, under strain, these films exhibit negative longitudinal magnetoresistance and a chiral transport, signatures consistent with the emergence of massless and correlated Dirac fermions driven by symmetry-breaking distortions. These findings establish strained niobates as a compelling platform for exploring topological and correlated electronic states. The synthesis and transport measurements were conducted at the Materials Science and Technology Division, Oak Ridge National Laboratory.

Keywords: Correlated topology, oxide, niobate, chiral transport

https://www.linkedin.com/in/jeongkeun-ryan-song-628783113/

8.2 Focused Si++ ion irradiated nanometer sculpting and vortex pinning in a topological superconductor heterostructure FeTe0.75Se0.25/Bi2Te3

Debarghya Mallick** 1, Sujoy Ghosh2, An His Chen1, Qiangsheng Lu1, Liam Collins2, Simon Kim1, Gyula Eres1, Ivan Kravchenk2, Stephen Jesse2, Steven Randolph2, Scott Retterer2, Matthew Brahlek1, Robert G Moore1

1Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

2Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

**email of presenting author: mallickd@ornl.gov

FeTe0.75Se0.25/Bi2Te3 (FTS/BT) is a promising platform for hosting Majorana fermions, which are believed to revolutionize the field of fault-tolerant quantum computing. In this work, we used a focused ion beam (FIB) system equipped with Si++ ions to create a about 100 nm laterally damaged region on the microbridge of the FTS/BT heterostructure. We investigated the superconducting properties of this "superconductor-affected superconductor-superconductor" system, specifically focusing on its critical temperature (Tc) and critical current (Ic) as a function of Si++ ion dose. Measurements of Ic vs. magnetic field (B), at different doses reveal that the decline of Ic with increasing B, slows down at higher doses. This behavior suggests that defect-induced vortex pinning inhibits vortex motion, thereby reducing dissipation, which would otherwise degrade superconductivity. Our results demonstrate an effective method to enhance superconductivity against magnetic-field-induced suppression by nanostructuring with a focused Si++ ion beam. Additionally, this work suggests the future possibility of engineering a weak link by carefully tuning both the ion beam energy and dose. This could enable the formation of a superconductor-insulatorsuperconductor (SC-I-SC) Josephson junction (JJ), paving the way for the realization of fault-tolerant superconducting qubits.

8.3 Nanofabrication and integration of Quantum Spin Liquid materials into test structures and devices

Ciril Samuel Prasad1*, Sujoy Ghosh1, Steven J. Randolph1 and Stephen Jesse1

1 Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

* Corresponding author: samuelprasac@ornl.gov

Quantum Spin Liquids (QSLs) emerge in frustrated magnetic materials where spins remain disordered even at 0 K. The presence of quasi-particles, long-range entanglement, and topological order makes QSLs a promising material platform for building inherently fault-tolerant devices for the storage and processing of quantum information. Several recent reports have proposed schemes to test and leverage these unique properties of QSLs, the majority of which involve thermal transport measurements, considering the electrically inactive nature of QSLs. However, realizing such device schemes demands unconventional approaches to nanofabricate and integrate QSL materials into test structures that can reliably operate under cryogenic temperatures (< 2 K) and large magnetic fields (~ 8 T). In this presentation, I will discuss our recent progress in developing a mesoscale thermal transport measurement platform for testing QSLs that can operate under such constraints. I will describe our efforts towards developing ultrasensitive on-chip cryogenic thermal sensors, fabricating suspended nanostructures with minimal thermal leakage, and successfully integrating 2D QSL materials. The development of this platform enables the measurement and control of mesoscale local temperature gradients in QSLs with sub-mK precision, paving the way for further exploration of their fascinating properties and potential applications in quantum technology.

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Keywords: Quantum spin liquids, Thermal transport, Nanofabrication

www.linkedin.com/in/cirilsp/

8.4 Effect of precipitates formation and oxide particle on the grain boundary mobility assisted recrystallization in SS 316H alloy processed by L-PBF

Gyan Shankar a, Selda Nayir a, Peeyush Nandwana a

aMaterials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, United States of America

Stainless steel (SS) 316H was printed using laser powder bed fusion (L-PBF) for potential structural application in advanced nuclear reactors. It requires uniform and predictable microstructures and properties of printed parts to qualify for such critical application. Microstructural heterogeneities, localized strain gradients, columnar grain structures, and anisotropic properties are the inherent features of as-fabricated L-PBF parts. Heat-treatment of printed parts were carried out aiming to produce homogeneous equiaxed recrystallized microstructure. However, presence of elemental segregation (Cr and Mo), impurities oxide particles such as alumina, and formation of precipitates hinder recrystallization even at 1200 °C. These particles were found to pin the grain boundaries resulting in reduced recrystallization kinetics. Alumina particles were found to be most detrimental in reducing the grain boundary mobility due to its nano-size uniform distribution across the microstructure favoring the Zener pinning effect. This study, for the first time, elaborates the broad effect of nano oxide inclusions and Zener pinning on the recrystallization kinetics of L-PBF SS 316H alloy. The study showed that higher temperature annealing is beneficial to overcome the Zener pinning force and promote recrystallization. These findings provide a solution to the post-build processing of AM materials and its qualification for high temperature critical applications.

Keywords: L-PBF; Stainless steel 316H; Heat-treatment; Zener pinning; Microstructure evolution

Oral Session 9: Biology Sciences 2

9.1 Enhancing Single-Cell Mass Spectrometry: Comparing Liquid Vortex Capture and the Rapid Droplet Sampling Interface

Stephen C Zambrzycki[1], Vilmos Kertesz[1], John F Cahill[1]

[1] Bioanalytical Mass Spectrometry Group, Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

Corresponding author: cahilljf@ornl.gov.

Single-cell mass spectrometry aims to resolve cell-to-cell biochemical variation despite identical genotypes [1,2], but low analyte abundance and inefficient sampling hinder data quality. Single-cell measurements can uncover mechanisms driving cellular responses relevant to bioengineering, cellular manufacturing, and medicine.

We compared ion signal and analytical performance between two sampling approaches: Liquid Vortex Capture (LVC) and the Rapid Droplet Sampling Interface (RDSI). LVC uses continuous solvent aspiration through a vortex to capture, lyse, and electrospray the sample into the mass spectrometer [3]. RDSI delivers solvent flow to an electrospray syringe needle tip, where the cell is dispensed and sprayed with minimal dilution, enhancing ionization efficiency [4].

In collaboration with HP Life Science Solutions, we coupled the D100 single-cell printer to both interfaces to evaluate the sensitivity of dispensing standard solutions and cells. Single-cell detection of drugs and lipids was tested using Hep G2 cells incubated with amiodarone for 24 hours or atorvastatin for 10 minutes.

Preliminary results show a 10× boost in signal response with RDSI compared to LVC for both drugs and lipids in solution and single cells. These findings highlight RDSI as a promising tool to improve sensitivity and data quality in single-cell mass spectrometry.

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Keywords: Mass spectrometry, Single cells analysis, Bioanalytical chemistry, High-throughput analysis, Microfluidics

https://www.linkedin.com/in/stephen-zambrzycki-60360192/

9.2 Controlling Matric Potential In Microfluidics To Examine Microbial Dynamics In Unsaturated Porous Media

Shane Franklin, Scott Retterer, Amber Webb, Jennifer Morrell-Falvey

Corresponding Author: franklinsm@ornl.gov

The use of microfluidics for the study of soil microbial ecology is an emerging field. Most microfluidic studies of biological systems, however, have been performed under fully saturated conditions that are not representative of natural soil. Therefore, while microfluidics offer many unique capabilities that other methodologies cannot, they are not currently suited to address the effects of matric potential, an important variable defining the microbial moisture niche. Here, a methodology is presented that allows the user to control the aqueous conditions within microfluidics by manipulating matric potential using a hanging water column. The method relies on hydrophilic surface treatment of the microfluidic device using polyvinyl alcohol and incorporating small pores at the network boundaries, which serve as a porous plate analogue. The method was validated on a capillary bundle and then on a more complex pore network. A water retention curve was generated for the pore network over a matric potential range of 0 to – 5 kPa. Both the drainage and wetting curves were reproducible, as was the spatial configuration and number of fragmented moisture niches in the pore network, particularly on the drainage curve. Ultimately, the methodology provides realistic pore-scale moisture conditions that can be easily manipulated and maintained.

9.3 Improving the prediction and interpretability of microbial nutrient utilization phenotypes

Dileep Kishore[1]*, Priya Ranjan[1], Chris Neely[2], William Riehl[2], Marcin P. Joachimiak[2], Janaka N. Edirisinghe[3], José P. Faria[3], Myra B. Cohen[4], Zahmeeth Sakhaff[3], Pamela Weisenhorn[3], Dale A. Pelletier[1], Mitchel J. Doktycz[1], Robert W. Cottingham[1], Christopher S. Henry[3], Adam P. Arkin[2], Paramvir S. Dehal[2]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA;
[2]Lawrence Berkeley National Laboratory, Berkeley, CA;
[3]Argonne National Laboratory, Lemont, IL;
[4]Iowa State University, Ames, IA.

*Corresponding author: kishored@ornl.gov

Deciphering microbial nutrient utilization from genomic data is vital for understanding ecosystem niches. Current predictive models struggle with incomplete gene annotations and inconsistent training data. To overcome these challenges, we compiled a dataset of phenotypic information from 819 microbial genomes, analyzing their binary growth outcomes across 242 carbon sources. We created feature sets for machine learning using genomic annotations from multiple sources, including metabolic pathway features and protein functional data. Phenotype-specific classifiers were developed, and we assessed the influence of dataset characteristics and feature selection on prediction accuracy. Employing diverse pre-processing and selection strategies alongside a standardized evaluation framework revealed that dataset biases and phylogenetic distances significantly affected model performance. Our models performed better within datasets than across datasets, irrespective of feature representation. While no individual annotation source proved superior, biologically informed feature selection enhanced predictive performance and interpretability. Integration of multiple annotation sources improved model outcomes for approximately 82% of phenotypes, especially where single-source models fell short. These classifiers facilitate insights into microbial growth dynamics and metabolic pathways, underscoring the significance of feature selection and dataset composition in predictive modeling of microbial metabolism.

Keywords: machine learning, bacterial cultivation, microbial metabolism, environmental preferences

https://www.linkedin.com/in/dileep-kishore/

9.4 Predicting membrane permeability using realistic mammalian bilayers and LipidLure: a steered molecular dynamics pipeline

John Vant[1], Van Ngo[2], Debsindhu Bhowmik[1], Narendar Singh[1], Anuj Kapadia[1]

1 Computer Science and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

2 National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: bhowmikd@ornl.gov

Many key biological processes depend on the passive diffusion of molecules across lipid membranes. For example, drugs that are not actively transported must permeate the membrane to reach intracellular targets, ultimately affecting their bioavailability. The Inhomogeneous Solubility-Diffusion (ISD) model has been widely used to predict permeability by estimating free energy and diffusivity profiles across simplified bilayer models. However, these approaches often neglect the structural complexity of mammalian membranes, including heterogeneity and leaflet asymmetry. We introduce LipidLure, a high-throughput computational pipeline that leverages hundreds of steered molecular dynamics simulations to map free energy landscapes and local diffusivities across realistic membrane models. Our method shows strong agreement with experimental permeability data across a panel of drugs with varying membrane-crossing ability. Moreover, we demonstrate how lipid composition and asymmetry substantially modulate barrier heights and diffusivity profiles, revealing the importance of biologically accurate membranes in predictive permeability modeling.

Keywords: membrane permeability, molecular dynamics, drug transport, steered MD, lipid asymmetry

https://www.linkedin.com/in/john-vant-2481641a3/

9.5 Cost efficiency of US hydropower plants: A Stochastic Frontier Analysis

Gbadebo A. Oladosu1 and Yu Ma1*

1Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA

*Corresponding author: may3@ornl.gov

Despite its long-standing capacity contributions to the national electricity grid, the US hydropower industry currently faces pressures to reduce costs and improve its competitiveness. The goal of this study is to quantify the operation and maintenance (O&M) cost efficiency of US hydropower plants for benchmarking purposes and develop a better understanding of the underlying drivers to help identify cost reduction opportunities. Utilizing a proprietary annual performance and cost panel dataset of US hydropower plants from 2011 to 2019, we apply parametric stochastic frontier methods to estimate measures of cost efficiency and economies of scale. Results suggest that there is scope for cost efficiency improvements among US hydropower plants. All plants are cost inefficient to some degree, with the average efficiency estimates at around 67%. Larger plants, on average, are more cost efficient than smaller plants. There is no evidence of upward or downward trends in cost efficiency estimates over time, and the efficiency rankings do not dramatically change in a short period of time. The presence of economies of scale implies a need for innovative approaches/technologies to reduce the costs of operating and maintaining smaller hydropower plants, which also constitute most of the remaining hydropower potential.

Keywords: hydropower, cost efficiency, stochastic frontier analysis, economies of scale.

Oral Session 10: AI/ML 2

10.1 Optimization of rare earth elements recovery with large language models

Viktoriia Baibakova[1]* and Alexey Serov[1]

[1] Energy Conversion and Manufacturing Group, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: baibakovav@ornl.gov

The critical role of rare earth elements (REEs) in renewable energy and clean technologies necessitates efficient recycling methods to reduce ore dependence and ensure sustainable supply [1]. However, optimizing REE recovery and separation is challenging due to the complexity of experimental parameters, including REE type, sorbent properties, and operating conditions [2]. This work investigates the use of large language models (LLMs) to accelerate REE recycling process optimization. By analyzing extensive scientific literature, LLMs can uncover complex relationships and predict optimal experimental conditions, helping to reduce the parameter space for experimentalists [3]. We apply LLMs to assess existing research on REE extraction techniques, such as solvent extraction and leaching, to identify key parameters, highlight discrepancies, and discover promising new methods. Additionally, we propose developing autonomous Agents that combine LLM-derived insights with active learning to iteratively suggest experiments [4]. This system aims to minimize the number of required experiments, reducing time and resource demands. This abstract was authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy (DOE).

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Keywords: Rare earth elements, recycling, large language models, AI agents.

http://www.linkedin.com/in/viktoriia-baibakova
http://www.linkedin.com/in/alexey-serov

10.2 HARMONY: Evolutionary Design of Efficient Hybrid Transformer-Mamba-MoE Language Models Through Large-Scale Architecture Search

Emily Herron*, Sajal Dash, and Feiyi Wang

National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: herronej@ornl.gov

Mixture of Experts (MoE) enables efficient Large Language Model (LLM) training by sparsely activating a small subset of parameters for each token, enabling large model sizes without proportional computation increases. Similarly, hybrid architectures that combine attention with State-Space models, like Mamba, have demonstrated promising capabilities in handling long contexts while maintaining competitive performance. However, a comprehensive design principle behind designing experts or determining ideal combinations of architectural components is lacking. To address this challenge, we introduce Hybrid Architecture Research for Mamba, Optimized with Neural efficiencY (HARMONY), an evolutionary neural architecture search framework for designing efficient decoder-only language models that combine transformer attention mechanisms, Mixture-of-Experts (MoE) routing, and state space model (SSM) components. HARMONY explores a comprehensive architectural search space encompassing six attention variants, variable expert configurations, and Mamba SSM parameters, enabling the discovery of heterogeneous architectures that strategically balance performance and efficiency. Our multi-objective fitness evaluation considers both training loss and computational efficiency to identify optimal configurations. We deploy our search algorithm on the Frontier exascale supercomputer across thousands of GPUs, enabling exploration of a vast design space. Experimental results demonstrate that HARMONY discovers architectures that significantly outperform existing state-of-the-art models with comparable parameter counts. The best-performing discovered architectures reveal optimal mixing ratios between different attention types and Mamba layers, along with strategic expert routing patterns. We provide the HARMONY framework as an open tool for researchers to design efficient hybrid expert models tailored to specific computational constraints and performance requirements.

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Keywords: Neural Architecture Search (NAS), Hybrid Language Models, Mixture of Experts (MoE), State Space Models (Mamba), Evolutionary Algorithms

http://www.linkedin.com/in/emily-herron-ph-d-623b43aa/

10.3 Generalizing time-series modeling of stably stratified turbulence using parameterized neural ODE

Nasik Muhammad Nafi[1]*, Murali Gopalakrishnan Meena[1], Isaac Lyngaas[1], and Stephen M. de Bruyn Kops[2]

[1] National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2] Department of Mechanical and Industrial Engineering, University of Massachusetts Amherst, Amherst, MA, 01003, USA

*Corresponding author: nafinm@ornl.gov

Unsteady Reynolds-Averaged Navier-Stokes (URANS) based turbulence modeling often requires generalization across varying physical (usually non-dimensional) parameters — for example, the Reynolds and Froude numbers for stratified turbulence. Traditional models struggle to maintain predictive accuracy across these parameters due to their limited adaptability to parameter changes. In this work, we explore the application of Parameterized Neural Ordinary Differential Equations (PNODE) to enhance the flexibility and generalization capabilities of turbulence models within the URANS setting. PNODE extends the standard Neural ODE architecture by explicitly incorporating input-dependent parameters into the dynamical system, drawing motivation from parameterized ordinary differential equations. We aim to learn continuous-time dynamics conditioned on varying physical parameters through PNODE, enabling them to adaptively capture the diverse flow outcome. We demonstrate the potential of this approach by integrating PNODE into URANS closures for stably stratified turbulent flows undergoing multiple temporal regime changes and evaluating their performance across a range of Reynolds and Froude numbers. Preliminary results indicate improved predictive accuracy and robustness compared to conventional turbulence models. Our experiments used resources from Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory, which is a DOE Office of Science User Facility.

Keywords: Turbulence Modeling, Generalization, Time Series, Latent-dynamics Learning

http://www.linkedin.com/in/nasiknafi/

10.4 DIALED into Discovery: Autonomous Active Learning for Nanoscale-Ordered Materials Diffractometer Experiments

Ankit Shrivastava[1*], Marshall McDonnell[1], Lance Drane[1], Paul Laiu[1], and Stephen DeWitt[2]

[1]Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: shrivastavaa@ornl.gov

We present a Bayesian optimization-driven active learning workflow to detect a magnetic phase transition in a powder diffraction experiment on α-Fe_2O_3 (hematite), using the Nanoscale-Ordered Materials Diffractometer (NOMAD). Our goal is to stabilize the Morin transition temperature region where magnetic "spin-flop" transition occurs while minimizing the experimental time spent to fully characterize this region.

The underlying transition is characterized by changes in the concavity of peak intensity profiles as a function of temperature and is located using Bayesian optimization to identify extrema in the second derivative of peak intensity with respect to temperature. During optimization, a trained Gaussian process infers the second derivative of peak intensity, guiding exploration toward temperatures with high uncertainty and probable extrema. The process is repeated until a convergence is observed. This approach concentrates measurements near the most informative parts of the transition while minimizing the number of experiments.

Our approach uses the Interconnected Science Ecosystem (INTERSECT) and Distributed INTERSECT Active Learning for Experimental Design (DIALED), enabling real-time decision-making and closed-loop experimentation. This framework shows how Bayesian optimization can speed up phase boundary mapping in materials with path dependence and experimental limits, such as metastable or non-equilibrium quantum and soft matter systems.

Keywords: Bayesian optimization, Autonomous experimentation, Phase boundary mapping

http://www.linkedin.com/in/ashriva16/

10.5 Credit-Based Coordination for Resolving the Tragedy of the Commons in Autonomous Agent Networks

Qixing (Jason) Wang

Transportation Analytics and Decision Science, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: wangq1@ornl.gov

In large-scale autonomous agent systems, such as networks of autonomous taxis, individually rational decisions often lead to globally inefficient outcomes—an instance of the Tragedy of the Commons. Addressing this NP-hard problem in real time is a key challenge in optimizing decentralized intelligent systems. This paper introduces a dynamic, credit-based coordination mechanism that iteratively computes the marginal effect of each agent's decision on overall system congestion. By updating credits in response to these marginal effects, agents are incentivized to choose routes that incrementally shift the system toward a global optimum. This mechanism operates without centralized enforcement, instead using localized feedback signals to rapidly approximate optimal collective behavior. Through agent-based simulations on urban mobility networks, it demonstrates that this credit-driven approach significantly reduces computational time compared to static or heuristic strategies. Moreover, it enables emergent cooperative behavior among competing agents, mitigating the Commons dilemma efficiently and scalable. This framework offers a scalable model for collective intelligence in other distributed, agent-driven environments.

https://www.linkedin.com/in/qixing-w-a0a7562b/

Oral Session 11: Manufacturing

11.1 Macro- and micro-scale evolution of SS316L powders hot isostatically pressed (HIPed) at intermittent temperatures and pressures

Pavan Ajjarapu[1*], Fred List III[2], Subrato Sarkar[2], Jason Mayeur[2], Soumya Nag[1], Samuel Bell[1], Kevin Hanson[1], Ryan Dehoff[2]

[1] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2] Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: ajjarapuk@ornl.gov

Powder metallurgy–hot isostatic pressing (PM-HIP) is a dynamic thermo-mechanical manufacturing process that strives to fabricate near-net shaped parts with presumably isotropic properties. While the primary objective of PM-HIP has been to achieve fully-dense components for industrial applications, it is quintessential to understand the mechanisms and process variables governing powder densification, can distortion, and microstructural evolution during the HIP cycle. To this effect, SS316L powders were subjected to various HIP cycles involving intermediate temperatures, pressures and soak times and characterized at different length scales to elucidate property-structure-processing (PSP) relationships. The results from this study are expected to illustrate the influence of individual process parameters on microstructure-property correlations in HIPed components, thereby aiding metal part manufacturers and modellers make informed decisions in desiging PM-HIP cycles.

Keywords: Powder metallurgy, SS316L, Hot isostatic pressing.

http://www.linkedin.com/in/pavan-kumar-ajjarapu

11.2 Development of vinyl ester resin for unsupported direct-ink-write horizontal printing

Subhabrata Saha[1*], Nadim S. Hmeidat[1], Brittany Rodriguez[1], Akash Phadatare[2], Tyler Smith[1], Patrick Snarr[3], Steve Bullock[1], Vipin Kumar[1], Ahmed Arabi Hassen[1]

[1]Manufacturing Science Division, Oak Ridge National Laboratory, Knoxville, TN, 37932, USA
[2]Mechanical, Aerospace, and Biomedical Engineering Department, University of Tennessee, Knoxville, TN, 37996, USA
[3]Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

[*]Corresponding author: sahas@ornl.gov

This study presents the development of vinyl ester resin formulation featuring a dual-cure system designed for unsupported, horizontal direct-write 3D printing using robotic UV-assisted deposition. The dual cure system comprised of UV snap cure to rapidly solidify the resin and a slow latent peroxide cure for improving the strength and toughness with minimum shrinkage. To extend the printing time specifically for large structure a two-part resin system was developed. The formulation incorporates hybrid filler systems to tailor the rheological behavior enabling unsupported printing. The two-part system was engineered to be individually non-reactive yet maintain similar viscosities to ensure uniform mixing. The robotic setup included independently controlled pneumatic pumps for precise ratio control and dual UV sources at the print head to enable rapid snap curing upon deposition. Rheological and cure kinetics analysis validated the formulation design, and horizontal printing trials demonstrated the capability of this system to produce self-supporting structures without the need for auxiliary scaffold. The results delineate the potential of the current work in advancing DIW printing providing foundation for optimizing complex geometries and high-rate hybrid manufacturing.

Keywords: Direct-ink-writing, Vinyl ester resin, UV curing, Unsupported printing.

http://www.linkedin.com/in/dr-subhabrata-saha-5b18b013b

11.3 Microscale mechanical insights into AM 316 stainless steel using Nanoindentation

Geeta Kumari[1*], Stephen Taller[1], Caleb Massey[1]

[1]Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[*]Corresponding author: kumarig@ornl.gov

Additive manufacturing (AM) of metals, such as 316 stainless steel, is increasingly used in advanced engineering applications, including those in nuclear environments. Understanding how these materials behave at small scales is critical, especially when exposed to extreme conditions like radiation. In this study, nanoindentation was used as a powerful technique to explore the microscale mechanical properties of AM 316 stainless steel, both in irradiated and non-irradiated conditions. Nanoindentation allows for precise measurement of properties like hardness and elastic modulus at the sub-micron level; something traditional mechanical tests cannot resolve. This is particularly valuable for AM materials, which often exhibit localized variations in microstructure due to layer-by-layer fabrication. The technique enabled us to detect and compare the mechanical response of features such as melt pools and heat-affected zones. In irradiated samples, changes in these properties revealed insights into the effects of radiation damage. This work highlights nanoindentation as an essential tool for characterizing advanced materials, offering high-resolution insights that support material development, qualification, and performance prediction.

Keywords: Additive manufacturing, stainless steel, nanoindentation, irradiation.

http://www.linkedin.com/in/geeta-kumari/

11.4 Finite element analysis of additively manufactured textile-inspired braided metamaterials for high specific energy absorption and shape recovery

Ajay Jayswal, Polyxeni P. Angelopoulou, Sargun Singh Rohewal, Logan T. Kearney, Sumit Gupta, Christopher C. Bowland, Michael D. Toomey, Amit K. Naskar*

[1]Carbon & Composites Group, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

*Corresponding author: naskarak@ornl.gov

Mechanical metamaterials (MMs) are engineered structures whose unique mechanical properties arise from their specific geometric arrangement, often featuring lattice-like patterns. Conventional designs, such as honeycomb and re-entrant auxetic structures, are prone to failure at sharp corners and joints due to stress concentrations during deformation. To overcome these issues, braided MMs inspired by textiles have been explored. In this study, cylindrical braided metamaterials (CBMMs) with two different unit cell designs—diamond and regular—were fabricated using fused deposition modeling (FDM) 3D printing. The process created layered assemblies of intertwined nylon strands fused at contact points, forming a robust structure. Computational models were developed to predict the deformation behavior of these CBMMs under various loading conditions, including quasi-static compression, cyclic, and creep loading at room temperature. Simulations and experiments revealed that diamond CBMMs exhibited stress softening at 30% compressive strain, supporting ~440 N, while regular CBMMs withstood ~250 N at 50% strain. Additionally, diamond CBMMs demonstrated superior creep resistance and higher energy absorption under cyclic loading compared to the regular CBMMs, although the latter showed better shape recovery (~80%) than the diamond design (~60%). These findings offer pathways for designing lightweight mechanical devices capable of enduring sustained loads while optimizing energy absorption and recovery properties.

Keywords: Cylindrical braided metamaterials, quasi-static compression, cyclic loading, specific energy absorption, creep, finite element analysis.

http://www.linkedin.com/in/ajayjayswal/

11.5 Additive manufacturing of functionally graded materials

Abdul Sayeed Khan[1], Brian Jordan[2], Yousub Lee[3], James Haley[2], Soumya Nag[1,*]

[1]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, 37830, TN, USA
[2]Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, 37830, TN, USA
[3]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, 37830, TN, USA

[*]Corresponding Author: nags@ornl.gov

Placing the right material at the right place provides a unique opportunity to utilize the capabilities of different materials in a multi-material system. Materials with extreme capabilities are, however, often complex to form a unitary compatible system and are not easy to manufacture. Combined with the powder based directed energy deposition additive manufacturing strategy, this research explores the possibilities of achieving functionally graded superalloys towards refractory alloys. The design, development and preliminary material characteristics explore possible path functions for avoiding brittle intermetallic phases between nickel based IN718 and niobium based C103 alloys. Such functionally graded materials (FGMs) are sought to provide site-specific properties of super alloys at one end and refractory alloys on the other end crucial for energy, aviation, and space sectors.

Keywords: Directed energy deposition, functionally graded materials, refractory alloys.

http://www.linkedin.com/in/abdul-sayeed-khan-17386248/

Oral Session 12: Nuclear Science 2

12.1 Characterization of irradiated Inconel 718 using in-situ SEM-EBSD analysis

Soyoung Kang[1]*, Maxim Gussev[2], Tim Lach[1], and David McClintock[3]

[1] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[2] Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[3] Neutron Technologies Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

Corresponding author: kangs1@ornl.gov

Inconel 718 was chosen for the proton-beam windows (PBWs) at the Spallation Neutron Source because of its resistance to corrosion and radiation damage. Post-service ex-situ tensile tests showed that both uniform and total elongation increase with irradiation dose. To elucidate this phenomenon, in-situ tensile testing was performed in a scanning electron microscope equipped with electron backscatter diffraction (SEM-EBSD) on PBW material with a radiation dose of 2–10 dpa. Several regions of interest (ROIs) were selected, and sequential EBSD mapping of the same ROIs during deformation captured the microstructural evolution. Deformation mechanisms were analyzed with misorientation parameters such as kernel average misorientation (KAM) and grain reference orientation deviation (GROD). As the material plastically deformed, KAM increased along grain boundaries, indicating dislocation pile-ups due to geometrically necessary dislocations (GNDs). GROD—which measures the misorientation between a point and its grain's average orientation—showed grains that bent or rotated; "hot spots" appeared near grain boundaries in the GROD maps. Correlating these parameters with plastic strain across different irradiation doses provided dose-dependent deformation behavior. The results provided a better understanding of the deformation mechanisms of irradiated Inconel 718 and the ductility enhancement reported in earlier experiments.

Keywords: 718 alloy, proton beam window, spallation neutron source, deformation mechanisms, in-situ SEM-EBSD.

12.2 Understanding hydrogen retention behavior through revealing local phase fraction variations in YH_2

Shaileyee Bhattacharya[1] *, M. Nedim Cinbiz[2] and David J. Sprouster[3]

[1] Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[2] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

[3] Department of Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, NY, 11794, USA

*Corresponding author: bhattacharya@ornl.gov

Nuclear microreactors are low power and transportable advanced reactors designed for remote or off-grid locations [1]. A key challenge in their design is the selection of moderator materials suitable for high temperature and space-constrained environments. Metal hydride-based moderators are promising due to their high hydrogen retention capacities and compact geometries [2,3]. Sub-stoichiometric yttrium dihydride (YHx) not only exhibits hydrogen retention at elevated temperatures [4], but also has high thermal stability and radiation resistance, which makes it a candidate neutron moderator for microreactor applications. However, fast neutron flux can induce hydrogen redistribution and eventual loss from the hydrides, compromising moderator effectiveness. To investigate this, YHx specimens with hydrogen-toyttrium ratios between 1.69 and 1.83 were subjected to neutron irradiation over a range of temperatures. Post-irradiation analysis of the specimens using high resolution synchrotron X-ray diffraction revealed enhanced metallic yttrium peak intensities and a corresponding decrease in the hydride phase peak intensities in the samples irradiated at higher temperatures, suggesting hydrogen depletion. Notably, the lattice parameters of all the specimens remain unchanged, indicating structural stability. An overview of the experimental results, highlighting the importance of local phase fraction variations in yttrium hydrides and their implications for microreactor applications, will be presented.

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Keywords: Microreactors, neutron moderators, yttrium hydrides, synchrotron X-rays, hydrogen retention

www.linkedin.com/in/shaileyee-bhattacharya

12.3 Maximizing Uranium recovery using monoamide extractants

Jopaul Mathew*, Marcy Lamb, Santa Jansone-Popova

Chemical Sceinces Division, Oak Ridge National Laborator, Oak Ridge, 37831, USA

nlnj@ornl.gov

The increasing global focus on sustainability has catalyzed a surge in nuclear energy demand, highlighting the urgent need for effective reprocessing of spent nuclear fuel (SNF). This process is crucial for managing nuclear waste and advancing nuclear power generation. The conventional plutonium uranium reduction extraction (PUREX) process relies on tri-n-butyl phosphate (TBP) as an organic extractant [1,2]; however, TBP presents several challenges, including non-compliance with the CHON principle and vulnerability to high radiation fields. These factors complicate purification efforts [3,4]. In response, the Group Actinide Extraction (GANEX-I) process employs monoamides, [5] with *N, N*-di-2-ethylhexyl-isobutyramide DEHiBA showing promising results in uranium and plutonium separation. This study focuses on developing novel monoamide ligands with optimized alkyl groups to enhance uranium separation efficiency. The alkyl group sizes are tailored to maintain strong U/Pu selectivity, and their degradation produces byproducts that are easily removable from the organic solvent, minimizing impact on U and Pu separation efficiency. This presentation will discuss these new organic extractant candidates and their performance in uranium dissolution, highlighting their potential role in sustainable nuclear waste management.

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Keywords: Uranium, Chemical Separations, TBP, Monoamide, dissolution

https://www.linkedin.com/in/jopaul-mathew-233573191/

12.4 Molten Salt Thermophysical Properties – Measurements and Database

Ryan Chesser[1]*, Nick Termini[1], Anthony Birri[1]

[1] Nuclear & Extreme Environment Measurements Group, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: Ryan Chesser, chesserrj@ornl.gov

Renewed interest in molten salt as heat transfer fluids and nuclear fuels has invited a greater demand for well-characterized thermophysical properties such as viscosity and thermal conductivity. Knowledge of these properties is necessary to design safe and reliable power systems. Our group focuses on experimental methods for the development of property measurements in chloride, fluoride, and actinide-bearing salts. Viscosity measurement is performed with a rolling ball technique, relating the terminal velocity of the descending ball to the viscosity of the molten salt. The thermal conductivity measurement utilizes a variable gap apparatus to measure the heat transfer across a layer of molten salt with controllable thickness. Experiments are performed at several temperatures. Correlations are developed to capture the influence of temperature on the thermophysical salt properties. These correlations are incorporated into the thermophysical arm of the molten salt thermal properties database (MSTDB-TP) managed by ORNL. This database serves as a repository for all available molten salt property measurements. These data are ranked using a six-factor quality assurance assessment developed by Idaho National Laboratory. Where sufficient high-quality duplicate data permits, reference correlations are established for each system. This presentation will focus on experimental methods and results, and the progress in developing MSTDB-TP.

Keywords: Molten Salt, Viscosity, Thermal Conductivity, Correlations, Database

http://www.linkedin.com/in/ryan-chesser-7b2772105

Posters

Factors governing thermal transport in carbon fibers reinforced nylon 6 composites for thermal management applications

Ajay Jayswal [a], Kai Li [b, *], Ercan Cakmak [c], Logan Kearney [a], Sumit Gupta [a], Kashif Nawaz [b], Amit Naskar [a, *]

[a] Carbon and Composites Group, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

[b] Multifunctional Equipment Integration Group, Buildings and Transportation Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

[c] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

*Corresponding author: lik1@ornl.gov (Kai Li)

*Corresponding author: naskarak@ornl.gov (Amit Naskar)

A thermally conductive light-weight material with enhanced mechanical properties and thermal stability is desirable for heat exchanger applications to promote the safety, reliability and functionality of the devices. To achieve this goal, this study focused on designing polymer composites with carbon fiber reinforced in semi-crystalline thermoplastic polyamide 6 matrix. The melt-mixing process followed by strategically designed compression molding process was adopted. Various fiber contents (10 wt%, 20 wt%, and 30 wt%) of different fiber lengths (0.25 inch and 0.5 inch) were explored to optimize the fiber content based on mechanical properties. In addition, the factors such as crystallinity, interfacial interaction, fibers distribution that affect the thermal conductivity of samples were studied. The out-of-plane thermal conductivity improved by 43.50 % by the incorporation of 20 wt% of CFs of 0.5-inch fiber length in the PA6 matrix as compared to that of neat PA6.

Keywords: Carbon fiber reinforced polymer composites, crystallinity, fiber orientation, thermal conductivity.

LinkedIn: https://www.linkedin.com/in/ajayjayswal/

Leveraging Exascale Computing for Scalable Drug Discovery: Integrating Multiscale Simulations and AI-Driven Molecular Design

Bharath Raghavan

Advanced Computing for Chemistry and Materials Group, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The high costs and failure rates associated with the traditional drug discovery underscore the necessity for innovative computational approaches in the early stages of drug design.[1] Integrating computer-aided drug design (CADD) and artificial intelligence (AI) methodologies can streamline this process. However, given the complexity of the simulations, these methods can be often prohibitively expensive to run. Thus, computational methods that scale well on exascale machines like Frontier can greatly aid in drug discovery.[2] This presentation explores two complementary strategies harnessing exascale capabilities to enhance drug discovery:

1. **MiMiC Framework for Scalable Multiscale Simulations**
   The MiMiC framework employs a multiple-program multiple-data (MPMD) model, utilizing Message Passing Interface (MPI) for efficient inter-program communication.[3] By coupling quantum mechanical (QM) and molecular mechanical (MM) simulations, MiMiC facilitates high-throughput, scalable simulations of large protein-ligand complexes. This approach not only aids in target identification but also refines docking predictions by providing detailed thermodynamic and kinetic insights into ligand binding processes.

2. **AI-Driven Molecular Generation in Solution**
   I discuss a technique for the AI-based generation of novel molecules and protein-ligand complexes in solution. This method leverages established work on machine learning-interatomic potentials and graph neural networks (GNNs) to allow for a highly scalable training process. This could potentially allow for de novo drug design and facilitate the hit identification stage of drug discovery.[4]

Collectively, these methodologies represent could paradigm shift in drug discovery, demonstrating how exascale computing can be leveraged to accelerate the identification and optimization of therapeutic candidates.

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Systems analysis for the development of cost competitive technologies

Chandra Sekhar Somayajula
Chemical Process Scale-Up Group, Energy and Industrial Processes Section, Manufacture Science Division, Energy Science and Technology Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
Corresponding author: somayajulac@ornl.gov

Developing cost-competitive and sustainable technologies presents significant challenges, and Oak Ridge National Laboratory (ORNL) addresses these through comprehensive systems analysis that spans a cradle-to-grave framework—from material extraction to product end-of-life. This approach integrates mass and energy balances, process engineering design, resource assessment, market analysis, and logistics to identify challenges and opportunities for cost improvements. Data gap challenges are mitigated by frequent, close interactions with researchers and industry partners to exchange information and to ensure impactful outcomes.Notable successful implementations of process modeling and scenarios analysis include cost benefits from sustainable technologies such as, biomass conversions to produce transportation fuels, conversion of atmospheric CO2 into valuable products, recycling and reusing post-end-of-life wood-based construction materials, and economic analysis of redox flow batteries. Furthermore, some applications beyond ORNL include predictive maintenance using condition monitoring and state estimation, as well as energy system modeling to assess profitability of power plant systems in the dynamic energy market. The adaptable nature of our process modeling and economic analysis methodologies allows us to tailor our approach to any system of choice, which will be showcased, thereby supporting research teams in meeting their project milestones and goals.

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Keywords: Technoeconomic analysis, process modeling and simulation, scenario analysis, state estimation.
LinkedIn: https://www.linkedin.com/in/chandrasekharsomayajula

Structural Characterization of Chitosan-Immobilized Carbonic Anhydrase with Contrast Variation SANS

Chathurika Kosgallana[1], Wellington Leite[2], Jong Keum[2,3], Yue Yuan[3] and Flora Meilleur[1,2*]
[1]Molecular and Structural Biochemistry, North Carolina State University, NC, 27695, USA
[2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[3] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
*Corresponding author: meilleurf@ornl.gov

Enzymatic immobilization within solid supports enhances enzyme stability and reusability, which is crucial for industrial applications. Chitosan, a biodegradable polymer derived from chitin, forms stable matrices that improve enzyme retention and provide mechanical strength when applied to textiles. Although chitosan-enzyme mixtures show catalytic potential, their nanoscale structural organization remains largely unexplored, yet it is essential for improving material performance. To investigate the spatial distribution of carbonic anhydrase (CA) within the chitosan matrix, we employed small angle neutron scattering (SANS) and small angle X-ray scattering (SAXS). SANS enables contrast variation through the use of deuterated chitosan and protiated CA in varying D_2O/H_2O solvent mixtures, allowing differentiation of components with similar chemical compositions. This approach facilitates detailed analysis of structural parameters such as size, shape, and spatial arrangement. SAXS provides complementary information on the overall morphology and uniformity of the hybrid complexes. In this work, we will discuss the methodology for contrast matching in SANS, analyze scattering data to extract structural features, and compare SANS and SAXS results to build a comprehensive picture of enzyme distribution within the chitosan matrix. This structural understanding is critical for guiding the design of more effective immobilized biocatalytic materials.
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Keywords: Enzyme-immobilization, Small-angle Neutron Scattering, Small-angle X-ray Scattering
Linked In: https://www.linkedin.com/in/chathurika-kosgallana/

Using process monitoring to identify voids and heat accumulation in laser powder bed fusion additive manufacturing

Christine Cummings*[1,2], Chase Joslin[1,2], Gerald Knapp[1,3], Amirkoushyar Ziabari[1,4], William Halsey[1,4], Luke Scime[1,2], Zackary Snow[1,2]
[1]Manufacturing Demonstration Facility, 2350 Cherahala Blvd, Knoxville, TN 37932
[2]Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[3]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[4]Electrification and Energy Infrastructures Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
*Corresponding author: cummingscm@ornl.gov

There is a growing need for quality assurance of parts produced with laser powder bed fusion (LPBF) additive manufacturing. LPBF is capable of creating complex geometries and low-weight performance parts for applications in aerospace, medical, energy and other critical industries. Due to the complexity, shape, and/or size of parts constructed with LPBF, traditional methods of nondestructive evaluation (NDE) can be ineffective or impossible. In situ monitoring of the LPBF process could be an alternative or supplement to these traditional NDE methods. To use in situ imaging/sensing for part qualification, however, understanding the link between detected process anomalies and material flaws is required.

Like other additive processes, LPBF parts are built layer-by-layer. On each layer, the machine distributes a thin layer of powder and uses a laser to selectively melt a slice of the part. This process repeats to create a 3D object. In this work, process monitoring images of parts were captured each layer after melting and after recoating the next layer of powder.

A dynamic multilabel segmentation convolutional neural network classified the image pixels as one or more anomaly types. This work focused on swelling, an anomaly where overbuilt material protrudes though the recoated powder and is identifiable in the post-recoat images. While swelling is a known phenomenon, the mechanisms driving swelling and the link between swelling and flaws is not well studied. We find that swelling can be an indicator of heat accumulation due to nonoptimal processing parameters or scan strategy. Additionally, swelling can be an indicator of probable void locations. We identify specific swelling signatures linked to clusters of small voids, a single large lack-of-fusion void, and clusters of large lack-of-fusion voids. These insights can be used as a framework for the interpretation of swelling anomalies for quality assurance and towards the qualification of LPBF parts.
Keywords: Additive manufacturing, laser powder bed fusion, process monitoring, flaws

Investigating size limitations of single particle inductively coupled plasma mass spectrometry in nano and microparticle research

Delaney H. Ryan,1,2* Sarah Szakas1, Benjamin T. Manard1
1Chemical and Isotopic Mass Spectrometry Group, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
2School of Civil & Environmental Engineering, Clemson University, Clemson, SC, 29634, USA
*Corresponding author: ryandh@ornl.gov

Single Particle Time of Flight Inductively Coupled Mass Spectrometry (spICP-TOFMS) is an analytical technique that allows users to analyze suspensions one particle at a time. spICP-TOFMS can easily quantify and identify nanoparticles of various sizes and compositions. This is especially useful for samples where particle size and composition are unknown prior to analysis. There are element/isotope dependent size limitations for nano and microparticles in spICP-TOFMS. For example, spICP-TOFMS has been proven to detect 20 nm solid Au nanoparticles, but the upper boundary remains relatively unknown. We explore this upper size limit by using Au particles with diameters ranging from 20-400 nm to investigate the instrument's linear dynamic range, ionization efficiency, and the effect of different integration times on the signal obtained on a per-particle basis. The results of this experimentation can aid in unsupervised analysis of particles, mixtures of particles with various size distributions, and particles analysis within a matrix. This is especially important for single cell analysis of microorganisms, which can be > 2 μm in size, as spICP-TOFMS can allow scientists to gain insight into their uptake mechanisms for heavy metals.
Keywords: spICP-TOFMS, nanoparticles, limit of detection
LinkedIn: https://www.linkedin.com/in/delaneyhryan, https://www.linkedin.com/in/sarah-szakase112233, https://www.linkedin.com/in/benjamin-t-manard-4464a967

Liquid extraction surface sampling mass spectrometry for detection of adsorbed microbial metabolites across polymer-modified surfaces

Emily A. Kurfman,[1] Vilmos Kertesz,[1] Charini Maladeniya,[2] Zhefei Yang,[2] Spenser R. Brown,[1] Jennifer L. Morrell-Falvey,[1] John F. Cahill[1]*
[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
*Corresponding author: cahilljf@ornl.gov

To aid in developing surfaces that can better control biofilm formation, a better understanding of the mechanisms of bacterial attachment to surfaces is necessary. In this work, we use mass spectrometry (MS) techniques to identify molecular components in bacterial exudates that may promote bacterial persistence across polymeric surfaces designed to reduce biofilm formation. Silicon wafer samples were either modified with antifouling zwitterionic polymers or left unmodified as a control. The surfaces were incubated with exudate from *Pantoea* sp. YR343 bacteria for four hours and rinsed with water to remove unadhered compounds before sampling. A liquid microjunction surface sampling probe (LMJ-SSP) system was interfaced with MS to collect and measure surface extracts. Using this method, unmodified surfaces and those modified with poly(1-(3-sulfonatopropyl)-2-vinylpyridinium) or poly(1-(dimethyl amino)N-oxide methacrylate) that were incubated in bacterial exudate were found to have specific compounds adsorbed to the surface. A series of related ions, *m/z* 552.3, 580.3, 608.4, and 636.4, was detected in higher abundance on unmodified surfaces.

These ions were concentrated from *Pantoea* exudate for further investigation using tandem MS and are hypothesized to be lipid products of oxidative stress. Further study of these compounds' adsorption to surfaces could help increase our knowledge of biofilm formation.
Keywords: mass spectrometry, microbes, biofilms
LinkedIn: https://www.linkedin.com/in/emily-kurfman

One-pot bioconversion of PET plastic using a thermophilic microbe

Komal Sharma Agrawal*, Austin L. Carroll, Naga Sirisha Parimi, William G. Alexander, Carrie A. Eckert, Adam M. Guss*
Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
*Corresponding authors: komal@ornl.gov , gussam@ornl.gov

Polyethylene terephthalate (PET) is a major component of unrecycled plastic waste, presenting an opportunity for conversion into valuable products. We engineered the thermophilic bacterium *Parageobacillus thermoglucosidasius* to (1) depolymerize PET into terephthalic acid (TPA) and ethylene glycol (EG), (2) utilize EG for growth, and (3) convert TPA into a value-added product. Thermophilic PETases were engineered with secretion tags to hydrolyze PET into TPA and EG at 55°C. Since thermophilic pathways for TPA and EG assimilation are unknown, we employed selective enrichment to isolate thermophiles capable of metabolizing these monomers and used systems biology to identify relevant catabolic genes. An EG degradation pathway was introduced into *P. thermoglucosidasius*, enabling growth on EG at 55°C, with further enhancement via adaptive laboratory evolution. TPA catabolism was enabled by integrating genes for its conversion to protocatechuic acid (PCA), and additional genes routed PCA into the tricarboxylic acid cycle, allowing TPA to serve as the sole carbon source. Integration of all modules enabled *P. thermoglucosidasius* to convert PET powder directly into PCA in minimal medium at 55°C. This was supported by novel genetic tools including a strong thermophile-specific promoter and characterization of restriction-modification systems, laying the foundation for high-temperature, single-organism PET bioprocessing.
Keywords: PET biodegradation, consolidated bioprocessing, synthetic biology, thermophilic pathway engineering.
LinkedIn: https://www.linkedin.com/in/komal-sharma-ag/.

Examining EBC coating systems on SiC substrates in varying high temperature steam oxidizing environments

Kristyn D. Ardrey*, Michael J. Lance, Mackenzie J. Ridley
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
*Corresponding author: ardreykd@ornl.gov

Abstract content
The study of Si-bond coat TGO properties in EBC systems on SiC/SiC CMC substrates is crucial for understanding coating failure and lifetime, as TGO growth at the EBC/Si bond coat interface can cause spallation [1][2]. Various SiC substrates (CVD β-SiC, sintered α-SiC, reaction-bonded SiC) are used in lab-scale investigations, but their impact on TGO microstructure and chemistry remains unclear. This research aims to systematically assess how different SiC substrates affect TGO properties in high-temperature steam environments, with the goal of refining EBC testing protocols. Additionally, limited research exists on state-of-the-art EBC systems in high-temperature, high-pressure steam environments, making studies of Y-doped $Yb_2Si_2O_7$ coatings on SiC substrates limited for high pressure exposures. This research will address this gap in the literature and explore the effects of Y-doping in EBCs in a high-pressure environment and its potential to enhance coating stability and resistance to failure.
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Keywords: EBCs, SiC-CMCs, thermally grown oxide, high temperature corrosion, rare-earth silicates
LinkedIn: https://www.linkedin.com/in/kristyn-ardrey-953061128

Travel Patterns and Characteristics of Millennial Population in New York State

Latif Patwary1*, Melrose Pan1, Majbah Uddin1, Tim Reuscher1
1 Buildings and Transportation Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA
*Corresponding author: patwarya@ornl.gov

Millennials (born 1981–1996) represent the largest segment of the U.S. population, surpassing baby boomers. Their distinct lifestyle, technology use, and transportation preferences significantly impact urban planning and infrastructure development. Understanding millennial travel patterns is crucial for policymakers aiming to accommodate evolving transportation demands. Using data from 2009, 2017, and 2022 National Household Travel Surveys, this study analyzes sociodemographic characteristics and travel behaviors of millennials in New York State, comparing them with older generations (Gen X and baby boomers) and younger cohorts (Gen Z). Results show millennials consistently make fewer daily trips than Gen X and baby boomers, though this gap has narrowed over the past decade. The study identifies a range of factors that shape the travel behavior of millennials. Key influences include gender, driving status, employment, travel party size, household income and size, vehicle ownership, and the built environment. For instance, in 2017, millennials across all regions dedicated a significant portion (~28%) of their trips to work, which is the highest across all generations. They also led in adopting ridesharing, online shopping, and micromobility solutions. The study findings necessitate multimodal and technology integrated transport strategies to meet millennials' evolving mobility preferences.

Keywords: Millennials, Travel Behavior, Mobility Trends, Urban Planning

LinkedIn: https://www.linkedin.com/in/alp20/

Flow through a U-Bend: Comparing Four Turbulence Models with Experimental Results

Louis Dagobert[1,2*], Alexander DeMarco[2], Vincent Nyagilo[2], Barbara Zavala[2]
1 Nuclear Nonproliferation Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
2 Thomas J. Watson College of Engineering and Applied Science, Binghamton University, Binghamton, NY, 13850, USA
*Corresponding author: dagobertla@ornl.gov

Magnetic resonance velocimetry (MRV) is an emerging flow-measuring technique. It uses magnetic resonance imaging (MRI) to obtain the velocity fields in flows. Elkins and Alley (2007) listed the many applications of MRV in analyzing engineering flows. Benson et al. (2020) demonstrated that MRV can measure a three-dimensional, three-component velocity field of water going through a tight U-Bend. Han et al. (2021) have done simulations in ANSYS Fluent representing that experimental setup and have found that simulation results agreed with Benson's experiment. The objective of this project was to reproduce the flow simulated by Han et al. (2021). Three of the turbulence models employed by Han et al. (2021) were used by the participants in this project. The results between both groups were nearly the same. The fourth turbulence model used in this project was the Reynolds stress model (RSM). When all the results were compared to the measurements made by Benson et al. (2020). It was found that each turbulence model excelled at predicting certain regions of the flow, while noticeably falling short in other regions. The SpalartAllmaras (SA) model gave reasonable predictions throughout the entire flow.

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Keywords: Magnetic Resonance Imaging (MRI), Magnetic Resonance Velocimetry (MRV), Computational Fluid Dynamics (CFD), Reynolds Stress Model (RSM), ANSYS Fluent

Linked In: https://www.linkedin.com/in/louis-dagobert

Constitutive and Inducible Oleoresin Defenses Share Genetic Architectures and Mechanisms in *Pinus taeda*

Mallory Morgan[1,2], Jared Westbrook[1,3], Salvador Gezan[4], Tania Quesada[1], Robert Sykes[5,6], Timothy S. Johnson[7], Gabriela Madrid[2], Matthew Lane[8], Alice Townsend[8], Christopher Dervinis[1], Thomas A. Colquhoun[7], John M. Davis[1], Daniel Jacobson[2], Gary F. Peter[1]

[1] School of Forest, Fisheries, and Geomatics Sciences, University of Florida, Gainesville, FL
[2] Computational and Predictive Biology Group, Oak Ridge National Laboratory, Oak Ridge, TN
[3] The American Chestnut Foundation, Asheville, NC
[4] VNS International, Hemel Hempstead, UK
[5] National Renewable Energy Laboratory, Golden, CO
[6] Los Alamos National Laboratory, Los Alamos, NM
[7] Department of Environmental Horticulture, University of Florida, Gainesville, FL
[8] Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee-Knoxville, Knoxville, TN

Corresponding author: gfpeter@ufl.edu

We characterized the genetic architecture of constitutive and induced oleoresin flow and stem wood terpene content with quantitative genetic analyses and genome wide association studies (GWAS) in two clonal populations of *Pinus taeda*. Genetic analyses with ten oleoresin-related traits show polygenic inheritance and trait-to-trait correlations provide strong evidence for shared genes regulating constitutive and induced oleoresin flow. We identified high- and low-yielding genotypes to validate our quantitative genetic models. We discovered 236 SNPs significantly associated with oleoresin flow, resin canal number, and terpene composition, across two populations using multiple SNP sets and models. We used a systems-level approach to understanding gene function by exploring orthologous gene-gene interactions with multiplex network learning to uncover the shared genetic basis of constitutive and inducible defense. Our GWAS identified pine genes likely involved in essential defense mechanisms, including seven genes in terpene biosynthesis, four genes in pathogen recognition and immune priming, six genes regulating transcriptional responses to biotic stress, and five putative regulators of cambial meristem reprogramming and cell differentiation. Our approach leverages orthology and multiplex networks derived from experimental and predictive evidence to enable in-depth interpretation of gene modules that move beyond the one-trait-one-gene paradigm and demonstrate that breeding programs can simultaneously enhance terpene composition, constitutive and inducible oleoresin flow, and growth performance for improved resistance and biofuel potential.

Keywords: loblolly pine, quantitative genetics, genome wide association study (GWAS), plant immunity, systems biology

LinkedIn: https://www.linkedin.com/in/mallory-morgan-03728592/

Extending ExaDigiT's Resource Allocator and Power Simulator (RAPS) for Scheduling and Synthetic Workload generation

Matthias Maiterth, Wesley H. Brewer, Feiyi Wang, [1]
[1]Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
Corresponding author: maiterthm@ornl.gov

Digital Twins of HPC Systems help to model and understand a systems behavior [1,2]. Traditional approaches of evaluating scheduling are limited to post-deployment analysis of the systems in action, or scheduling simulators, which generally do not model associated HPC. For what-if scenarios using data center digital twins, the integration of scheduling simulators provide additional parameters, expanding the state space of study. This work presents progress on the integration of schedulers and datacenter digital twins. The poster shows the current state, as implemented in the ExaDigiT Project [3], and shows extensions for the integration of scheduling simulation and the use of public datasets within the framework, as well as work on synthetic workload generation.

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Scheduling Simulators, Digital Twin, Data Center Digital Twin, System Simulator, Distributed Systems Simulation, Batch Scheduling

LinkedIn: https://www.linkedin.com/in/matthiasmaiterth

Temperature-dependent Neutron Diffraction Study of a New Piezoelectric

Mohit Chandra[1, *], Brooke N. Richtik[2], Michelle Dolgos[1, 2], and Alicia Manjón-Sanz[1]
1Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
2University of Calgary, 2500 University Drive NW, Calgary, AB, T2N 1N4 Canada *Corresponding author: chandram@ornl.gov

Piezoelectric ceramics generate an electric charge in response to mechanical stress and vice versa [1, 2]. Lead Zirconate Titanate, Pb(Zr1-xTix)O3 (PZT), is the current industry standard and the basis for almost all generators, actuators, sensors and related applications critical in today's technology. PZT ceramics exhibit a relatively low operating temperature, normally only used below a temperature of 350 °C. This fact is due to phase instability and piezoelectric performance decrease around and above their curie temperature (Tc) of 350 °C for PZT [1]. However, there is insufficient research on materials for high-temperature piezoelectric applications, yet they have important applications in the critical equipment of aeroengines and nuclear reactors in harsh and high-temperature conditions [2]. Achieving high piezoelectric performance alongside a high Tc remains a major challenge. Here, we propose to synthesize and investigate the structure-property relationships of high Tc advanced functional ceramics [3, 4] using neutron powder diffraction measured on the POWGEN beamline of the Spallation Neutron Source, Oak Ridge National Laboratory [5]. Such relationships are critical to the design and optimization of piezoelectric devices.

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Keywords: Piezoelectric, High Curie temperature, Bismuth-based perovskite, Structural phase transition
LinkedIn: mohit-chandra-bb29491b6

Extraction and stimuli-driven release of superhydrophilic oxyanions using amphiphilic iminoguanidine ligand

Nabarupa Bhattacharjee, Radu Custelcean, Jeffrey D. Einkauf*
Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830, USA
*Corresponding author: einkaufjd@ornl.gov

Superhydrophilic oxyanions (SO_4^{2-}, SeO_4^{2-}, CrO_4^{2-}) are extremely difficult to separate from aqueous solutions owing to their high free energies of hydration. Nevertheless, their targeted separations are a crucial part in the processing of legacy nuclear waste, oil production, and desalination. Various high-affinity synthetic receptors have been reported to achieve selective oxyanion separation through molecular recognition; however, relatively fewer can overcome the Hofmeister bias to liquid-liquid extraction (LLE) of these ions, especially from increasingly complex and dilute mixtures. Additionally, achieving high affinity and selectivity often leads to difficulties in releasing (stripping) the captured ion without generating dilute waste streams and large amounts of secondary wastes. Herein, we address this issue by designing an amphiphilic, photoactive iminoguanidine ligand (SGPyDIG) appended with long alkyl chains. This ligand can be readily synthesized as a chloride salt in one step and its high solubility in non-polar solvents (1,2- dichloroethane) make it a desirable candidate for LLE. SGPyDIG can facilitate selective (~90 %) removal of oxyanions from aqueous

solution over chloride. This remarkable selectivity may be attributed to a combination of two factors: (1) oxyanion recognition through hydrogen bond interaction of the guanidinium core of the ligand and (2) through formation of large aggregates in the non-polar solvent. Additionally, when stimulus in the form of light or heat is used, a triggered release (~89 %) of the captured ion is achieved. This work establishes a sustainable liquid-liquid separation system for challenging superhydrophilic oxyanions, which in turn can help inspire future advances in critical separations.
Keywords: oxyanions, liquid-liquid extraction (LLE), iminoguanidine.

A machine learning model for predicting nonlinear 1D saturated potentials from linear gyrokinetic simulation data

Preeti Sar1*, Sebastian De Pascuale1, Harry Dudding2, Gary Staebler1
1 Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA
2 United Kingdom Atomic Energy Authority, Abingdon, Oxfordshire, United Kingdom
*Corresponding author: sarp@ornl.gov

Turbulent instabilities are a primary driver of transport in the core of tokamak plasma. Nonlinear gyrokinetics represents the most accurate plasma turbulence modelling paradigm available, having been extensively validated against experiments to accurately simulate local turbulent fluxes. However, full fidelity gyrokinetic simulations are computationally expensive making it impractical for use in integrated modelling simulations, in which one is required to simulate many flux surfaces over confinement timescales. Quasilinear models such as TGLF and QuaLiKiz are instead used for this purpose, which bypass the expense of calculating the fluxes in the nonlinear gyrokinetic system by instead solving for the linear response of the plasma instabilities, which is then combined with an estimation of the magnitude of the saturated potentials, giving the largest contribution to the fluxes, via a saturation rule to provide calculations in greatly reduced time. The latest quasilinear saturation rule, SAT3 [1], is an accurate model of the saturated potential for an enhanced CGYRO database that encompasses most common ITG and TEM turbulence regimes found in experiments. It does not however represent a complete description of turbulent plasma transport and will perform less reliably in a parameter space far from its empirical regression. In this work, we formulate a generalized framework to predict the magnitude of the 1D saturated potentials against the poloidal wavenumber from local linear simulation growth rates and frequencies, using a neural network architecture trained on a database of high-resolution nonlinear CGYRO simulations. This database is the same as the one used in SAT3 and will be expanded by adding more simulation runs over new parameter ranges. Hence, the resulting neural network model is targeted to generalize well within ITG and TEM turbulence regimes. A machine learning fit that models the squared potentials more accurately will improve the calculation of the total energy and particle fluxes as well as considerably reduce the simulation time in integrated modeling.

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Keywords: Gyrokinetics, machine learning, saturated potentials, quasilinear models, CGYRO, tokamak core transport
LinkedIn: https://www.linkedin.com/in/preeti-sar-29143417/

Leveraging thermal fluctuations to investigate the spin dynamics of quantum magnets

Pyeongjae Park[1]*, G. Sala[2], Daniel M. Pajerowski[3], Andrew F. May[1], James A. Kolopus[1], D. Dahlbom[3], Matthew B. Stone[3], Gábor B. Halász[1]* and Andrew D. Christianson[1]*
[1] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[2] Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
[3] Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
*Corresponding author: parkp@ornl.gov, halaszg@ornl.gov, christiansad@ornl.gov

Low-dimensional or frustrated quantum ($S = 1/2$) magnets exhibit strong quantum spin fluctuations, leading to complex spin dynamics that challenge conventional spin-wave analysis and complicate the identification of microscopic spin models using neutron scattering. However, raising the temperature moves these systems into a regime dominated by classical thermal fluctuations, making their dynamical properties more amenable to semi-classical analysis. In this presentation, we introduce an approach that leverages thermal fluctuations to study the momentum and energy-resolved spin dynamics of quantum magnets, using the Landau-Lifshitz dynamics (LLD) framework implemented in the Su(n)ny software package [1]. We will outline a standardized simulation protocol designed for modelling finite-temperature spin dynamics [2, 3] and present its successful application to the inelastic neutron scattering results of two model systems: the $S = 1/2$ square lattice Heisenberg antiferromagnet $Zn_2VO(PO_4)_2$ [2] and the $S = 1/2$ XXZ triangular lattice antiferromagnet $Ba_2La_2CoTe_2O_{12}$ [4]. Notably, this approach has successfully determined spin Hamiltonians by fitting energy-resolved excitation spectra in the paramagnetic phase while also capturing the attenuation of quantum spin dynamics–such as continuum excitations–due to thermal fluctuations. We will conclude by discussing the broad potential of this LLD-based approach for advancing cutting-edge research in quantum magnetism.

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Keywords: Quantum magnetism, Inelastic neutron scattering, Spin dynamics simulations

Ablate and Illuminate: High-Resolution Bioimaging with LA-ICP-TOFMS

Sarah Szakas[1], Benjamin Manard[1]
[1]Oak Ridge National Laboratory
Corresponding author: szakasse@ornl.gove

Bioimaging via laser ablation inductively coupled plasma time-of-flight mass spectrometry (LA-ICP-TOFMS) has become a method of choice to investigate metal accumulation and distribution in a variety of tissue and biological samples. Benefits of using a TOF mass analyzer include the ability to monitor multiple nuclides/isotopes in a single laser pulse, as well as detect micro-scale inclusions via fast integration time (2 ms). This allows for precise, high-resolution images for elemental and isotopic mapping. Maps of mouse brain cross-sections were used to optimize laser mapping conditions for both human lung and ovarian tissues. Lung tissues from both smokers and nonsmokers were compared, and ovarian tissues were obtained from patients with and without ovarian cancer. By detecting the full mass range (m/z 6 to 258), elements of interest can be used to differentiate each sample. LA-ICP-TOFMS was also used to examine plant-microbe interfaces by abating the cross section of roots. The maps obtained show the accumulation of microbes around the roots from the detection of endogenous metals.

Keywords: Laser ablation, ICP-MS, mass spectrometry

LinkedIn: www.linkedin.com/in/sarah-szakas-e112233

Discrepant impact of CNTs as additive on lubricant tribological performance

Wenbo Wang[1], Xiaoqian Wang[2], Chanaka Kumara[1], Harry M. Meyer[3], Ning Ren[2], Jacob Bonta[2], Edward Murphy[2], Roger D. England[2], James A. Haynes[1], Jun Qu[1,*]
1. Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
2. Valvoline Global Operations, Lexington, KY, 40509, USA
3. Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
*Corresponding author: qujn@ornl.gov & Equal contribution

Cabron nanotubes (CNTs), used as lubricant additives in a non-polar base oil, demonstrated discrepant effects on wear protection in two common tribological tests: four-ball unidirectional sliding and HFRR ball-on-flat reciprocating sliding.

The CNT surface was functionalized with a phenyl ligand and a dispersant (PIBSI) was used to achieve stable suspension and dispersion before tribotesting. In the four-ball test, PIBSI alone did not provide effective wear protection but the CNTs effectively reduced wear loss. However, in the HFRR test, the PIBSI alone led to strong wear reduction but the addition of CNTs had no further improvement. This discrepancy was hypothetically attributed to the different wear protection mechanisms by the PIBSI and CNTs, which responded distinctively under different testing conditions. Additional unidirectional and reciprocating sliding tests with matched Hertzian contact pressures supported the hypothesis. Further analysis of worn surface morphology and tribofilm composition reinforced the proposed wear mechanisms. Fundamental understanding gained in this study provided insights into the potential benefits and limitations of using CNTs in lubrication.

Keywords: Carbon nanotubes (CNTs), Dispersant, Lubricant additives, Wear, Contact pressure

LinkedIn: https://www.linkedin.com/in/wenbo-wang-5a98b6118/

Understanding Wetting Behavior of Graphite by Water Contact Angle Measurement

Wenqi Li[1,*], Gang Seob Jung[2], Jose' David Arregui-Mena[3], Lianshan Lin[3], Jisue Braatz[4], Cristian Contescu[3], Jun Qu[3] and Nidia Gallego[1]

1 Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA
2 Computer Sciences & Engineering Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA
3 Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA
4 Isotope Science & Enrichment Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA
Corresponding author: gallegonc@ornl.gov

In this study, we use Highly Oriented Pyrolytic Graphite (HOPG) as a model of graphitic material. A goniometer equipped with an environmental chamber was employed to measure the water contact angle of HOPG. The chamber enables precise control of temperature and humidity during measurements, allowing accurate assessment of wetting behavior under well-controlled conditions. Based on our contact angle measurements and comparison with previous studies, we believe the intrinsic wettability of graphitic materials is hydrophobic. Additionally, the initially hydrophilic nature observed on freshly cleaved HOPG surfaces can be attributed to oxygencontaining functional groups formed at surface defects during exfoliation, as well as wetting transparency effect driven by van der Waals forces from the underlying graphene layers. Molecular dynamics (MD) simulations reveal that exposing a fresh surface will trigger an irreversible structure defect, such as ripples and wrinkles, on the top graphene layer, driven by defect relaxation at grain boundaries and the release of interlayer confinement. As exposure time increases, these structural deformations grow and the distance between the top graphene layer and the underlying layers expand, which leads to significant increase in water contact angle over time and the transformation of surface behavior from hydrophilic to hydrophobic.

Keywords: Graphite, Contact Angle, Wetting Behavior.

LinkedIn: https://www.linkedin.com/in/wenqi-li-19a522aa/

Hybrid quantum/classical algorithms for exotic quantum chemistry

Zachary W. Windom*, Daniel Claudino

Computational Sciences & Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
*Corresponding author: windomzw@ornl.gov

The exact solution to the electronic Schrödinger equation represents the "holy grail" of quantum chemistry, as such knowledge would enable *ab initio* prediction of all material properties. Despite being the formal objective, practical applications require compromises between computational tractability and approximation fidelity. To this end, ansätze based on low-rank coupled cluster (CC) theory provide experiment-quality predictions for "well-behaved" systems using classical algorithms that scale polynomially with system size. However, systems involving more exotic electron correlations demand higher wavefunction resolution, which can be computationally prohibitive on classical hardware. Quantum computers, by contrast, are anticipated to overcome this limitation. Nevertheless, trade-offs between fidelity and affordability will persist for the foreseeable future, given the current limitations of quantum hardware—namely, a restricted number of qubits and significant error rates. To address this, we propose a hybrid algorithm that first optimizes low-rank unitary coupled cluster (UCC) ansätze on a quantum computer, and then uses a classical computer

to correct for the missing electron correlations [1–3]. We show that this approach yields more accurate and affordable predictions, representing a practical intermediate between current computing technologies and fault-tolerant quantum computers.

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Keywords: Unitary coupled cluster theory, perturbative corrections, hybrid computing

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