12TH ANNUAL
OAK RIDGE POSTDOCTORAL ASSOCIATION
RESEARCH SYMPOSIUM

JULY 11–12, 2024

TENNESSEE ROOMS

OAK RIDGE National Laboratory | U.S. DEPARTMENT OF ENERGY

CONTENTS

FOREWORD BY LABORATORY DEPUTY DIRECTOR FOR SCIENCE AND TECHNOLOGY

I want to thank the Oak Ridge Postdoctoral Association (ORPA) Executive Committee for bringing together the Laboratory community for the 12th Annual Research Symposium. This unique event offers a look at some of the great things happening across the Oak Ridge National Laboratory (ORNL) science and technology portfolio, providing a platform for colleagues from ORNL and our partner universities to convene, learn, and motivate each other. I am excited for what is ahead!

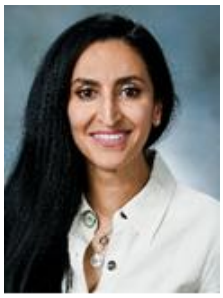
This year's symposium will give you a taste of the global challenges we're tackling as an institution. By leveraging the incredible acceleration in scientific innovation, we are working to harness the power of artificial intelligence and quantum, addressing the worldwide effects from climate change, and delivering advancements to enable a clean energy future.

To truly make an impact in these areas and beyond, we utilize team science—pulling in people with diverse expertise and different experiences—to turn big ideas into discoveries and solutions important for our mission. As a PhD student, I was fortunate to have the opportunity to experience this at a national laboratory, and it has certainly influenced my career path. Over the next couple of days, I encourage you to learn more about the breadth of research ongoing at ORNL and how multi-disciplinary teams are tackling some of the most pressing challenges of our time. I also encourage you to talk with those outside your area to better understand the challenges they are working on and consider how you could potentially collaborate. The connections and network you create now could shape your career, your research, and its impact.

I hope you enjoy this year's symposium!

Dr. Susan Hubbard
Deputy Director for Science and Technology

FOREWORD BY OFFICE OF RESEARCH EDUCATION DIRECTOR



I'm pleased to welcome you to ORNL's 12th annual ORPA Research Symposium! The Oak Ridge Postdoctoral Association Executive Committee has curated an exceptional program, offering a platform for sharing groundbreaking research and engaging with the work of peers. It's impressive to see such a diverse range of presentations and posters featured this year—a testament to ORPEX's dedication to delivering a dynamic scientific agenda and to your commitment to sharing your research.

This year, we are introducing six distinguished keynote speakers who will share their insights and experiences, providing valuable perspectives on various research topics. Additionally, we are introducing Innovation Hours, a new segment designed to foster creativity and collaboration with industry partners.

I extend my heartfelt gratitude to ORPA's Research Committee chairs, Aniket Pramanik and George Yumnam, and Laurie Varma from the Office of Research Education (ORE) for their meticulous organizing efforts; to all our postdoc and postdoc ally volunteers who have tirelessly worked to bring this program to fruition; and to the ORNL staff members who are generously serving as judges.

ORPA and the Executive Committee play a pivotal role in nurturing a robust scientific community at ORNL. Their activities span from welcoming new postdocs and providing essential information to fostering a sense of community through various social events, promoting volunteer opportunities to connect with the broader community, and facilitating career development through programs like the annual Research Symposium. Key events this year include the R U Feeling OK? activities, the Your Science in a Nutshell competition, Postdoc Appreciation Week, and the newly introduced Innovation Hours, which will take place on Friday afternoon during this year's symposium. Innovation Hours offers symposium attendees the opportunity to share their science with industry representatives keen on learning more about the world-leading research being undertaken here at ORNL by our postdocs and early-career staff. Through a holistic approach, ORPA ensures that postdoctoral researchers are well-prepared for the next steps in their careers and remain actively engaged during their tenure at ORNL.

This year, the Executive Committee continues to build connections with postdoc associations at other national laboratories, particularly with Idaho National Lab. Their commendable efforts are set to expand these relationships, enhancing the collaborative spirit and programmatic success that define our postdoc community. ORPA's sustained efforts uphold ORNL's reputation as a premier institution for postdoctoral research—a place where you can emerge as leaders in your fields and forge professional relationships that transcend disciplinary boundaries. The excellence of ORNL's postdoc experience directly contributes to ORNL's standing as a global research leader.

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

Best wishes,

Moody Altamimi
Director, Office of Research Education

FOREWORD BY THE ORPA PRESIDENT

On behalf of the Oak Ridge Postdoctoral Association (ORPA), I am honored to welcome you to the 12th Annual Research Symposium! This year's event holds a special significance as it coincides with ORPA's 10th anniversary of fostering and supporting postdoctoral researchers at ORNL.

The symposium provides a valuable platform for postdoctoral researchers and early-career scientists at ORNL to showcase their ongoing work. Through presentations, posters, and dedicated networking sessions, researchers will spark stimulating discussions and explore potential collaborations across various scientific disciplines at ORNL. 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.

This year's symposium promises to be even more enriching, with the exciting addition of representatives from several esteemed companies and universities joining us for Innovation Hours, scheduled for the second day of our symposium. This unique opportunity will allow researchers to connect with potential employers and gain valuable insights into the industry and academia landscapes. To further facilitate these connections, we will have a dedicated space for researchers and company representatives to engage in more in-depth discussions.

The success of this symposium would not be possible without the invaluable 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.

Thank you for your participation in the 12th Annual ORPA Research Symposium.

Sincerely,

Huixin (Anna) Jiang
President, ORPEX24

FOREWORD BY THE ORPA RESEARCH CO-CHAIRS

Welcome to the 12th Annual ORPA Research Symposium!

As co-chairs of the Oak Ridge Postdoctoral Association (ORPA), it is our pleasure to join in welcoming you to this year's symposium. This event not only marks our 12th symposium but also celebrates a decade of ORPA's commitment to fostering the professional and personal growth of postdoctoral researchers at ORNL. The symposium serves as a dynamic platform where postdoctoral researchers and early-career scientists can present their cutting-edge work through presentations, posters, and interactive networking sessions. These activities are designed to spark insightful discussions and pave the way for interdisciplinary collaborations within ORNL. Such interactions are integral to our mission of nurturing a collaborative research environment.

This year, we are particularly excited to introduce Innovation Hours on the second day of the symposium. This new addition will feature representatives from various companies, offering a unique opportunity for attendees to network with potential employers and gain valuable perspectives on careers in both industry and academia.

We would like to extend our heartfelt thanks to Dr. Moody Altamimi, Director of the Office of Research Education (ORE), and Laurie Varma, Early Career Programs Specialist in ORE, for their unwavering support and guidance. Their dedication to ORPA and their commitment to the professional development of our postdoctoral researchers are instrumental to the success of this symposium.
Thank you for
being a part of the 12th Annual ORPA Research Symposium. We look forward to the engaging presentations and fruitful discussions that this event will undoubtedly bring.

Best regards,

George Yumnam and Aniket Pramanik
Research Co-chairs, ORPEX24

VOLUNTEERS ACKNOWLEDGEMENT

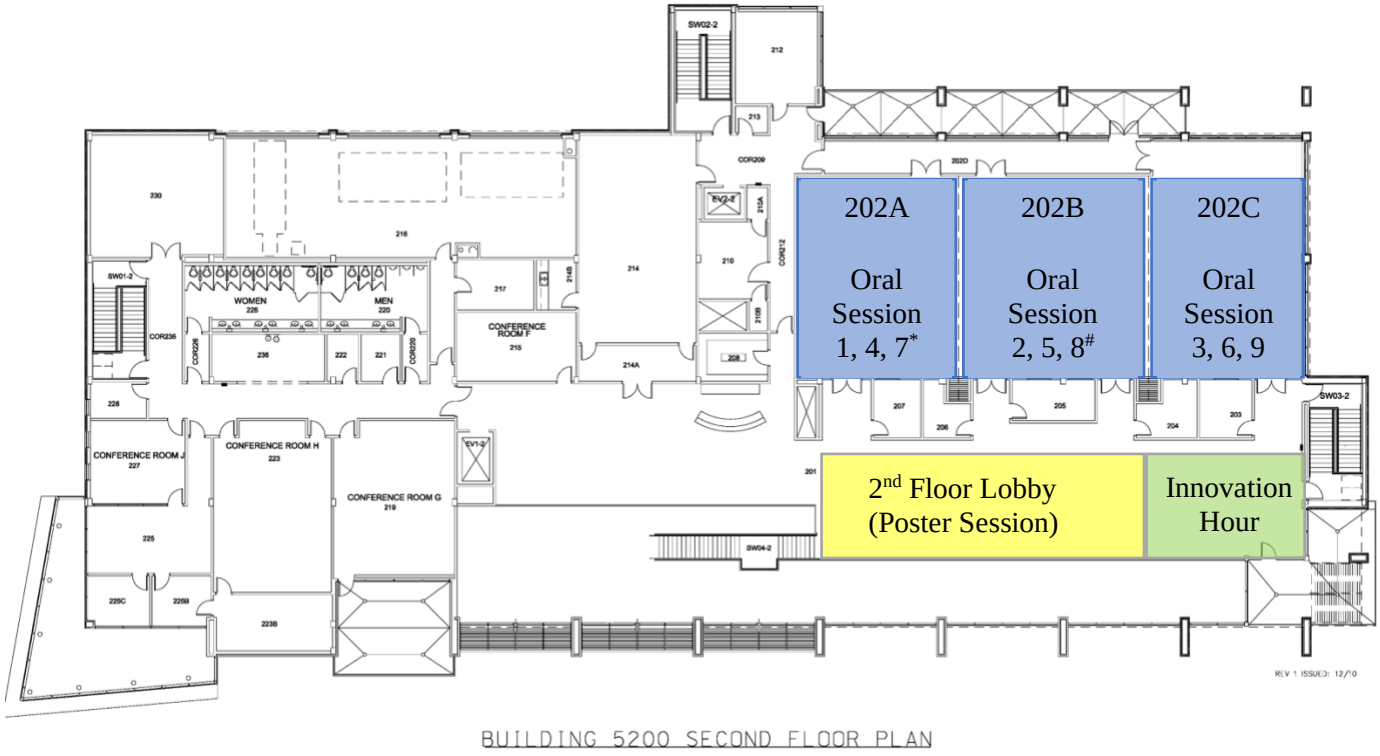
We are extremely thankful to all the volunteers who helped organize this symposium including the ORPEX24 board members.

List of Volunteers who contributed to making to the symposium a success.

Arvind Ganesan
Ajay Jayswal
Huixin Anna Jiang
Pavan Ajjarapu
Aubrey Fine
Nadim Hmeidat
Bo Xiao
Duygu Vargun
Ryan Morelock
Elise Phillips
Polyxeni Angelopoulou
Ritin Mathews
April Armes
Celestin Bourgery
Tanvir Sohail
Aaron Onufrak
Samuel Fagbemi
Jayasai Rajagopal
Qiangsheng (Johnson) Lu
Parul Raghuvanshi
Christianna Brantley

EVENT LOCATION AND CONTACTS

Event contact	George Yumnam (yumnamg@ornl.gov) and Aniket Pramanik (pramanika@ornl.gov)
Location	ORNL Conference Center, Building 5200, Tennessee Rooms (A/B/C) and 2nd Floor Lobby



BUILDING 5200 SECOND FLOOR PLAN

*All Keynote Sessions: 202A
Boxed Lunch (11th July): 202 B

OAK RIDGE POSTDOCTORAL ASSOCIATION 12TH ANNUAL RESEARCH SYMPOSIUM

AGENDA

JULY 11, 2024 (DAY – 1)			
09:00 – 09:10	Room 202A	**Stephen Streiffer (ORNL Director)**	Lab Director's address and Welcome Remarks
09:10 – 09:20	Room 202A	**Aniket Pramanik** and **George Yumnam**	Research Symposium Plan and Welcome Remarks
09:30 – 10:15	Room 202A	**David Sholl *(Keynote 1)***	Net-zero by 2050: Can we get there?
10:15 – 10:30	BREAK		

	Oral Session 1 (Biological Sciences) Room 202A	**Oral Session 2 (Materials Science - 1) Room 202B**	**Oral Session 3 (Materials Science - 2) Room 202C**
10:30 – 10:45	**Biruk Feyissa** *Microbial DNA fragments (MDF) integration into the host Populus trichocarpa nuclear genome alters plant traits*	**Tanvir Sohail** *Tuning Skyrmion Physics for Next-Generation Spintronics*	**Puspa Upreti** *Impact of phonon coupling to electric field on thermal transport in a relaxor ferroelectrics*
10:45 – 11:00	**Celestin Bourgery** *Discovery and engineering of nylon hydrolase for nylon recycling*	**Yuchen Jiang** *Magnetohydrodynamic pressure drop in nuclear fusion blanket*	**George Yumnam** *Enhanced magnetic-disorder driven magnon softening of TbSb via Y-doping*
11:00 – 11:15	**April Armes** *Deciphering Microbial Communication in Microbial Community Assembly*	**Ernesto Camilo Z. Suarez** *Electrochemical characterization of sulfur catholytes used in redox flow batteries*	**Yueh-Chun Wu** *Nanoscale magnetic ordering dynamics in a high Curie-temperature ferromagnet*
11:15 – 11:30	**Elise Phillips** *Layered regulation of the Cas9 nuclease significantly reduces leaky, incidental expression*	**Achutha Tamraparni** *Experimental Investigation and Performance Characterization of PCM Integrated Finned Tube Heat Exchanger for Building Heating and Cooling Applications*	**Jane Chen** *Te-vacancy enhanced superconduc1vity in hybrid interface $FeTe_{1-x}Se_x/Bi_2Te_3$ grown by molecular beam epitaxy*
11:30 – 11:45	**Kewei Chen** *Linking hydrologic exchange flow and biogeochemical modeling to quantify methane emission from rivers*	**Lynda Amichi** *Resolving Heterogeneous Hydrogen Fuel Cell Catalyst Degradation at the Nanoscale via Automated 3D Electron Tomography*	**Thomas Ruland** *Improving Reactor Decay Heat Data*

11:45 – 12:00	**Lynnicia Massenburg** *Cryo-EM, SANS and SAXS reveal structural insights on subunit-subunit and lobe-lobe interactions from Physcomitrium patens cellulose synthase 5*	**Jordan Stanberry** *MicroExtraction-ICP-MS for the Direct Analysis of Nanoparticles Loaded on a Solid Surface*	**Bogdan Dryzhakov** *Enhancing aluminum nitride's ferroelectric switch through irradiation-engineered defects*

12:00 – 12:30	LUNCH RECESS		
12:30 – 13:15	Room 202 A	**Vittorio Badalassi (*Keynote 2*)**	Designing Fusion Reactors with Supercomputing
13:15 – 13:30	BREAK		

	Oral Session 4 (Chemistry) Room 202A	**Oral Session 5 (AI / ML) Room 202B**	**Oral Session 6 (Manufacturing 1) Room 202C**
13:30 - 13:45	**Subhamay Pramanik** *Capturing Promethium in Solution*	**Malgorzata Makos** *Reaction Pathways Search using Adaptive-Learning Global Optimization and Generative Adversarial Networks*	**Pavan K Ajjarapu** *Convergent Manufacturing of 316L Stainless Steel Hot Isostatically Pressed (HIP) Canisters*
13:45 – 14:00	**Jopaul Mathew** *Revolutionizing Uranium Recovery: Monoamides for enhanced U/Pu Separation*	**Ganesh Narasimha** *Automated structure discovery via active learning in STM.*	**Gyan Shankar** *Effect of laser melt schedule on the microstructure of additively manufactured IN718*
14:00 - 14:15	**Nicholas Gregorich** *A Membrane Contactor Enabling Energy-Efficient CO2 Capture from Point Sources with Physical Solvent*	**Maria Mahbub** *AI-Powered Insights: Streamlining Injection Drug Use Detection in Clinical Notes*	**Jeff Brookins** *Precipitation Behavior in an FCC Multi-Component Alloy Using Single Laser Tracks*
14:15 - 14:30	**Ana Belen Cueva** *SMART Lixiviants for the Selective Leaching of Rare Earth Metals*	**Aniket Pramanik** *A Learnt Half-Quadratic Splitting-Based Algorithm for Fast and High-Quality Industrial Cone-beam CT Reconstruction*	**Geeta Kumari** *Stress Relief Optimization for Laser Powder Bed Fusion Printed 316H Stainless Steel*
14:30 - 14:45	**Huixin Jiang** *Quaternary Ammonium Salt Coated Air Filter for Bioaerosol Removal from Building Indoor Air*	**Anthony Hong Cheol Lim** *In Silico Investigation on the Effects of Sub-Cellular Ac-225 Spatial Distribution on Tumor Cells and Biological Outcomes*	**Komal Chawla** *3D-printed car bumper with design and material optimized through AI-based inverse optimization framework*
14:45 - 15:00	**Harisree Krishnamoorthy** *Pulse shape discrimination techniques for the LEGEND experiment*		**Bhagya Prabhune** *Employing Machine Learning for Predicting Melt-pool Geometry in Additive Manufacturing*

15:00 – 15:15	BREAK		
15:15 – 16:00	Room 202 A	**Leah Broussard (*Keynote 3*)**	Understanding the beta-decay (and other strange disappearances) of the neutron
16:00	ADJOURN		

JULY 12, 2024 (DAY – 2)			
09:00 – 09:10	Room 202A	**Moody Altamimi Director ORNL ORE**	Welcome Remarks
09:10 – 09:20	Room 202A	**Aniket Pramanik** and **George Yumnam**	Research Symposium Agenda and Announcement
09:30 – 10:15	Room 202A	**Bronson Messer - II *(Keynote 4)***	Understanding Stellar Explosions: A Problem for the World's Most Powerful Computers and for Team Science
10:15 – 10:30	BREAK		

	Oral Session 7 (Building & Transportation) Room 202A	**Oral Session 8 (Health / Medicine) Room 202B**	**Oral Session 9 (Manufacturing - 2) Room 202C**
10:30 – 10:45	**Hevar Palani** *Evaluating the Impact of Window Replacement on Air Infiltration of Residential Buildings*	**Jordan Tschida** *Evaluating Algorithmic Bias on Biomarkers of Breast Cancer Pathology Reports in Six SEER Registries*	**Ritin Mathews** *Control of machining-induced residual stress via tool geometry and process parameter modification*
10:45 – 11:00	**Md Masudur Rahman** *Net-zero carbon fuel reactivity on commercial oxidation catalysts for emissions control*	**Jayasai Rajagopal** *Development of a workflow to calculate organ-at-risk dosimetry for targeted radiopharmaceutical therapy applications*	**Jordan Wright** *Advanced Manufacturing of PIP-Based SiC-SiC CMCs*
11:00 – 11:15	**Zhenlei Liu** *Balancing Health and Efficiency: Indoor Air Quality and Energy Efficient Homes*	**Abhishek Shivanna** *Ensuring Equity in AI Healthcare: A Study on Racial Bias in Cancer Site Classification Models*	**Nadim S. Hmeidat** *Rapid Energy-Efficient Manufacturing of High-performance Thermoset Polymer Composites via Self-Energized Frontal Polymerization Chemistry*
11:15 – 11:30	**Mengjia Tang** *Algorithms for increasing automation in installing prefabricated components for building envelopes*	**Avishek Bose** *Predicting drug effects from high-degree asymmetric drug data sets*	**Wenbo Wang** *Marine Turbine Lubrication Additives: Ionic Liquids with High Lubricity and Eco-Friendliness*
11:30 – 11:45		**John Wyatt Vant** *Cellular Interactions at Scale: GPU-Accelerated Simulations for Cancer Therapy Optimization*	**Daniel Suarez** *Liquid Metal MHD modelling for fusion applications*

11:45 – 12:30	LUNCH RECESS		
12:30 – 13:15	Room 202 A	**Prasanna Balaprakash (*Keynote 5*)**	ORNL's AI Initiative: Advancing Secure, Trustworthy, and Energy-Efficient AI for Science

13:15 – 15:15	Lobby	POSTER SESSION		**INDUSTRY BOOTHS (Lobby)**
15:15 – 16:00	Room 202 A	**Melanie Mayes (*Keynote 6*)**	Experiences and Lessons from Career in the Environmental Sciences	
16:00 – 16:30	Room 202 A	**Closing Ceremony**		

POSTER PRESENTATIONS

Sl. No.	Presenter	Poster Title
1	Bharat Sharma	Simulating CO2 Responses of Secondary-Succession Forests at Duke and Oak Ridge FACE Experiments with ELM-FATES-CNP
2	Bailey Murphy	Ground Truthing Land Surface Models: A Multi-Data Approach for Validation
3	Stephen Zambrzycki	Furthering Capabilities in Single Cell Metabolomics Using Single Cell Printing-Liquid Vortex Capture-Mass Spectrometry
4	Matthias Maiterth	Building Blocks of a Digital Twin for an Exascale Supercomputer
5	Eric Lee	Comparing Machine Learning and Deep Learning Models for Pediatric Anxiety Classification using Temporal, Structured, and Environmental Data from Electronic Health Records
6	Steven Hespeler	Temporal Analysis of ML/DL Techniques for Fault Detection in Cyber-Physical Systems Using Controller Area Network Data
7	Shiwanka V. Wanasinghe	Opacifiers to improve thermal performance of polyisocyanurate (PIR) foams
8	Latif Patwary	Estimating Gasoline Consumption for the Recreational Boating Sector in the U.S.
9	Ginu R. George	Insights into packed bed reactors by multi-scale reactor simulation approach
10	Soyoung Kang	Deformation mechanisms of Addictive Manufacturing 316SS using in-situ mechanical test with SEM-EBSD
11	Daniel Felton	Reproducible Surface-Enhanced Raman Spectroscopy of Nanodiamonds
12	Jordan Roach	Optical Vibrational Spectroscopic Signatures Related to U3O8 Production Processes
13	Huixin Jiang	Ultra-conductive Copper-Carbon Nanomaterial Composites through Brush Coating
14	Isaiah Dishner	Sequence-property relationships of periodically structured copolyamides
15	Mary Danielson	CO2 Capture from Seawater via a Novel Hollow Fiber Contactor
16	Janet Meier	Evaluation of a proposed Low melting point Element-Assisted Nucleation (LEAN) mechanism in dilute Al-Zr alloys micro-alloyed with Sn, Si, In, and Sb
17	Qiangsheng (Johnson) Lu	Direct Observation of an Interfacial Topological Superconducting States in FeTeSe-Bi2Te3 Heterostructure
18	Arvind Ganesan	Porous Liquids as Precursor for Mixed-Matrix Membrane (MMM) Synthesis

KEYNOTE 1: NET-ZERO BY 2050: CAN WE GET THERE?

David Sholl

Executive Director and Vice Provost
University of Tennessee-Oak Ridge Innovation Institute

The US and many other countries have embraced goals of reaching net-zero GHG emissions by 2050. I will discuss the far-reaching implications of this goal for the nation's economy, and examine the urgent need to develop scalable net-negative technologies that can be deployed in the next decade.

Biography

David Sholl is the Executive Director and Vice Provost of the University of Tennessee Oak Ridge Innovation Institute (UT-ORII), Director of the Transformational Decarbonization Initiative at the Oak Ridge National Laboratory, and the Editor-in-Chief of *AIChE Journal*. From 2022-2023 he was a Strategic Policy Advisor for DOE's Office of Clean Energy Demonstrations. From 2013-2021 David was the School Chair of Chemical & Biomolecular Engineering at Georgia Tech. He has published over 400 papers and several books. David was on the Board of Directors of AIChE from 2019-2021 and in 2020 chaired the inaugural Gordon Research Conference on Chemical Separations. In 2024 he was elected to the National Academy of Engineering.

KEYNOTE 2: DESIGNING FUSION REACTORS WITH SUPERCOMPUTING

Vittorio Badalassi

Distinguished R&D Staff Member, Thermal Hydraulics group
Reactor and Nuclear Systems Division
Oak Ridge National Laboratory

The blanket is a complex and fundamental component for future fusion power reactors, yet none has been built and tested; the current TRL level of one of the most studied blanket concepts (the Dual Coolant Lead Lithium Blanket, quite popular in DOE FES) is only two. Despite this, all the fusion startups want to pick a blanket concept and design it in detail. In this presentation, I will show how modelling and simulation, particularly the Fusion Energy Reactor Models Integrator (FERMI) simulation framework, may reduce the risk of deploying technology from such a low technology readiness, and I will present a new blanket concept.

FERMI is an integrated simulation environment under development for the coupled simulation of the plasma, first wall, and blanket of fusion reactor designs. The FERMI's original goals are to shorten the overall design cycle while guaranteeing unprecedented accuracy, thus integrating fusion design activities, facilitating an optimal reactor design, and reducing development risks. These goals are achieved by coupling single-physics solvers into a multiphysics simulation environment (FERMI). The Integrated Plasma Simulator (IPS)–FASt TRANsport (IPS-FASTRAN) simulation framework is used for the following: plasma physics, MCNP/Shift codes for neutron and photon transport, OpenFoam for computational fluid dynamics and magnetohydrodynamics (MHD), HyPerComp Incompressible MHD solver for Arbitrary Geometry (HIMAG) for dual-coolant lead-lithium (DCLL) blankets, and DIABLO for structural mechanics simulations. These codes are coupled using the open-source library named precise Code Interaction Coupling Environment (preCICE). FERMI's features are tested with the analysis of the liquid immersion blanket (LIB) [proposed in the Affordable Robust Compact (ARC)–class tokamak design], the DCLL blanket [proposed in the Fusion Pilot Plant (FPP) design], and other benchmark cases. The calculated figures of merit are the tritium breeding ratio, material activation, displacements per atom, shutdown dose rate, heat deposited in the vacuum vessel and blanket, temperature hot spots, and displacements caused by swelling and creep. A critical technical problem is multiphysics code coupling, which is tackled here, and the first three-dimensional (3D) simulations of the DCLL-FPP and LIB-ARC blankets are presented. FERMI represents the first effort to perform 3D simulations of nuclear fusion first wall and blankets in a fully coupled multiphysics manner, and it shows the way to derisk the detailed design of blankets.

Finally, I will present the patent pending "Nested Pebble Bed Blanket", a revolutionary blanket concept that may solve most issues affecting existing blankets concepts.

Biography

Dr Vittorio Badalassi is a Distinguished R&D Staff Member in the Thermal Hydraulics group - Reactor and Nuclear Systems Division at Oak Ridge National Laboratory. Vittorio received his PhD (2004) in

chemical engineering at the University of California, Santa Barbara and trained in Innovation and Entrepreneurship Business Management at the Imperial College London Executive Program. He is a Chartered Engineer with international experience and a proven record for success in R&D, industrial consulting, R&T management and startup funding/operation; he is a recognized expert in modelling and simulation (CFD) and in Nuclear Thermal Hydraulics, with further expertise in the aerospace and chemical sector; he has worked in numerous technical positions for R&D institutions (Royal Society Industry Fellow at Imperial College/Rolls-Royce), in industry (Chief Nuclear Safety Engineer at the PALLAS reactor) and startups (Founder and CTO of his company in the UK). He sourced funding (up to 4Mn$), managed multi-cultural engineering teams in both industry and academia, and had direct exposure to senior executives in corporations. Author of highly cited papers and patents, and winner of prestigious academic awards.

At ORNL he is developing, demonstrating, and qualifying predictive simulation software for nuclear thermal hydraulics and safety applications through leveraging high-fidelity computational fluid dynamics (CFD), reduced-order thermal-hydraulic models, and advanced data analytics; further, he is leading and setting up the strategy and the investments on computational fluid dynamics for the whole laboratory. In particular, he is the PI of the ARPA-E FERMI project which is delivering a digital twin of Fusion reactors.

KEYNOTE 3: UNDERSTANDING THE BETA-DECAY (AND OTHER STRANGE DISAPPEARANCES) OF THE NEUTRON

Leah Broussard

Research Scientist, Neutron Symmetries group
Physics Division
Oak Ridge National Laboratory

The neutron's transformation into a proton, electron, and antineutrino--a process called beta decay--should be well described by the Standard Model of Particle Physics. Precision measurements of observables in beta decay provide a robust and comprehensive test of our understanding of the weak interaction, one of the four fundamental forces in nature. However, experimental results are currently in significant tension with predictions. The Nab experiment, now commissioning at the Spallation Neutron Source, will perform the world's best determination of the correlation between the electron and antineutrino in neutron beta decay. This correlation, along with the neutron beta-decay lifetime, is used in one of the most precise tests of our model of the weak interaction. I will describe how Nab's novel approach will both improve precision of this test and shed light on experimental discrepancies. I will also discuss recent searches for exotic transformations of the neutron, proposed to explain anomalies such as the neutron lifetime puzzle, and the potential implications for our understanding of how matter evolved in the universe.

Biography

Leah Broussard received her B.S. in computer science from Tulane University with majors in math and physics. She received her M.A. and Ph.D. at Duke University using nuclear and neutron beta decay to characterize aspects of the weak interaction, and for her thesis performed the most precise measurement of the 19Ne half-life. As a Seaborg Postdoctoral Fellow at Los Alamos National Laboratory, she developed detector systems to study neutron beta decay products and she explored novel applications using ultracold neutrons for actinide science. She joined Oak Ridge as a Wigner Fellow in 2016, where she spear-headed a new program looking for exotic interactions of the neutron and continued detector development for further neutron beta decay studies. She received a DOE Early Career Award in 2019 in part to characterize key aspects of the detector performance for next generation neutron beta decay experiments. Today she is co-spokesperson for the Nab experiment, which promises the most precise determination of key parameters in neutron beta decay.

KEYNOTE 4: UNDERSTANDING STELLAR EXPLOSIONS: A PROBLEM FOR THE WORLD'S MOST POWERFUL COMPUTERS AND FOR TEAM SCIENCE

Bronson Messer II

Director of Science, OLCF
National Center for Computational Sciences
Oak Ridge National Laboratory

The study of exploding stars touches on a variety of questions including the origin of the chemical elements, the formation of neutron stars and black holes, the generation of gravitational waves, and more. At ORNL, we model supernovae—both core-collapse and thermonuclear types—using extreme-scale computational resources. I will discuss some of the recent triumphs and challenges associated with gaining this understanding. I will also outline how this work relies heavily on having a team of people capable of attacking all the physical and computational issues inherent in the problem.

Biography

Bronson Messer is a Distinguished Scientist and the Director of Science at the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory. He is also Joint Faculty Professor in the Department of Physics & Astronomy at the University of Tennessee. His primary research interests are related to the explosion mechanisms and phenomenology of supernovae, especially neutrino transport and signatures, dense matter physics, and the details of turbulent nuclear combustion. In addition, he has worked on the application of machine learning algorithms to the analysis of galaxy merger simulations and on performance modeling and prediction for high-performance computing architectures. Prior to joining ORNL, Dr. Messer was a Research Associate in the Department of Astronomy & Astrophysics at the University of Chicago, where he was Deputy Group Leader for Astrophysics in the ASC Center for Astrophysical Thermonuclear Flashes.

Dr. Messer is a member of the American Astronomical Society and he recently served on the American Physical Society's Committee on Informing the Public (2018-2020). In 2020, he was awarded the Department of Energy Secretary's Honor Award for his part in enabling the COVID-19 High Performance Computing Consortium. Dr. Messer holds undergraduate and graduate degrees from the University of Tennessee, earning his PhD in physics in 2000.

KEYNOTE 5: ADVANCING SECURE, TRUSTWORTHY, AND ENERGY-EFFICIENT AI AT SCALE FOR SCIENTIFIC DISCOVERY

Prasanna Balaprakash

Distinguished R&D Scientist
Director of AI Programs
Oak Ridge National Laboratory

We will present an overview of the Oak Ridge National Laboratory's Artificial Intelligence Initiative, which aims to advance the domains of science, energy, and national security. At the core of this initiative are two fundamental thrusts: transformative science applications and cross-cutting assurance. The application thrust focuses on developing AI methods to accelerate scientific discoveries, while the cross-cutting assurance thrust ensures that AI systems are secure, trustworthy, and energy-efficient. Secure approaches include alignment, privacy preservation, and robustness testing for AI models. Trustworthiness is achieved through validation and verification processes, coupled with advanced techniques in uncertainty quantification and causal reasoning. Meanwhile, energy efficiency is prioritized by developing scalable solutions, integrating edge computing technologies, and adopting a holistic co-design approach that optimizes the synergy between software and hardware resources. Through this initiative, we will demonstrate how ORNL is advancing the development and implementation of assured AI for scientific discovery that is impactful, secure, and sustainable.

Biography

Prasanna Balaprakash is the Director of AI Programs and a Distinguished R&D Scientist at Oak Ridge National Laboratory, where he directs research, development, and application of artificial intelligence and machine learning (AI/ML) to solve problems of national importance. Balaprakash's research interests span AI, machine learning, optimization, and high-performance computing. He serves as the AI lead for several significant DOE-funded projects. He received the U.S. Department of Energy's Early Career Award in 2018. Prior to his current role at ORNL, Balaprakash held several positions at Argonne National Laboratory, evolving from postdoctoral researcher to an R&D Group Leader within the Mathematics and Computer Science Division. Previously, he served as the Chief Technology Officer at Mentis SA in Brussels, Belgium. Balaprakash received his PhD in 2010 from CoDE-IRIDIA (AI Lab), Université Libre de Bruxelles, Brussels, Belgium, where he received Marie Skłodowska-Curie and F.R.S-FNRS Aspirant fellowships from the European Commission and the Belgian-French Community's National Fund for Scientific Research, respectively.

KEYNOTE 6: EXPERIENCES AND LESSONS FROM A CAREER IN THE ENVIRONMENTAL SCIENCES

Dr. Melanie A. Mayes

Distinguished Staff Scientist and Ecosystem Processes Group Leader
Environmental Sciences Division and Climate Change Science Institute
Oak Ridge National Laboratory

I will share my experiences and lessons learned from my career in the Environmental Sciences Division. I arrived at ORNL for a 4-month internship with the Oak Ridge Associated Universities, which morphed into a graduate research assistantship at the University of Tennessee focused on the fate and transport of radionuclides in weathered and fractured soils. At graduation, I accepted a post-Masters position at ORNL to work on radionuclide mobility in partially saturated soils from the US DOE's Hanford Reservation in Washington, which formed the basis of my PhD research. Program changes from the Office of Science reduced the emphasis on research on DOE's contaminated lands, and I became more engaged with climate research, since organic matter in soils constitutes a globally significant reservoir of carbon. I also learned that some of the gaps in climate prediction are due to uncertainties in how organic materials react with soils, so I transformed my research and built new collaborations to develop new models to better represent these processes. Along the way, I worked with neutron scientists, molecular dynamics modeling researchers, process and earth system modelers, and microbiologists to better understand soil and organic matter interactions. Currently, I am working with atmospheric and plant scientists to better understand interactions between green spaces and urban microclimate. I am also leading a team that is expected to develop a large-scale ecosystem manipulation experiment over the next decade.

Biography

Dr. Melanie Mayes is a Distinguished Scientist and Ecosystem Processes Group Leader with the Environmental Sciences Division and the Climate Change Science Institute at Oak Ridge National Laboratory, and a Joint Faculty with the University of Tennessee. She is a Fellow of the American Association for the Advancement of Science, and an Associate Editor of the journals Biogeochemistry and Frontiers in Soil Science. Current research involves carbon and nutrient cycling in soils, forests, and urban environments, and investigative approaches for soil mercury contamination. She is also an avid hiker, usually logging over 1000 miles in the Appalachian Mountains each year.

1. ORAL SESSION 1: BIOLOGICAL SCIENCES

O1.1: MICROBIAL DNA FRAGMENTS (MDF) INTEGRATION INTO THE HOST POPULUS TRICHOCARPA NUCLEAR GENOME ALTERS PLANT TRAITS

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The integration of organelle and microbial DNA into nuclear genomes played a crucial role in the evolution of eukaryotes. Initially, we discovered a nuclear-encoded genomic region, PRL-1, containing a microbial DNA fragment (MDF) associated with non-photochemical quenching photosynthesis parameters using a genome-wide association study in 743 Populus trichocarpa accessions. Higher expression of PRL-1 facilitated anterograde signaling between the nucleus and plastid, leading to increased expression of Rubisco, enhanced photosynthesis, and up to 35% greater plant height and 88% biomass in poplar accessions under field conditions. Overexpression of PRL-1 in hybrid Poplar species and Arabidopsis resulted in up to a 200% increase in plant height and a 50% increase in seed yield in the case of Arabidopsis. We extended our genome-wide survey of foreign DNA fragments in Poplar to identify additional genomic regions with MDF footprints. We identified approximately 12,000 DNA fragments from organelle transfers and diverse organisms. Out of these, we further characterized two genes in P. trichocarpa. Integrating MDF added molecular functions, such as transcriptional role, to the genes and enhanced Poplar productivity. Our findings suggest MDF in the host plant's nuclear genome can increase genomic diversity and impact plant productivity across different species, benefiting plant breeding.

O1.2: DISCOVERY AND ENGINEERING OF NYLON HYDROLASE FOR NYLON RECYCLING

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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. 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. 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. However, some of these enzymes possessed interesting properties of activity and substrate selectivity that had never been demonstrated before. The engineering of these enzymes should also make them compatible with more realistic conditions for degrading more complex materials such as commodity plastics. This 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.

O1.3: DECIPHERING MICROBIAL COMMUNICATION IN MICROBIAL COMMUNITY ASSEMBLY

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Bacterial communities play a pivotal role in many ecosystem processes including nutrient cycling, plant growth, and stress tolerance. Plant-associated bacteria are well known for their diverse metabolic capabilities contributing to the range of interactions among bacterial species. The impact of microbe-microbe interactions on multispecies community structure and dynamics is poorly understood. Cell-to-cell signaling in the form of quorum sensing (QS) often regulates extracellular enzyme production, biofilm formation, competence, and secondary metabolite production contributing to microbe-microbe interactions. A prevalent class of signaling molecules essential to QS are acyl homoserine lactones (AHLs). AHL-mediated QS circuits are common to plant-associated bacteria, suggesting a crucial role AHLs play in microbe-microbe interactions. Here we examine how AHLs mediate microbial interactions in a 10-member synthetic community isolated from *Populus deltoides.* In our previous work, this 10-member community stabilized over time in passage experiments and the final community structure was unchanged despite differences in initial inoculum ratios. Most (60%) community members encode genes associated with the production and response to AHLs. To explore the role of AHLs in microbial community structure and dynamics, we disrupted microbial cell-to-cell signaling using purified AiiA-lactonase, an enzyme that cleaves the lactone ring. Initial experiments in a defined minimal medium found inhibiting AHL signaling altered microbial community structure after 48 hrs. AiiA-lactonase dependent inactivation of AHL signals was confirmed using a hypersensitive bioreporter and mass spectrometry. Current efforts focus on assessing the effects of AHL inactivation on microbial community structure, pairwise interactions, biofilm formation, and secondary metabolite production of the 10-member synthetic community in passage experiments. Elucidating the role of AHLs in structuring this synthetic community will provide valuable insights into the intricate relationships involved in mediating microbial community assembly. This research has the potential to contribute meaningful knowledge in unraveling the multifaceted factors governing microbial community assemblage.

O1.4: LAYERED REGULATION OF THE CAS9 NUCLEASE SIGNIFICANTLY REDUCES LEAKY INCIDENTAL EXPRESSION

Elise Phillips

Biosciences Division, Oak Ridge National Laboratory

Inducible promoters are known to "leak," or exhibit low levels of uninduced gene expression. While this leaky expression is negligible in most contexts, leaky expression of Cas9 in the presence of a guide RNA results in up to 99.99% cell death. This extensive cell death makes library maintenance and storage infeasible, and limits Cas9 use in some species. Hypothetically, a multicomponent regulation scheme could reduce promoter leak and, in turn, prevent unwanted Cas9 activity. In this work, we demonstrated a significant improvement in uninduced nuclease activity by combining post-transcriptional control elements with inducible promoters to drive Cas9. The production of a "leakless" inducible Cas9 construct will enable easier, more robust methodologies for working with large, diverse genome editing or gRNA libraries.

O1.5: LINKING HYDROLOGIC EXCHANGE FLOW AND BIOGEOCHEMICAL MODELING TO QUANTIFY METHANE EMISSION FROM RIVERS

Kewei Chen

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CH4 emissions from inland water are highly uncertain in the current global CH4 budget, especially for rivers and streams due to sparse measurements and the uncertainty of measurements caused by turbulent water flow. To address this challenge, we developed a process-based model to estimate CH4 flux at the air-water interface using the attributes available in the national hydrography data set. It calculates the annual mean flux of VHEF, CH4 production in sediments, and CH4 transport in the river channel in a sequential manner. Model performance is evaluated by CH4 efflux observed at the Hanford reach of the Columbia River. We show that reach-wise sediment hydrologic and biogeochemical conditions estimated from the national hydrography data set could serve as a good indicator of CH4 emissions from rivers. Aerobic methane oxidation and export to the downstream are the dominant ways of total CH4 loss for the large lowland river. The hotspots of CH4 emissions are likely to be at the reaches with fine sediments and slow channel velocity. This study demonstrates the possibility of quantifying CH4 emissions at the reach scale and the modeling framework has the potential to be extended to the basin scale to improve estimates of CH4 emissions from lotic inland water.

O1.6: LINKING HYDROLOGIC EXCHANGE FLOW AND BIOGEOCHEMICAL MODELING TO QUANTIFY METHANE EMISSION FROM RIVERS

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Cellulose is one of the most abundant biopolymers for food, fiber and fuel. This versatile fiber is made by plant cellulose synthase, a plant membrane protein with a structural architecture that is not fully understood. PpCesA5 from an early moss plant Physcomitrium patens has been the protein of interest due to PpCesA5-specific homooligomerization. Plant CesAs can form trimers and a hexamer of trimers called cellulose synthase complexes (CSCs). Our 2.8 Å PpCesA5 trimer cryo-electron microscopy (cryo-EM) structure showed concerted flexibility between the PpCesA5 subunits, and also revealed a novel tether pin that tethers the intrinsically disordered N-terminal domain (NTD) of PpCesA5 to the protein main body. The structural conformation of the tethered NTD infers loop formation and lobe-lobe interaction, but cryo-EM was unable to detect intrinsically disordered regions in PpCesA5. Small angle neutron scattering (SANS) showed that the NTD forms extended loops formed by the tether pin. This PpCesA5 NTD region was isolated and further characterized using small angle X-ray scattering (SAXS). Contrary to previous knowledge on NTD dimerization, NTD formed extended monomers further supporting an extended NTD conformation in PpCesA5. Overall, new oligomerization mechanisms are revealed that inform rational design of biofuels and biomaterials.

2. ORAL SESSION 2: MATERIALS SCIENCE 1

O2.1: TUNING SKYRMION PHYSICS FOR NEXT-GENERATION SPINTRONICS

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The rapid advancement of technology demands innovative memory and logic devices. Traditional devices, with their high volatility, increased power consumption, and slow speeds, have driven the exploration of topological magnetic defects—such as monopoles, domain walls, vortices, and skyrmions—as potential candidates for future spintronic applications. Among these, skyrmions, induced by chiral interactions in non-centrosymmetric magnetic compounds or thin films, stand out for their exceptional promise. These nanoscale structures can be manipulated, created, and annihilated, making them ideal for advanced information storage and logic applications. Their soliton nature, stabilized by the Dzyaloshinskii-Moriya interaction (DMI), allows for size manipulation, leading to higher information density compared to other topological defects. This study presents a numerical micromagnetic analysis of equilibrium energy in B20 materials, such as FeGe, examining the effects of varying skyrmion core and anisotropic DMI influence. By tuning these parameters, we can achieve control over skyrmions motion, stability and dynamics, enabling the customization of spin topologies for spintronic applications. Furthermore, we investigate the influence of magnetic fields on the energy landscape, offering insights into the design of nextgeneration memory devices. This work underscores the transformative potential of skyrmions in revolutionizing the emerging field of skyrmionics.

O2.2: MAGNETOHYDRODYNAMIC PRESSURE DROP IN NUCLEAR FUSION BLANKET

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In the nuclear fusion reactor blanket design involving liquid metals (LMs), one of the challenges is the magnetohydrodynamic (MHD) effect associated with electroconductive LM flowing under the strong plasma-confining magnetic field, such as high MHD pressure drop. In fully developed 2D MHD flows, the pressure drop is related to induced electric currents closing in cross-sectional planes. In the 3D flows, such as flows in access ducts, where magnetic field has a fringe zone, or inlet/outlet manifolds, where geometry changes an additional pressure drop appears called the 3D MHD pressure drop due to electric currents closing in the flow direction. In this study, two MHD pressure drop correlations have been established based on the 3D data computed with COMSOL-Multiphysics and using the least squares method and linear regression analysis, including MHD flow in manifolds and a fringing magnetic field. The developed

correlations allow for calculations of the MHD pressure drop as a function of the dimensionless flow parameters, such as the Hartmann and Reynolds number. In addition, MHD liquid metal flows in a blanket supply system featuring a coaxial radial duct, expansion/contraction region, poloidal ducts and U-turn zone were computed in two cases of electrically conducting and insulating walls.

O2.3: ELECTROCHEMICAL CHARACTERIZATION OF SULFUR CATHOLYTES USED IN REDOX FLOW BATTERIES

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The current state-of-the-art vanadium-based Redox flow battery (RFB) suffers from the cost associated with the vanadium material used as catholytes (positive electrolyte). Redox active materials based on sodium-sulfur, Na-S, catholytes are considered a cheaper alternative. However, one of the limitations of sulfur-based RFBs is that during their operation, they degrade, generating insoluble products. We have found that incorporating phosphorus into the Na-S molecule structure improves its stability and solubility, thereby increasing the volumetric capacity of the battery. Our work focused on the synthesis and electrochemical characterization of the new Na-P-S catholytes. The synthesis method implemented was based on wet synthesis, which, in contrast with mechanochemical methods, reduces the amount of energy invested in the synthesis process. The electrochemical properties of Na-P-S catholytes were compared using cyclic voltammetry. During reduction/oxidation cycles, Na-P-S exhibited electrochemical irreversibility. However, they displayed stable cycling performance for up to 100 cycles. This behavior is consistent with measurements on RFBs containing a Na-P-S catholyte. Preliminary flow cell measurements on Na-P-S catholyte using a solid/liquid hybrid RFB configuration show reversible voltage profiles after the formation step with deep discharge. This work demonstrates that Na-P-S catholytes represent a promising material for high-energy, low-cost redox flow batteries.

O2.4: EXPERIMENTAL INVESTIGATION AND PERFORMANCE CHARACTERIZATION OF PCM INTEGRATED FINNED TUBE HEAT EXCHANGER FOR BUILDING HEATING AND COOLING APPLICATIONS

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In the United States, the building sector accounts for 40% of all energy use, and buildings are responsible for more than two-thirds of electricity consumption. Thermal energy storage (TES) using phase change materials (PCMs) offers unique benefits in storing and releasing large amounts of energy from the latent

heat of phase transition. TES technologies based on PCMs could enable flexibility of buildings' thermal demand, shave peak load, and provide energy savings to the end user. Herein we investigate the thermal performance of a PCM-based heat exchanger that is designed to offset buildings' heating and cooling loads. We integrate the PCM-based heat exchanger with thermally anisotropic building envelopes (TABEs), where the TABE can redirect natural thermal energy from a building using hydronic loops to TES. In this work, we describe an experimental apparatus for two 5-gallon fin and tube heat exchanger systems integrated with a commercially available organic PCM that is subjected to heated and cooled boundaries. Experimental observations provide insight into the role a TES system can play in offsetting a building's heating and cooling demand and also offer a means to characterize the performance of PCMs for building applications. The scale and study presented in this work will help in the design of future thermal storage systems optimized for storage capacity while also accounting for overall system costs for building applications. The developed method and apparatus provide a means to investigate and characterize thermal storage systems at the gallon scale, which can help in the design of future energy storage systems optimized for cost and energy savings.

O2.5: RESOLVING HETEROGENEOUS HYDROGEN FUEL CELL CATALYST DEGRADATION AT THE NANOSCALE VIA AUTOMATED 3D ELECTRON TOMOGRAPHY

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The loss of platinum (Pt) electrochemically active surface area (ECSA) is a critical degradation mode that often becomes a limiting factor for heavy-duty proton exchange membrane fuel cell vehicles. High surface area carbon supports have been shown to improve Pt dispersion and limit detrimental ionomer-electrocatalyst interactions due to their large interior pore volume. In this work, using automated scanning transmission electron tomography, we compare the degradation of nanoparticles located on the interior versus exterior surfaces of the carbon support following a catalyst specific accelerated stress test (AST) of 90,000 voltage cycles between 0.6 V to 0.95 V. Our results reveal a notable increase in average particle size for both interior and exterior Pt catalyst particles, with a slightly higher increase in both particle size distribution and specific surface area for the particles located on the exterior carbon surface. The high interior fraction of Pt observed at the beginning of test is maintained following the AST test, along with a notable increase in carbon pore size. The results shed light on the degradation mechanisms affecting electrochemical properties and the enhanced particle accessibility at lower relative humidity.

O2.6: MICROEXTRACTION-ICP-MS FOR THE DIRECT ANALYSIS OF NANOPARTICLES LOADED ON A SOLID SURFACE

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Nanoparticles have become a topic of interest among many fields of science and industry in recent years; demand for nanoparticle analysis has increased in response. The capabilities of Single Particle Inductively Coupled Plasma Mass Spectrometry (SP-ICP-MS) for the analysis of nanoparticles has become significantly more advanced in recent years.

Among SP-ICP-MS methods, laser ablation is the sole method for direct ICP-MS analysis of particles from a solid surface. In this work, we develop a new ICP-MS based method for the analysis of particles loaded on a solid surface. We use a modified Advion Plate Express to extract nanoparticles directly from a solid surface, and introduce them to a quadrupole ICP-MS in a single step, providing a new avenue for the analysis of nano-particles. We term this novel technique Microextraction ICP-MS (ME-ICP-MS). It is in the early phases of development, and here we investigate how parameters such as solution flow rate, and solvent system affect transport efficiency and the overall efficacy of the method. Additionally, we investigate the potential for particle sizing. Next we compare and contrast the commercial extraction probe head with one designed and machined here at Oak Ridge National Laboratory.

3. ORAL SESSION 3: MATERIALS SCIENCE 2

O3.1: IMPACT OF PHONON COUPLING TO ELECTRIC FIELD ON THERMAL TRANSPORT IN A RELAXOR FERROELECTRICS

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Relaxor-based ferroelectrics PMN-xPT have been extensively studied due to their giant electromechanical coupling that is utilized in sensors and ultrasound applications. The application of an external electric field impacts the structure on multiple scales ranging from induced local atomic displacements to polar nanoregions and longer-range ferroelectric domain alignments. These structural responses influence the phonon dispersion (group velocities) and lifetimes, and, consequently, the thermal transport properties. With this motivation we have investigated the response of thermal transport properties to electric fields using a two-pronged approach. Inelastic neutron scattering measurements with ARCS were used to determine the phonon properties and single crystal diffuse scattering measurements on CORRELI were used to correlated with the changes in the local structures induced by electric field poling PMN-30PT at the Oak Ridge National Laboratory Spallation Neutron Source. We gratefully acknowledge the collaboration with Joseph P. Heremans group at Ohio State University. This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

O3.2: ENHANCED MAGNETIC-DISORDER DRIVEN MAGNON SOFTENING OF TBSB VIA Y-DOPING

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Understanding disorder in magnetic systems is an important endeavor as disorder influences thermodynamic and transport properties crucial for the development of current and future technologies. Magnetic systems with a cubic crystal structure, such as TbSb ($S = 7/2$, 9.7 μB), offer a simple yet effective platform for studying magnetic disorder via doping with a nonmagnetic element, such as yttrium. Y-doping reduces the Néel temperature in TbSb and enables studying the interplay of disorder and magnetic excitations as a function of doping concentration. We study the effect of disorder on the magnetic excitations as function of Y-doping in TbSb by combining inelastic neutron scattering and linear spin wave theory (LSWT). Increasing the doping soften and broaden the magnons in TbSb until the percolation threshold in Tb0.6Y0.4Sb, where the system no longer remains antiferromagnetic. Numerical simulation of the spin waves in TbSb based on LSWT and classical spin dynamics reveal the transformation of spin waves and crystal field excitation as a function of Y-doping. Our study provides new insights into the

behavior of magnons in disordered magnetic materials and highlights the potential for further research in this field.

O3.3: NANOSCALE MAGNETIC ORDERING DYNAMICS IN A HIGH CURIE-TEMPERATURE FERROMAGNET

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Investigating spin fluctuations, which are the dynamic deviations of a magnetic system from its equilibrium state, represents a critical frontier in condensed matter research. This yields invaluable insights into magnetic coupling and elucidates the properties around the magnetic instability or quantum critical points. Nitrogen-vacancy (NV) defects in diamonds stand out as a promising quantum sensing platform with relaxometry techniques that allow converting magnetic noise into optical signals. The recent development of scanning NV techniques has demonstrated remarkable visualization of nanoscale magnetic texture. Such a scanning technique also enables the study of spin fluctuations at the nanoscale when an atomic single-NV is brought into proximity and locally interacts with local magnetic textures. Hence, we seek to demonstrate the NV scanning relaxometry as an efficient tool to probe the spin fluctuations locally near the phase transition of Sr2FeReO6 (SFRO), a double perovskite oxide that has recently attracted attention as a stoichiometrically tunable ferromagnetic insulator/metal with high Curie temperature. Characterizing the magnetic order and dynamics of the system near phase transition serve as a successful demonstration of the scanning NV relaxometry technique and provide insight into the magnetic coupling mechanism of high Curie-temperature ferromagnetic double perovskite oxide.

O3.4: TE-VACANCY ENHANCED SUPERCONDUCTIVITY IN HYBRID INTERFACE $FETE_{1-x}SE_x/BI_2TE_3$ GROWN BY MOLECULAR BEAM EPITAXY

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Hybrid interfaces of topological insulators and s-wave superconductors are great candidates for realizing Majorana bound states (MBSs) which have been projected to have paradigm-changing possibilities in quantum computing. The epitaxial $FeTe_{1-x}Se_x/Bi_2Te_3$ platform possess the necessary parameters for topological states and provides wide range of tunability. Recently, monolayer of superconducting FeTe1-xSex (x = 0.25) grown on the Bi_2Te_3 was reported to exhibit emergent topological interfacial Dirac states at the Fermi energy. Pushing to lower Se levels reduces disorder, which is critical for interrogating Majorana

bound states, yet pure FeTe is not superconducting. Here we systematically investigate how modifications to the molecular beam epitaxy growth of Bi_2Te_3 and $FeTe_{1-x}Se_x$ enable tailoring both superconductivity and topological properties at low Se doping levels. Low temperature transport measurement, angle resolved photoemission spectroscopy, Rutherford backscattering spectrometry and X-ray diffraction are combined to unravel the roles of band structure, crystallinity, composition and superconductivity which can be tailored as a function of growth conditions. This study will reveal the complex relation of strain and charge at $FeTe_{1-x}Se_x$ / Bi_2Te_3 interface which will hopefully create a robust platform for realizing MBSs and advancing quantum devices.

O3.5: IMPROVING REACTOR DECAY HEAT DATA

Thomas Ruland

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A large fraction of the heat generated by a nuclear reactor is from unstable fission products undergoing β decay on their way back to stability. This heat is known as decay heat and while the reactor is operating it accounts for ~10% of the heat generated but is 100% of the heat generated after reactor shutdown, planned or accidental. Proper understanding of reactor decay heat is vital to the safe operation of nuclear reactors as well as informing the design of next-generation reactors, and this understanding requires precise and accurate β-feeding intensities for the decaying fission products. Historical measurements of β-feeding intensities using high-resolution detectors are often troubled by low g-ray efficiencies, which can result in incomplete β-feeding intensities. This generally causes the low-energy level β feedings to be over-predicted while the higher energy levels are under-predicted. These discrepancies can be corrected using high-efficiency total absorption detectors such as ORNL's Modular Total Absorption Spectrometer (MTAS). We've measured the β-feeding intensities for the well-produced A=105 mass chain using MTAS at Argonne National Laboratory, and results on the impact to reactor decay heat as well as the contribution to the reactor antineutrino flux for the A=105 isobars will be presented.

O3.6: ENHANCING ALUMINUM NITRIDE'S FERROELECTRIC SWITCH THROUGH IRRADIATION-ENGINEERED DEFECTS

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Aluminum nitride (AlN) is a promising wurtzite ferroelectric semiconductor for memory applications, but its high coercive fields, often exceeding breakdown voltage, pose a challenge. Reducing the domain switching energy barrier is crucial, and defects such as Al and N vacancies and their complexes with native

impurities like oxygen and carbon play a significant role in ferroelectric switching dynamics. In this study, we utilize cathodoluminescence (CL) to probe the optical signatures of defect chemistries and correlate them with AlN's ferroelectric behavior. CL excites color centers through ionization processes, overcoming low optical interaction cross-sections of defects in AlN's wide bandgap (>6 eV) and revealing nanoscale heterogeneity. We employ dose-dependent helium ion irradiation to induce local structure changes and modulate defect density and type. CL spectra show irradiation-dose-dependent changes in defect chemistry, suggesting a gradual evolution of existing defects favoring nitrogen vacancy formation and reducing oxide complexes. Functional atomic force microscopy measurements measure a steep decrease in ferroelectric coercive field and a significant enhancement of piezoelectric coefficient with increasing irradiation dose. By leveraging He-ion irradiation to enhance potential nucleation sites, we reduce the switching barrier by >40% and demonstrate the critical role of defect states in engineering ferroelectric properties in AlN thin films.

4. ORAL SESSION 4: CHEMISTRY

O4.1 CAPTURING PROMETHIUM IN SOLUTION

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Lanthanides play a huge role in US economic, energy, and national security due to their prevalent applications in advanced technologies. Separating trivalent lanthanides is a massive task due to highly expensive methods and environmental challenges. Promethium is the most elusive member of the lanthanide family, a row of 15 metals marooned in the periodic table's southern territories. Discovered in 1945, the element was named after the Titan Prometheus, who stole fire from the gods in Greek mythology. Researchers estimate that less than 1 kilogram of it currently exists naturally in the Earth's crust, and its radiation has previously been harnessed to power pacemakers and spacecraft. Despite its importance, Pm has been conspicuously absent from the experimental studies of lanthanides, impeding our full comprehension of the so-called lanthanide contraction phenomenon, a fundamental aspect of the periodic table quoted in general chemistry textbooks. My present work involves the design and synthesis of diglycolamide (DGA) ligand to chelate radioactive promethium (147Pm radionuclide with a half-life of 2.62 years), making a stable chemical 'complex' — a compound in which three surrounding molecules girdle central Pm3+ ion.1 This feat of synthesis enabled the team to study how the element bonds with other atoms in a water solution. Due to the limited availability of radioisotope 147Pm, a surrogate crystal of [Sm(DGA)3][Sm(NO3)6]·3C2H5OH was developed. The homoleptic Pm3+ complex in an aqueous solution was studied using synchrotron X-ray absorption spectroscopy and quantum chemical calculations to establish promethium's coordination structure and bond distances. These fundamental insights allow a complete structural investigation of a full set of isostructural lanthanide complexes, ultimately capturing the lanthanide contraction in solution solely based on experimental observations. Our results showed accelerated shortening of bonds at the beginning of the lanthanide series, which can be correlated to the separation trends shown by diglycolamides. Lately, we have also been focusing on synthesizing redox-active DGA ligands, which could lead to the development of new environmentally friendly and efficient separation of trivalent lanthanides.

O4.2 REVOLUTIONIZING URANIUM RECOVERY: MONOAMIDES FOR ENHANCED U/PU SEPARATION

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Reprocessing of spent nuclear fuel (SNF) plays a crucial role in both nuclear waste management and the expansion of nuclear power generation for electricity production. Efforts are underway to develop an efficient uranium recycling methods. The PUREX process utilizes tri-n-butyl phosphate (TBP) to extract uranium and plutonium from SNF. TBP has drawbacks such as not following the CHON principle, vulnerability to radiation, production of harmful degradation products, and high solubility in aqueous phase. Monoamides in GANEX-I process resolve some difficulties, but significant nitric acid consumption in both processes persists. Among different monoamides, DEHiBA yields efficient U/Pu separation. The structure of the monoamide, particularly the size of the alkyl groups, holds considerable importance. This study focuses on developing new monoamide ligands with refined alkyl groups to enhance uranium and plutonium separation. One ligand stood out for its effectiveness compared to DEHiBA. Using UV-Vis spectroscopy, significant results were observed in direct dissolution tests. The promising ligand underwent various chemical stability assessments. This presentation will discuss the findings, including insights from solvent extraction, direct dissolution tests, and chemical stability evaluations.

O4.3 A MEMBRANE CONTACTOR ENABLING ENERGY-EFFICIENT CO2 CAPTURE FROM POINT SOURCES WITH PHYSICAL SOLVENT

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Greenhouse gas contributions to global climate change have generated interest in separating carbon dioxide (CO2) from wet flue gas streams. To address this challenge, absorption of CO2 via environmentally friendly, green solvents, has emerged as a useful technique due to their reusability, high absorption capacities, and favorable economics. Compared to commercially available carbon capture processes that utilize ionic liquid and amine-based technologies, membrane-based carbon capture with diethyl sebacate (DS) is cheaper, easily regenerated, and presents high capacity for industrial level carbon capture. Despite its advantageous properties, little research has investigated DS as a solvent for carbon capture. To absorb CO2 from flue gas streams, a scalable, energy-efficient, hollow fiber membrane (microporous polypropylene and polyvinylidene fluoride) contactor (HFMC)-based process was designed with low-cost and high surface area to provide high interfacial area for effective CO2 capture. Gas chromatograph measurements of this system demonstrated effective capture of CO2 while rejecting nitrogen. A purity of 95.3% CO2 was achieved using DS, with a permeate flux over one magnitude greater than deep eutectic

solvent in this same system. Results from this work underscore the importance of utilizing green solvents in HFMC-based separation processes for effective carbon capture and provides a pathway toward practical deployment.

O4.4 SMART LIXIVIANTS FOR THE SELECTIVE LEACHING OF RARE EARTH METALS

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Rare earth elements are vital in several cutting-edge technologies for clean energy applications, electronics, automobiles, among others. Particularly, La, Ce, Pr, Nd, Sm, Eu, Tb, Dy, and Y are the base of technology development due to their application in permanent magnets, batteries, and Phosphors. Monazite is one of the key minerals containing REEs phosphates mainly. The common industrial practice for monazite treatment is cracking with hot, concentrated NaOH which converts phosphates into hydroxides. Hydroxides, though insoluble in water, have an opposing solubility bias to phosphates, resulting in light REEs being more soluble than heavy REEs. After cracking, REE hydroxides are acid leached following several intensive rounds of solvent extraction. The process is known to be energy intensive, inefficient, and environmentally strenuous. Thus, tailor-made lixiviants have been synthesized for the precise thermodynamical discrimination between large, light REEs and small, heavy REEs. Taking advantage of the characteristics of several lixiviants selective leaching of light REEs has been accomplished, while heavy rare earths remain in the solid phase, allowing for a selective, efficient enrichment and separation.

O4.5 QUATERNARY AMMONIUM SALT COATED AIR FILTER FOR BIOAEROSOL REMOVAL FROM BUILDING INDOOR AIR

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Indoor air quality (IAQ) is critical for occupants' health and gains lots of attention because of the frequent break out of inspiratory infectious diseases caused by airborne microorganisms, or bioaerosols. Applying biocidal air filters in buildings is a good strategy to prevent and stop inspiratory infectious diseases. It is necessary to develop biocidal air filters. In this study, a simple spray-coating method was used to fabricate biocidal air filters to remove and kill bioaerosols. The commercially available biocidal agent Goldshields 75 was sprayed on polypropylene filters, and the fabricated filters showed significant inhibition growth of Micrococcus luteus and Escherichia coli. The filter showed high biocidal ability after being fabricated for 3 months. The coated filters have higher than 99.9% of both bacterial and virus filtration efficiencies. These results suggest the potential of Goldshields 75 coated filters in improving the IAQ, and this simple spray-coating method provides a new way to produce biocidal air filters.

O4.6 PULSE SHAPE DISCRIMINATION TECHNIQUES FOR THE LEGEND EXPERIMENT

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The discovery of Neutrinoless double beta decay (0νββ) would have profound implications for neutrino physics and cosmology. It would provide unambiguous evidence for the Majorana nature of neutrinos, lepton number non-conservation and the absolute neutrino mass scale. The Large Enriched Germanium Experiment for Neutrinoless ββ decay (LEGEND) searches for 0νββ in the 76Ge isotope. The LEGEND-200 phase that is presently operational at high-purity Germanium (HPGe) detectors with excellent energy resolution immersed in liquid argon, allowing the rejection of backgrounds external to the Ge detector. The pulse shape analysis plays a critical role in distinguishing bulk 0νββ events from multi-site events and surface backgrounds that arise from gamma rays and other sources. This is crucial to maximize the sensitivity of the experiment to 0νββ and other physics events. I will discuss the status of the experiment, various pulse shape discrimination (PSD) cuts that have been employed and their impact on the signals and the backgrounds.

5. ORAL SESSION 5: ARTIFICIAL INTELLIGENCE / MACHINE LEARNING

O5.1 REACTION PATHWAYS SEARCH USING ADAPTIVE-LEARNING GLOBAL OPTIMIZATION AND GENERATIVE ADVERSARIAL NETWORKS

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The search for reaction pathways is a crucial aspect of chemistry. It involves exploring the energy landscape of complex chemical reactions to identify the reactants, transition states, and products. However, this task is incredibly challenging, as it requires navigating a vast potential energy surface with multiple possible outcomes.

In this work, an adaptive learning global optimizer combined with a machine learning algorithm to explore the potential energy surface and identify the reaction pathways. The global optimization algorithm allows for the determination of low-energy minima for large systems while the generative adversarial networks have been successfully used for the prediction of the transition states between a given set of reactants and products. Here, we combine the two computational schemes to connect a large set of possible reactants, transition states, and products, together with calculated energies at the DFT level.

This approach aid in the discovery of new reactions, optimization of existing reactions, the prediction of reaction outcomes, and extraction of generalized system descriptors. Moreover, it can facilitate the development of more efficient and sustainable chemical processes, contributing to the advancement of the chemical industry.

O5.2 AUTOMATED STRUCTURE DISCOVERY VIA ACTIVE LEARNING IN STM

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Scanning tunneling microscopy (STM) is a widely utilized technique for high-resolution imaging of materials at the atomic level and assessing their surface energies. However, achieving optimal imaging conditions is a time-intensive process due to the ultra-sensitive interaction between the tip and the surface. Moreover, the conventional approach involves a step-by-step imaging process, and understanding property correlations typically relies on the operator's interpretation aided by auxiliary spectroscopic data, thus limiting efficiency. We present a Bayesian optimization-based framework that autonomously enhances imaging conditions in real-time. Additionally, we introduce a probabilistic deep learning model to automatically deduce relationships between material structures and electronic properties. This data-

driven approach dynamically guides STM exploration towards regions corresponding to specific material properties. The method utilizes sparse-sampling to construct property-space efficiently with minimal data, as little as 1% compared to conventional hyperspectral imaging. Further, we demonstrate a multi-scale framework for property-guided structure discovery by autonomously identifying the structural origins of observed material properties. Our investigations reveal unique correlations of electronic properties with local defect density, surface terminations, and point defects. The deep-learning framework allows the possibility of studying and inducing dynamic processes such as matter manipulation for assembling artificial structures.

O5.3 AI-POWERED INSIGHTS: STREAMLINING INJECTION DRUG USE DETECTION IN CLINICAL NOTES

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Injection drug use (IDU) is a critical health concern in the United States and internationally, entailing numerous associated health risks. Therefore, identifying people who inject drugs early can reduce the likelihood of these issues arising. However, extracting information about any possible IDU from a person's electronic health records can be difficult because the information is often in text-based general clinical notes rather than provided in a particular section of the record or as numerical data. Manually extracting information from these notes is time-consuming and inefficient. Although natural language processing can efficiently extract this information from unstructured data, there are no validated tools. To address this gap in clinical information, we design the first question-answering (QA) framework to extract information on IDU from clinical notes for use in clinical operations. Our framework involves two main steps: (1) generating a gold-standard QA dataset and (2) developing and testing the QA model. We use data curated from the US Department of Veterans Affairs (VA) Corporate Data Warehouse to construct the dataset for developing and evaluating the QA model. Our study aims to enhance the accurate and efficient detection of people who inject drugs, extract relevant information, and ultimately facilitate informed patient care.

O5.4 A LEARNT HALF-QUADRATIC SPLITTING-BASED ALGORITHM FOR FAST AND HIGH-QUALITY INDUSTRIAL CONE-BEAM CT RECONSTRUCTION

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Industrial X-ray cone-beam CT (XCT) scanners are widely used for scientific imaging and non-destructive characterization. Industrial CBCT scanners use large detectors containing millions of pixels and the subsequent 3D reconstructions can be of the order of billions of voxels. To obtain high quality

reconstruction when using typical analytic algorithms, the scan involves collecting many projections/views which results in large measurement times - limiting the utility of the technique. Model-based iterative reconstruction (MBIR) algorithms can produce high-quality reconstructions from fast sparse-view CT scans but are computationally expensive and hence are avoided in practice. Single-step deep-learning (DL) based methods have demonstrated that it is possible to obtain fast and high-quality reconstructions from sparse-view data, but they do not generalize well to out-of-distribution scenarios. In this work, we propose a half-quadratic splitting-based algorithm that uses convolutional neural networks (CNN) to obtain high quality reconstructions from large sparse-view cone-beam CT (CBCT) measurements while overcoming the challenges with typical approaches. The algorithm alternates between the application of a CNN and a conjugate gradient (CG) step enforcing data-consistency (DC). The proposed method outperforms other methods on the publicly available Walnuts dataset.

O5.5 IN SILICO INVESTIGATION ON THE EFFECTS OF SUB-CELLULAR AC-225 SPATIAL DISTRIBUTION ON TUMOR CELLS AND BIOLOGICAL OUTCOMES

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Purpose: Ac-225 targeted therapy offers intense, localized radiation dose at the subcellular level. The precise positioning of Ac-225 within cells is vital for effective tumor control. This study aims to simulate the effects of sub-cellular localization of Ac-225 on tumor cells and predict biological outcomes.

Methods: The tumor volume in this study consists of a sphere and was fully packed with fibroblast cells that consist of a cell nucleus. The tumor volume was simulated with three Ac-225 localization regimes in TOPAS: zero, fifty, and ninety-five percent in intracellular and the remainder in extracellular space. The radiation-induced damage of the tumor model's cell nucleus was simulated with TOPAS-nBio; further repair kinetics were evaluated with MEDRAS to provide lethal chromosome aberration events and cell survival curves.

Results: Given an equivalent dose of 1 Gy to the tumor volume, the average alpha particle tracks crossing the nucleus increased from 0.78 to 2.31 tracks from zero to ninety-five percent intracellular radiation. The lethal chromosome aberration events ratio increased four times, and relative biological effectiveness in dose at ten percent survival was six times.

Conclusion: The higher Ac-225 yield in intracellular space increased alpha tracks in the nucleus and lethal events to the cell.

6. ORAL SESSION 6: MANUFACTURING - 1

O6.1 CONVERGENT MANUFACTURING OF 316L STAINLESS STEEL HOT ISOSTATICALLY PRESSED (HIP) CANISTERS

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Metal additive manufacturing (AM) evolved over the last decade to serve the current manufacturing needs. However, the tradeoff between cost, lead time, part complexity, size, and scalability for parts produced via AM versus powder metallurgy (PM) is still a point of contention. This talk demonstrates the feasibility of a combined AM + PM approach to fabricate metal parts which benefit from the intrinsic advantages of both AM and PM. Powders of 316L stainless steel (SS) were poured into canisters fabricated via (1) conventional extrusion, (2) laser powder bed fusion (LPBF), and (3) blown powder directed energy deposition (BP-DED) and then degassed and subjected to HIPing. Post-HIP specimens were characterized for microstructure, physical, and mechanical properties. This study provides a preliminary overview of the opportunities and challenges associated with the AM + PM approach and offers valuable insights that can further guide the fabrication of complex, large-scale metal components.

O6.2 EFFECT OF LASER MELT SCHEDULE ON THE MICROSTRUCTURE OF ADDITIVELY MANUFACTURED IN718

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Laser powder bed fusion (L-PBF) has enabled the fabrication of intricate and geometrically complex structures that are not achievable using conventional processes. It also offers the potential to facilitate multi-length scale design across the atomic- through macro-levels due to far from equilibrium thermal conditions. However, these systems lack the throughput for scalability. Rotary powder bed fusion (L-RPBF) systems are being investigated as possible routes for scaling to larger deposition areas and significantly increasing the deposition rate of traditional L-PBF. In this work, IN718 test coupons were fabricated using a dual laser L-RPBF system to study the effect of laser melt frequency and schedule on as-fabricated microstructures. Coupons were printed using either one of two lasers or alternating between both. These variations offer insights into; 1) systematic differences between lasers and 2) effects of laser cycling. With a 1 rpm bed rotation frequency, coupons fabricated by alternating between lasers experienced a melt every 30 or 90 seconds, with each layer experiencing differing thermal boundary conditions. The variation in melt-pool and microstructural features, such as grain size, shape, crystallographic orientation, and dislocation density were examined. The alternating laser-head melt schedule resulted in grain refinement at higher laser power.

O6.3 PRECIPITATION BEHAVIOR IN AN FCC MULTI-COMPONENT ALLOY USING SINGLE LASER TRACKS

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Structural and functional alloys have traditionally occupied competing design spaces; as mechanisms for strengthening the former often degrade the latter. However, recent work by Han et al. demonstrated that multi-component alloys can overcome these limitations, enabling the co-optimization of soft magnetism and high toughness [1]. This performance is achieved by tailoring the size of an ordered, paramagnetic nanoprecipitate. By overcoming structural-functional property trade-o#s, electromagnetic applications that experience a stress or impact can utilize new alloy design strategies for resilient components. For parts such as generator cores, additive manufacturing has been used to fabricate complicated geometries and tailored microstructures: minimizing the limitations of deformation-based processing. By varying the solidification rates and thermal gradients, site-specific control over the precipitating phase can influence both magnetic and mechanical properties. Here, we showcase an initial investigation into an AlFeCoNiTa-based alloy for laser-based processing. Strategies based on energy density were employed to alter solidification rates: controlling nucleation kinetics. Transmission electron microscopy showcased the ability to control the nucleation of sub-5 nm, spheroidal, L12 precipitates. Based on this work, we provide evidence that this alloy system is amenable to either in situ or post-process heat treatments to obtain the desired structure-properties-performance.

O6.4 STRESS RELIEF OPTIMIZATION FOR LASER POWDER BED FUSION PRINTED 316H STAINLESS STEEL

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Additive Manufacturing (AM) has significantly enhanced the capability to efficiently manufacture complex parts for various extreme environment applications. However, post-processing optimization, particularly heat treatment, remains a challenge. On one hand, full solution annealing often fails to preserve the grain structures unique to AM. Conversely, conventional stress-relief (SR) heat treatments often fail to completely remove deleterious residual stresses without over-sensitizing the material. This work aims to fine-tune the SR parameters for Laser Powder Bed Fusion (LPBF) printed 316H stainless steel to promote dislocation recovery without complete intragranular cellular annihilation. Through systematic experimental designs, we have explored a range of temperatures from 650°C to 850°C and varied the duration up to 6 hours to assess microstructural evolution. Advanced characterization techniques, including X-ray Diffraction (XRD) for dislocation density, and electron microscopy (SEM, TEM) for cellular structure analysis, have been employed to support our findings.

O6.5 3D-PRINTED CAR BUMPER WITH DESIGN AND MATERIAL OPTIMIZED THROUGH AI-BASED INVERSE OPTIMIZATION FRAMEWORK

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Metal This work focuses on designing lightweight lattice structures with tailored mechanical responses for a car bumper through finite element (FE) simulations and machine learning (ML) framework. We carried out FE simulations on representative volume element of bumper with seven different lattice geometries to generate training dataset for ML model. To provide tunability of materials in terms of stiffness and elasticity, we considered five different blends of 20% carbon fiber (CF) reinforced acrylonitrile butadiene styrene (ABS) and thermoplastic polyurethane (TPU). Periodic boundary conditions were applied to simulate mechanical properties of the entire bumper under two different loadings. We extracted stress-strain curve, critical mechanical properties from each simulation and corresponding design parameters (lattice type and materials) were considered as training dataset. ML model was trained using dataset through Gradient Boosting package in Python to conduct inverse design for predicting optimized lattice geometry and material blends. Given the target mechanical properties provided by Ford Motor, the inverse model generates design parameters for the bumper. We obtained an optimized design incorporating the optimal combination of lattice type and material blends for enhancing bumper performance. The ML framework and design optimization carried out in this work will guide industries for planning and selection of appropriate materials for applications involving multi-functionality.

O6.6 EMPLOYING MACHINE LEARNING FOR PREDICTING MELT-POOL GEOMETRY IN ADDITIVE MANUFACTURING

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In additive manufacturing of metals, parts are built layer by layer using a process that involves the formation of a molten pool of metal, called the melt pool. Predicting the dimensions of the melt pool is crucial for ensuring product quality, avoiding defects, and predicting microstructure. Traditionally, the melt-pool dimensions are determined using computationally intensive CFD-based melt pool simulations, which can take hours or even days to complete, rendering real-time prediction of the melt pool dimensions impractical. To address this challenge, we propose a machine learning approach based on convolutional neural network (CNN) models to predict the melt-pool dimensions by utilizing infrared in-situ camera images. This method can enable rapid prediction of the melt pool dimensions, thus facilitating on-the-fly adjustments

7. ORAL SESSION 7: BUILDING AND TRANSPORTATION

O7.1: EVALUATING THE IMPACT OF WINDOW REPLACEMENT ON AIR INFILTRATION OF RESIDENTIAL BUILDINGS

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Air infiltration through building envelopes accounts for 30% of the energy used for heating and cooling in residential buildings. Many of U.S. homes were constructed before the 1960s, feature windows lacking modern insulation and proper installation, leading to problems like air leakage and drafts causing inadequate ventilation, increasing indoor air pollution, and adversely affecting the health of residents. However, a significant research gap exists in understanding the impact of window systems on overall airtightness. Therefore, the objective of this project is to analyze and compare the impact of air leakage on air infiltration of residential houses. To achieve that, this study is performed in three tasks: (1) perform blower door tests to estimate the air leakage through the existing windows before and after window replacements; (2) compare the air infiltration results of the buildings before and after window replacements; and (3) recommend adjustments to energy codes, such as the IECC, to include specific guidelines for window installations in residential buildings. The results from the first 10 tested houses revealed uniform improvements in air leakage reductions, approximately 10%, after window replacements. This finding underscores the need to evaluate the impact of window upgrades on residential buildings and advocate for policy changes.

O7.2: NET-ZERO CARBON FUEL REACTIVITY ON COMMERCIAL OXIDATION CATALYSTS FOR EMISSIONS CONTROL

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Rail, marine and off-road transportation sectors are hard to electrify due to longer uptime needs, large travel distances, and lack of charging facilities in remote locations. The “U.S. Blueprint for Transportation Decarbonization” has identified the use of sustainable liquid fuels or net-zero carbon fuels as a promising alternative to achieve decarbonization of these sectors. To ensure emissions compliance and to identify unique emissions control challenges and opportunities with net-zero carbon fuels, a systematic study evaluating the reactivity of different net-zero carbon fuels on commercial diesel oxidation catalysts (DOC) was conducted.

In this communication, an automated synthetic exhaust flow reactor was used to measure the light-off temperatures of alcohols and a C10 diesel surrogate fuel (baseline) over hydrothermally aged, commercial Pd+Pt DOC as per industry guidelines. Ethanol (EtOH) and methanol (MeOH) oxidation were studied in the presence of water vapor and carbon monoxide (CO) by using state-of-the-art in-situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) technique to investigate the formation of surface intermediates and effects of adsorbed CO on alcohol reactivity. The investigation showed formation of strongly adsorbing acetate and formate species which were stable on the catalyst surface up to 275ºC and 225ºC during EtOH and MeOH oxidation, respectively.

O7.3: BALANCING HEALTH AND EFFICIENCY: INDOOR AIR QUALITY AND ENERGY EFFICIENT HOMES

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To achieve nearly net zero energy use, future buildings must be more airtight, which often leads to lower ventilation rates to minimize energy consumption. However, maintaining adequate ventilation according to ASHRAE Standard 62.2 is crucial for ensuring acceptable indoor air quality (IAQ). This presentation will explore strategies for creating comfortable and healthy indoor environments while maintaining energy performance of buildings. It will address common pollutants and their potential impacts on occupant health. The presentation will include a detailed analysis to illustrate the generation and transport of indoor pollutants with and without kitchen ventilation using the CONTAM simulation. Emissions of pollutants from various types of food and their transport within a residential building will be examined. Additionally, this presentation will evaluate the use of air purification technologies and novel materials to improve IAQ, adhering to the ventilation rates required by ASHRAE Standard 62.2 for residential buildings.

O7.4: ALGORITHMS FOR INCREASING AUTOMATION IN INSTALLING PREFABRICATED COMPONENTS FOR BUILDING ENVELOPES

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In the prefabricated construction industry, components for building envelopes are manufactured offsite and installed onsite. The installation process often requires intensive labor to meet the required tolerance, which is checked after the installation is completed. To reduce the cost due to labor and corrections, a tool named “Real-Time Evaluator” (RTE) using a single total station is being developed to provide real-time feedback on the position of the component during installation relative to the as-designed position. Two algorithms

were developed: one is to align the physical building facades and components with the digital space regardless of how the total station is set up, and the other one is to give instructions on how to move and rotate the component to the desired position. Lab-scale experiments were conducted to test the two algorithms, and it was found that an accuracy meeting the industry recommendation was achieved.

8. ORAL SESSION 8: HEALTH/MEDICINE

O8.1 EVALUATING ALGORITHMIC BIAS ON BIOMARKERS OF BREAST CANCER PATHOLOGY REPORTS IN SIX SEER REGISTRIES

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This work evaluated bias in a biomarker prediction algorithm trained using electronic pathology reports from 178,121 female breast cancer patients. Bias was evaluated across five categories: US State, race, Hispanic ethnicity, age at diagnosis, and residential socioeconomic status. We utilized the Framework for Exploring Scalable Computational Oncology (FrESCO) on 594,875 electronic pathology reports from the National Cancer Institutes (NCI) Surveillance, Epidemiology, and End Results (SEER) registries to train a Multi-Task Convolutional Neural Network (MT-CNN) algorithm to classify patients by their biomarker status. Algorithmic bias was evaluated using a balanced error rate (BER) quantifying the average error across classes, with values higher than 1.25 representing an inequality across classes. We found some evidence of algorithm bias in our models; however, this bias was primarily centered around BER differences between the US States and not patient characteristics. The lowest BER corresponds to the US State that contributes the most data (Seattle). We found no significant algorithmic bias in biomarker classification. Bias deep learning models could lead to health disparities and potential harm to patients. Our results suggest that, even when utilizing large amounts of data from multiple states, algorithm bias should be evaluated.

O8.2 DEVELOPMENT OF A WORKFLOW TO CALCULATE ORGAN-AT-RISK DOSIMETRY FOR TARGETED RADIOPHARMACEUTICAL THERAPY APPLICATIONS

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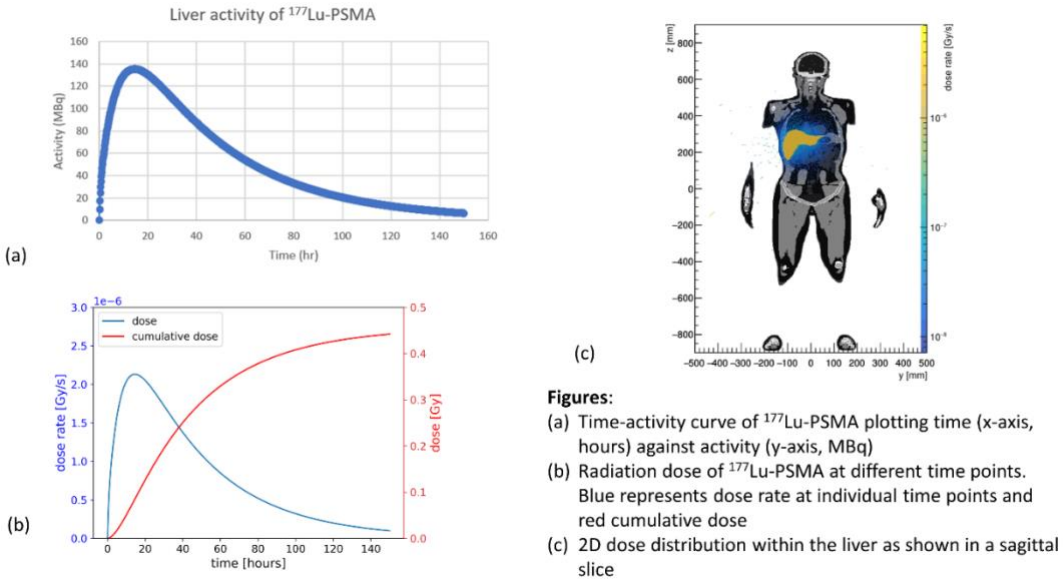
We describe a workflow to calculate radiation dose from targeted radiopharmaceutical therapy to organs-at-risk (OARs). Targeted radiopharmaceutical therapy provides a method to directly target and treat cancers. An associated concern is radiation dosage to healthy organs-at-risk (OARs). In this work, a workflow was developed to calculate OAR dosimetry for different patient geometries and radiopharmaceutical agents. The computational workflow was implemented for a 177Lu-PSMA-617 radionuclide and liver dosimetry. First, patient geometry and organ volume was defined by an anthropomorphic phantom (XCAT, Duke University). Next, a physiologically based pharmacokinetic (PBPK) model was implemented with six compartment models for tumor volume, blood volume, and target OARs including the liver. The PBPK model output was in terms of time versus activity. Then, the activity

curve from PBPK and liver geometry from the phantom were imported into a Monte Carlo radiation transport code module (GEANT4) to calculate time-relative and cumulative dose. For this demonstration, a 24 BMI female adult patient was injected with 3 GBq of 177Lu-PSMA-617. After initial injection, activity reached a peak value of 135.4 MBq in the liver at 14.5 hours. At the same time point, a peak dose rate of 2.13e-6 Gy/s. Total cumulative dose was measured at 0.44 Gy.



Figures:
(a) Time-activity curve of ^{177}Lu-PSMA plotting time (x-axis, hours) against activity (y-axis, MBq)
(b) Radiation dose of ^{177}Lu-PSMA at different time points. Blue represents dose rate at individual time points and red cumulative dose
(c) 2D dose distribution within the liver as shown in a sagittal slice

O8.3 ENSURING EQUITY IN AI HEALTHCARE: A STUDY ON RACIAL BIAS IN CANCER SITE CLASSIFICATION MODELS

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The integration of artificial intelligence (AI) in cancer diagnostics has significantly advanced the precision of tumor classifications. Yet, the potential for these models to inadvertently encode inherent biases, particularly racial bias, presents a substantial challenge. This study investigates the presence and impact of such biases within cancer site classification models using Hierarchical Self-Attention Network (HiSAN)-generated embeddings. Our methods involved analyzing a dataset of over 2.7 million electronic pathology reports from six National Cancer Institutes (NCI) Surveillance, Epidemiology, and End Results (SEER) Registries. We examined the feature importance scores from HiSAN-generated embeddings to detect any significant overlap between features used in cancer site classification and those influencing race predictions. This approach aimed to identify and quantify racial biases embedded within the AI models. Additionally, we implemented a mitigation strategy by pruning the overlapping features identified and subsequently reassessed the models' performance to ensure diagnostic integrity was maintained. Results showed minimal feature overlap and low cumulative importance scores affecting race predictions, indicating a negligible influence of racial information on clinical outcome predictions. After pruning these features, the models retained high diagnostic accuracy, affirming the clinical utility and fairness of the HiSAN embeddings. Our

findings demonstrate that HiSAN-generated embeddings can classify cancer sites effectively without significant racial bias, ensuring the fairness and reliability of AI tools in clinical settings.

O8.4 PREDICTING DRUG EFFECTS FROM HIGH-DEGREE ASYMMETRIC DRUG DATA SETS

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Tangible understanding of unknown drug responses in the human body has always been uncertain during the drug development phase. Modeling drug effects before physical trials is indispensable but poses a set of computational challenges. Machine learning (ML) models for drug effects prediction often encounter minimal impacts in using data sets that contain disparately distributed drug effect vectors with complex correlations between them. On top of that, training individual learning models and incorporating their prediction results for a wide spectrum of drug effect vectors is beyond practicality. Such an implication sheds light on employing this challenge as multi-prediction problems that would predict all drug effects at a time supporting effective experimentation and simple demonstration. Consequently, high data imbalance and data sparsity are causing impediments to ML architectures such as graph neural networks (GNN) to learn from high dimensional drug effect vectors as targets. We developed graph neural networks for drug effect prediction as multi-label and multi-regression problems and introduced a guideline to address highly imbalanced and asymmetric molecular graph data sets using an oversampling strategy and then compared the results with other sampling strategies.

O8.5 CELLULAR INTERACTIONS AT SCALE: GPU-ACCELERATED SIMULATIONS FOR CANCER THERAPY OPTIMIZATION

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In the realm of advancing cancer treatment strategies, computational modeling proves to be an invaluable tool. Current targeted radiotherapies are not personalized to individual patients, and combination therapy courses are often based on past successes. Our work seeks to leverage high-performance computing architectures to optimize the course and dosages of combination therapies for cancer patients. Specifically, we are exploring the use of XCAT phantom models to create patient-specific digital twins, enabling personalized agent-based cellular simulations. Our approach involves parallelizing cellular interactions and therapies to significantly scale up simulations. By incorporating patient-specific data, such as tumor location, size, and microenvironment, we aim to create realistic cancer scenarios. These digital twins act as virtual clinics for testing various combination treatments. Through these simulations, we gain insights into cellular dynamics, treatment response, and potential side effects. Our ultimate goal is to identify optimal

therapeutic strategies tailored to individual patients by integrating computational research with clinical practice.

9. ORAL SESSION 9: MANUFACTURING - 2

O9.1 CONTROL OF MACHINING-INDUCED RESIDUAL STRESS VIA TOOL GEOMETRY AND PROCESS PARAMETER MODIFICATION

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Distortion generated in machined, monolithic, thin-walled aerospace components due to residual stresses leads to significant material and economic waste in the manufacturing industry. Inherent residual stress (IRS) present in stock materials combines with machining-induced residual stress (MIRS) to influence the final machined part distortion. It is hypothesized that MIRS can be controlled through deliberate cutting tool geometry and process parameter modifications to negate the effect of IRS on distortion, consequently resulting in distortion-free parts. A finite element (FE) orthogonal cutting model is developed to study the influence of tool geometry and process parameters MIRS. Orthogonal cutting experiments are performed on Al 7075-T651 samples to measure cutting forces and MIRS via a cutting force dynamometer and a novel digital image correlation (DIC) based hole drilling technique, respectively. These data are utilized to validate the FE model. Increasing the depth of cut, tool tip radius, or rake angle is found to promote near-surface tensile stresses. Competing effects of material ploughing and temperature is shown to affect the type of RS and a window of variation of RS (up to ±400 MPa) is estimated, allowing for the control of MIRS through tool and process modification.

O9.2 ADVANCED MANUFACTURING OF PIP-BASED SIC-SIC CMCS

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While ceramic matrix composites (CMCs) exhibit exceptional mechanical and thermal resilience under extreme conditions, their manufacturing process remains inefficient due to numerous time-consuming steps. Traditional methods involve prepregging fiber cloth, shaping and layering in a mold, autoclaving, and several rounds of polymer infiltration and pyrolysis (PIP). Additive manufacturing (AM) presents a promising solution by consolidating these processes into a single operation. This innovative approach involves coextruding fiber tow and preceramic matrix, facilitating in-situ fiber impregnation and streamlining the production of complex-shaped CMC structures. Thus, this study focuses on optimizing CMC manufacturing via AM and advanced PIP densification. Several traditional CMC plaques and AM CMC bars underwent various PIP methods while monitoring their mass gains and material properties. Advanced PIP combined with AM promises significant time, energy, and labor savings in CMC manufacturing, enhancing material utilization

O9.3 RAPID ENERGY-EFFICIENT MANUFACTURING OF HIGH-PERFORMANCE THERMOSET POLYMER COMPOSITES VIA SELF-ENERGIZED FRONTAL POLYMERIZATION CHEMISTRY

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Thermoset polymer-matrix composites find widespread applications across industries such as aerospace, energy, and automotive. However, traditional curing and manufacturing methods for these composites are plagued by high costs, lengthy processing times, and energy-intensive procedures, leading to restricted design complexity and slow fabrication rates. The development of next-generation high-performance polymer composites for advanced manufacturing demands rapid, versatile, and energy-efficient manufacturing strategies. Frontal polymerization (FP) emerges as a promising alternative curing method, leveraging a self-sustaining exothermic reaction that moves through a monomer, transforming it into a hardened thermoset polymer. Since frontal curing solely relies on the initiating stimulus, the process demands significantly less energy, spanning several orders of magnitude less than conventional curing. This talk will begin with a brief overview of the origins and early applications of FP in composite manufacturing. Subsequently, it will proceed into recent research endeavors focusing on the development and processing of multifunctional composites cured through FP, exploring their diverse applications, including additive manufacturing. Finally, the discussion will extend to innovative avenues for implementing FP in wind energy, automotive, and other industrial sectors.

O9.4 MARINE TURBINE LUBRICATION ADDITIVES: IONIC LIQUIDS WITH HIGH LUBRICITY AND ECO-FRIENDLINESS

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Tidal energy is able to generate clean, sustainable electricity via turbomachinery and stands out as a promising source in the portfolio of renewable energy sources. Meanwhile, the development of environmentally acceptable lubricants (EALs) for marine turbomachinery is crucial to reducing the risk of conventional lubricants threatening marine ecosystems due to leakage or spillage incidents. Recently, eco-friendly and high-lubricity ionic liquids (ILs) have been successfully invented at Oak Ridge National Laboratory and being further developed as additives for tidal turbine gearbox lubrication. Compared with the commercial baselines, the ‘not toxic’ and ‘readily biodegradable’ IL-additized lubricants performed more effectively in mitigating the friction, rolling contact fatigue and wear loss. In addition, the mechanisms of wear and the protection resulting from the ILs have been discussed through surface and tribofilm analyses.

O9.5 LIQUID METAL MHD MODELLING FOR FUSION APPLICATIONS

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Nuclear fusion technology is rapidly evolving towards a commercialization phase expected to be reached during the next decade or two. However, there are still several technological challenges that must be solved in advance. Among the challenges are tritium breeding, reactor cooling, and radiation shielding, functions performed in the "breeding blanket." Although much research is still needed, using liquid metal to cope with these functions is a promising alternative. The liquid metal flow will interact with the existing strong magnetic field required to control the plasma. This interaction is known as magnetohydrodynamics (MHD), a key discipline to understanding the flow of electrically conducting fluids under a magnetic field. Strong heat deposition will promote buoyancy forces, generating instabilities which can modify the transport of tritium and heat. Inside the vacuum vessel, outside the breeding blanket, "plasma facing components" will receive extremely high heat fluxes. A film of liquid metal flow can cool the substrate and prevent material damage. Free-surface liquid metal MHD is therefore a discipline of high interest as well within the fusion community nowadays. This presentation summarizes current investigations at ORNL on computational fluid dynamics modeling of the liquid metal MHD flows involved in fusion technology at Fusion Energy Division

10. POSTER SESSION

P1: SIMULATING CO2 RESPONSES OF SECONDARY-SUCCESSION FORESTS AT DUKE AND OAK RIDGE FACE EXPERIMENTS WITH ELM-FATES-CNP

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Rising atmospheric CO2 can increase vegetation biomass production, which at the global scale can slow atmospheric CO2 growth rates. Elevated atmospheric CO2 (eCO2) experiments have gains in net primary productivity (NPP) and biomass. Significant component of global change has been the conversion of primary forests to secondary forests and several ecosystem-scale Free Air Carbon Dioxide Enrichment (FACE) experiments. Analysis of these FACE experiments indicated that the variability in the eCO2 response is related to the stage of stand development and progressive nitrogen limitation. We use ELM-FATES-CNP, size and time-since-disturbance structured vegetation demography model that integrates carbon and nutrient cycling to investigate nutrient constraints on eCO2 responses in even-aged forests. The primary objective of this study is to evaluate the performance of the ELM-FATES-CNP model against the observations from Duke and ORNL FACE experiments to ascertain how best to apply ELM-FATES-CNP to investigate stand structure and nutrient controls on ecosystem carbon responses to eCO2. Understanding the interactions of N availability for plant uptake and growth is necessary to improve predictive capabilities of models to simulate ecosystem C storage in response to eCO2. We compared net primary productivity (NPP) responses under simulated postdisturbance and counter-factual “equilibrium” forests at Duke and Oak Ridge.

P2: GROUND TRUTHING LAND SURFACE MODELS: A MULTI-DATA APPROACH FOR VALIDATION

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The Arctic is experiencing warming trends that surpass those observed elsewhere on Earth. Given the considerable carbon stored in permafrost that is susceptible to release, permafrost thaw has the potential to significantly impact global carbon cycling. However, Earth system model (ESM) predictions of climate change in Arctic regions are uncertain, due to the complexity of Arctic ecosystems and the historically limited availability of observational data. Arctic ecosystems are typically represented in a highly simplified manner. For instance, the Energy Exascale Earth System Model (E3SM) divides Arctic vegetation into two plant functional types (PFTs), deciduous shrub or grass. Recently, nine diverse Arctic PFTs were integrated into the E3SM land surface model (ELM), leveraging data from NGEE Arctic for parameterization. Here, we combined the new PFTs with plant community mapping to conduct spatially explicit simulations at a site in Alaska’s Seward Peninsula and compared model predictions to observations from three unique data streams (eddy covariance flux tower, high-resolution drone imagery,

satellite-based remote sensing) to evaluate whether refined representation of Arctic vegetation results in more realistic predictions of vegetation and carbon dynamics. Initial analysis reveals that the refined PFT representation produced more realistic patterns of vegetation biomass and land-atmosphere exchanges compared to the original model.

P3: FURTHERING CAPABILITIES IN SINGLE CELL METABOLOMICS USING SINGLE CELL PRINTING-LIQUID VORTEX CAPTURE-MASS SPECTROMETRY

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Single cell-resolved measurements are critical to understand the mechanisms that drive cellular response for applications in bioengineering and cellular manufacturing. Cell-to-cell heterogeneity in metabolite expression exist despite identical genotypes. Better tools to measure the diverse response of single cells to physical or chemical stimuli can lead to better engineering in biomanufacturing. In this study, we built a new single-cell printing-liquid vortex capture−mass spectrometry (SCP-LVC-MS) tool using the HP D100 single cell dispenser. The D100 offers rapid single cell analysis at a fraction of the cost and complexity of other SCP technologies. We evaluated the reproducibility of dispensing using the drug propranolol and showed relative standard deviations less than 10%. The D100 SCP-LVC-MS then characterized and detected Chlamydomonas microalgae and HepG2 liver carcinoma cells. Concurrently, a proof-of-concept in-capillary fluorescence detection capability was built for SCP-LVC-MS to enable simultaneous measure of fluorophores with mass spectral signatures. Immunofluorescence staining is the standard in molecular pathway elucidation. We want to couple the fluorescence data with SCP-LVC-MS to understand the mechanisms that drive single cell metabolomic response. Rhodamine 6G was used to calibrate the sensitivity of the system which exhibited a low µM detection sensitivity of a droplet of analyte administered to the LVC probe.

P4: BUILDING BLOCKS OF A DIGITAL TWIN FOR AN EXASCALE SUPERCOMPUTER

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This research poster presents our efforts of ExaDigiT (Exascale Digital Twin). The work first presents the general overview our digital twin system, which is split into Central Energy Plant (Facility) and HPC System (Supercomputer). The system incorporates simulators for the Resource Allocator and Power Simulator (RAPS) and a cooling Model built in Modelica, both of which ingest telemetry data collected from the system. The second part of the poster is the primary way of interacting with these systems, our 3d visual analytics model. The challenge here is to incorporate the different aspects of the Digital Twin into a AR/VR environment, coping with the scale and complexity of the system. This is done in Unreal Engine 5, where interaction with large component count and large data volume had to be tackled. We present the general visualization, from system overview, and central energy plant, down to the component

levels of the individual CPUs, GPUs and Memory. We show the telemetry ingestion and display, as well as triggering and presenting the simulation results of the Modelica cooling model inside and AR/VR environment using MS-HoloLens2.

P5: COMPARING MACHINE LEARNING AND DEEP LEARNING MODELS FOR PEDIATRIC ANXIETY CLASSIFICATION USING TEMPORAL, STRUCTURED, AND ENVIRONMENTAL DATA FROM ELECTRONIC HEALTH RECORDS

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This study investigates the utility of various machine learning (ML) and deep learning (DL) models to classify pediatric patients at risk of anxiety disorders from electronic health records (EHRs). Addressing the impracticality of manual EHR reviews, our approach targets proactive care by monitoring potential anxiety onset across 20 age groups. Each model is utilized on two datasets: 1) structured data and 2) structured plus environmental data, extracted from EHRs and preprocessed with temporal information. The results underscore the utility of both ML/DL models for early detection of pediatric anxiety disorders. The classical ML models provide a solid performance baseline with an AUROC score of 0.816 for eight-year-old children, and the RNN-based DL model shows a score of 0.857. We found that each model's performance varied by age group, underscoring the necessity of personalized model selection for optimal clinical predictive analytics. The findings of this study suggest that employing ML/DL models can significantly improve the classification process of pediatric anxiety disorders within EHR systems. The model's consistency and predictive accuracy promise future use in clinical settings to enhance decision-making and improve patient outcomes. Integrating such models into healthcare practices promises a shift towards more efficient, data-driven, and personalized care.

P6: TEMPORAL ANALYSIS OF ML/DL TECHNIQUES FOR FAULT DETECTION IN CYBER-PHYSICAL SYSTEMS USING CONTROLLER AREA NETWORK DATA

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This poster presents a comprehensive benchmark study on the efficacy of machine learning (ML) and deep learning (DL) techniques for fault detection within automotive systems, utilizing multivariate time series classification. Employing the first publicly available dataset featuring simulated faults in Controller Area Network (CAN) data, our research offers a data-driven framework to evaluate the ability of various models to identify system anomalies accurately and promptly. The benchmark explores the complex temporal dynamics of high-dimensional CAN data, establishing a methodical comparison across ML/DL methodologies. Results highlight the precision and speed of fault detection, dissecting the performance of each model, discussing the strengths and specific limitations when deployed in real-world diagnostic scenarios of cyber-physical systems. By analyzing robustness and performance metrics, we provide a nuanced insight into the potential of ML/DL for reliable system monitoring and fault diagnostics, setting the stage for future innovations in automotive technology and broader cyber-physical systems.

P7: OPACIFIERS TO IMPROVE THERMAL PERFORMANCE OF POLYISOCYANURATE (PIR) FOAMS.

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Advancement of PIR foam insulation in building and construction industry has drawn significant attention recently due to its exceptional low thermal conductivity and ability to improve energy efficiency. Current commercially available polyurethane rigid foams have thermal resistivity (Rvalue) of approximately 6 h.ft2 ·□F/Btu·in. However, thermal resistivity can be further improved by minimizing the radiative heat transfer through closed-cell foam. Therefore, the introduction of opacifiers that can scatter or absorb infrared, which lowers the IR transmissivity is an interesting way for a decrease in radiative heat transfer. In this study, Silicon Carbide, Zinc Oxide and Titanium Dioxide were introduced to the PIR foam and their impact on thermal performance were evaluated. Results showed that the thermal conductivity can be significantly reduced by optimizing the size and the percentage of infrared opacifier in the foam formulation. Long-term thermal performance and morphology of opacified foams were evaluated. The present work will provide a useful guidance for selecting relevant foam in view of higher thermal insulation performances of low-density PIR cellular foams.

P8: ESTIMATING GASOLINE CONSUMPTION FOR THE RECREATIONAL BOATING SECTOR IN THE U.S.

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The U.S. recreational boating industry has experienced unprecedented growth in recent years, driven by a surge in Americans' interest in outdoor recreation, mental well-being, and quality time with loved ones, particularly during the pandemic. Understanding the fuel consumption and associated costs of boat owners is crucial for estimating the economic significance and impact of various types and sizes of boats. This study analyzes data from the 2018 National Recreational Boating Survey (NRBS), national boating statistics, the 2012 NRBS trip survey, and economic value-added data on outdoor recreational activities to estimate gasoline consumption by the recreational boating sector at the state level. The analysis focuses on four types of boats: powerboats, sailboats, pontoon boats, and personal watercraft. Boating hours are computed from the number of registered boats, gasoline boat percentages, mean boating days, and hours per boating day. Adjustments are made for active engine hours based on literature and the 2012 NRBS trip survey. Fuel efficiency (gallons per hour, GPH) by boat type is then estimated from weighted horsepower and thermal efficiency information. Finally, state-level gasoline consumption estimates were derived by multiplying boat type GPH by active boating hours and the state's boat type shares. Growth factors are incorporated using economic value-added data to project future years' consumption. This approach provides a data-driven framework for estimating gasoline consumption in the U.S. recreational boating sector, facilitating informed decision-making on off-road transportation decarbonization and resource allocation.

P9: INSIGHTS INTO PACKED BED REACTORS BY MULTI-SCALE REACTOR SIMULATION APPROACH

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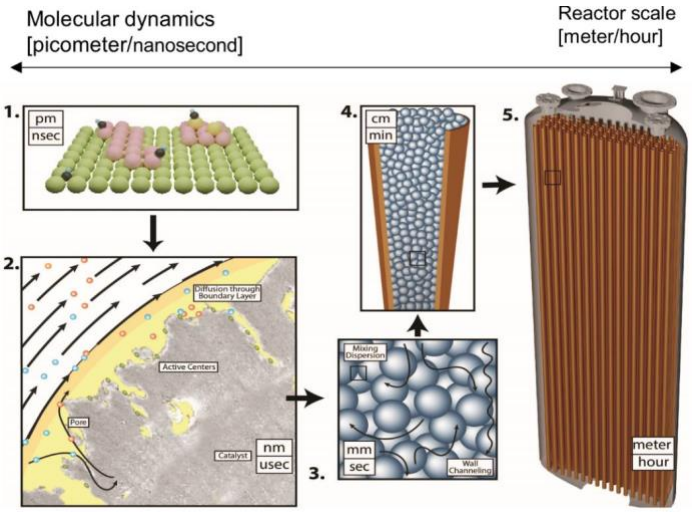
Today's chemical industries are facing daunting challenges due to high energy prices, changing feedstocks, limited resources, and the mounting pressure to adapt sustainable production methods. To handle these obstacles and to be resilient with ever changing market demands, chemical engineering community has always been in quest for novel ideas, including advanced reactor designs and process intensification approaches. Indeed, the chemical reactor systems are inherited with complex phenomena occurring on different length and time scales, and therefore gaining proper insights into reactors is cumbersome. This study demonstrates model informed scale-up strategies based on Computational Fluid Dynamics (CFD) for industrially relevant heterogenous catalytic packed-bed reactor systems. Albeit it is simple to construct, the packed-bed reactors have complex characteristics of heat/mass transfer and chemical kinetics. These interconnected transport and reaction features create a non-linear scale-up trajectory and hence require deep level of understanding from atomic scale to reactor scale. Figure 1 depicts a schematic representation of the underlining physics and chemistry in multi-scale from picometer/nanosecond to meter/hours. A CFD framework using COMSOL Multiphysics is presented, which is capable to bridge the varying scales and facilitates the successful scale up and technology transfer from lab-scale to commercial scale [2, 3]. Fig. 1 Illustration of different scales in a packed bed reactor (reproduced from ref. [1]).



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P10: DEFORMATION MECHANISMS OF ADDICTIVE MANUFACTURING 316SS USING IN-SITU MECHANICAL TEST WITH SEM EBSD.

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Additive Manufactured (AM) 316 austenitic stainless steel (316SS) is considered a structural candidate alloy for advanced nuclear reactors (e.g., sodium fast reactors). In this study, deformation mechanisms are observed using Scanning Electron Microscope (SEM)-Electron Backscatter Diffraction (EBSD) during insitu tensile tests to assess the mechanical integrity of the materials. The samples with two different orientations (vertical and horizontal) were cut into dog-bone tensile specimens. The EBSD dataset obtained during in-situ mechanical tests has advantages that can provide information about deformation (i.e., lattice rotation and active slip systems) depending on the local plastic strain. For example, the misorientation profiles within a grain show the evolution of dislocation accumulation due to plastic deformation. In addition, the grain orientation effect on twinning formation was observed for both samples at the higher strain (~15%). The inverse pole figure (IPF) identifies the orientation of the parent grain and twinning area. Also, the correlation of EBSD misorientation parameters (i.e., kernel average misorientation) and local plastic strain suggests predicting the deformation of materials. Lastly, two different orientations of samples result in different mechanical behaviors and fracture behaviors. Fractography was observed using SEM, and it showed that ductile fractures occurred dominantly for both samples.

P11: REPRODUCIBLE SURFACE-ENHANCED RAMAN SPECTROSCOPY OF NANODIAMONDS

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Impact events, such as explosions, produce a complex matrix of carbonaceous materials known as soot. The composition of soot can be effectively analyzed using Raman spectroscopy, which measures the intensities of the graphite band and the defect/disorder band. These measurements can elucidate the types of carbonaceous materials present in the soot. Notably, detonation nanodiamonds (DNDs), which are highly ordered carbon structures with an average crystal size of about 5 nm, are formed in high yields when the explosive Composition B is used. The presence of DNDs in soot can thus serve as an indicator of the type of explosive used. Traditional Raman spectroscopy typically requires extended collection times or specialized optics with UV excitation lasers to detect the ~1,332 cm−1 DND peak in soot. To address these challenges, surface-enhanced Raman spectroscopy (SERS) was employed. Samples of pure DNDs or soot were coated with a thin (~25 nm) layer of silver before measurement. This modification significantly amplifies the Raman signal from DNDs, enabling their detection using a 532 nm excitation laser in as little as 1 second. Additionally, SERS facilitates the identification of smaller DND aggregates compared with conventional Raman techniques.

P12: OPTICAL VIBRATIONAL SPECTROSCOPIC SIGNATURES RELATED TO U3O8 PRODUCTION PROCESSES

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Uranium ore concentrates (UOCs) are stable materials of high uranium density found early within the nuclear fuel cycle that allow for safe and easy transport. UOCs are typically converted to U3O8 for further processing and therefore may lose specific physiochemical characteristics relating to the materials source and processing history. In this work we explore the Raman spectra of eight oxide samples produced from various UOCs and processing pathways to examine the presence of spectroscopic signatures relating to the samples process history. Samples produced from AMEX and DAPEX processes show unique characteristics due to high concentration of αUO3 whereas samples sintered from metallic diuranates do not form pure α-U3O8 as a result of metallic ion inclusions. Single phase α-U3O8 oxide samples are obtained through sintering of ammonium diuranatate, ammonium uranyl carbonate and metastudtite intermediates. Raman spectra of these oxide samples show close agreement with pristine α-U3O8 spectra however deviations from the pristine spectra and each other are observed in the 300 – 460 cm-1 spectral range. These deviations are potentially attributed to lasting effects of process history and may serve as unique identifying signatures. Applied spectral center of mass (COM) calculations shows grouping of samples based on processing history.

P13: ULTRA-CONDUCTIVE COPPER-CARBON NANOMATERIAL COMPOSITES THROUGH BRUSH COATING

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Development of advanced conductors that can provide enhanced electrical and thermal conductivity, higher ampacity, and better mechanical strength is needed to reduce ohmic losses, transport power with smaller size and/or lightweight wires/cables and enable better thermal management across system components. Ultraconductive copper (UCC) composites that incorporate highly conductive carbon materials, e.g., carbon nanotubes (CNTs), into copper matrix is proven to be a promising strategy. In this study, we developed a commercially viable brush coating technology to incorporate CNTs on Cu substrate was developed to produce Cu-CNTs composites. The shear force during brushing action of bristles applied on Cu surface induces local alignment of the CNTs. Uniform CNTs coating was achieved after thermal treatment. Compared to Cu reference, our Cu-CNT composites demonstrate increased current carrying capacity and mechanical properties. Detailed characterizations were conducted to understand the mechanism. We believe our present approach could open new possibilities in designing advanced conductors for a broad range of electrical systems and industrial applications.

P14: SEQUENCE-PROPERTY RELATIONSHIPS OF PERIODICALLY STRUCTURED COPOLYAMIDES

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Although it is generally understood that altering monomer sequence can substantially impact bulk properties such as (semi)crystallinity and hydrophilicity, few studies to date have sought to quantify these sequence-property relationships. In this work, we use iterative synthesis to build sequenced diad, triad, and tetrad oligomers from a variety of diacid and diamine building blocks. These sequenced oligomers are subsequently polymerized through conventional solid-state polymerization, affording polyamides with high sequence specificity. We used nuclear magnetic resonance spectroscopy to confirm that monomer sequence is retained after polymerization, and molecular weight as measured by size exclusion chromatography was found to be comparable to polyamides synthesized from traditional diacid/diamine salts. Finally, we compared thermomechanical performance of sequenced copolyamides to their random counterparts using differential scanning calorimetry, dynamic mechanical analysis, tensile testing, and melt rheology. These results demonstrate the importance of monomer sequence in determining material performance. Future studies will seek to produce sequenced polymers more efficiently, and to explore additional chemistries and functionalization pathways to introduce new functionality

P15: CO2 CAPTURE FROM SEAWATER VIA A NOVEL HOLLOW FIBER CONTACTOR

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Climate change is the greatest societal and environmental danger we face today. With the massive amounts of carbon emitted every day, the solution to climate change will be a multifaceted one. In addition to reduction of greenhouse gas emissions, capture and removal of CO2 is a necessary step to remediation. While current work regarding CO2 capture centers on the gaseous sequestration, recent work has focused on removal of bicarbonates from seawater. Seawater absorbs about 40% of anthropogenic CO2 since the beginning of the industrial era with an effective CO2 concentration of 2.1 mmol kg^{-1} , or 0.095 kg m^{-3} in seawater, 140 times greater than in the atmosphere. We functionalized commercially available hollow fibers with ligands to selectively capture bicarbonates from seawater. Computational chemistry and DFT calculations aided in ligand identification to preferentially select for bicarbonates over other ions present in seawater. After bicarbonate binding, we show regeneration of the fibers through flowing an acidic solution (pH=6.5) through the fiber module to release gaseous CO2. Because the generated carbonic acid quickly degrades, the acidic buffer can be used, and reused infinitely, driving down cost. Our technology is the first reported fiber module capable of passive capture of bicarbonates from seawater.

P16: EVALUATION OF A PROPOSED LOW MELTING POINT ELEMENT-ASSISTED NUCLEATION (LEAN) MECHANISM IN DILUTE AL-ZR ALLOYS MICRO-ALLOYED WITH SN, SI, IN, AND SB

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Dilute Al-Zr alloys have shown great promise as a light-weight replacement for copper alloy in electric vehicle applications, but these alloys require aggressive heat treatments to obtain the necessary precipitation strengthening. The sluggish precipitation of the Al3Zr L12 phase has been shown to accelerate due to micro-alloying additions, such as Si. In our recent work, we found Sn micro-alloying additions both greatly accelerate the precipitation of Al3Zr L12 between 350°C and 450°C and facilitate the previously unreported nucleation of Al3Zr L12 at 200°C. To explain these finds, we proposed a new Low melting point Element-Assisted Nucleation (LEAN) mechanism for accelerating sluggish precipitation processes. To further validate the LEAN mechanism, first-principles calculations were used to select other elements, In and Sb, that may behave similar to Sn. This work assesses the effects In and Sb, in comparison to Sn and Si, have on the age-hardening and electrical conductivity behavior of an Al-0.2Zr alloy. The high temperature contribution of the LEAN mechanism is also evaluated through isothermal and 2-stage heat treatments.

P17: DIRECT OBSERVA-ON OF AN INTERFACIAL TOPOLOGICAL SUPERCONDUC-NG STATES IN FE(TE,SE)-BI2TE3 HETEROSTRUCTURE

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Topological superconductivity (TSC) has been proposed as an ideal platform for quantum computing qubits, as it could host Majorana-bound states with non-Abelian states. The interface between s-wave superconductor and topological insulator has been proposed to host Majorana-bound states, but yet hasn't been experimentally proved. Here, we use molecular beam epitaxy (MBE) to grow high-quality monolayer Fe(Te, Se) Se=20% on Bi2Te3 thin film. The existence and the location of the spin-polarized topological surface states are directly observed by the Spin and angle-resolved photoemission spectroscopy (SARPES system, and the topological surface states become superconducting at the same time with bulk states at the interface. In addition, based on the ARPES results and DFT simulations, the topological surface states don't hybridize with the Fe(Te,Se) electronic states, which is protected by the orbital selection between the states. The interfacial superconductance has been proved in our electronic transport and low-temperature scanning tunning microscopy (STM) measurements. This study indicates that the Fe(Te, Se)-Bi2Te3 is an ideal topological superconducting platform for further Majorana-based and non-Abelian electronic devices studies.

P18: POROUS LIQUIDS AS PRECURSOR FOR MIXED-MATRIX MEMBRANE (MMM) SYNTHESIS

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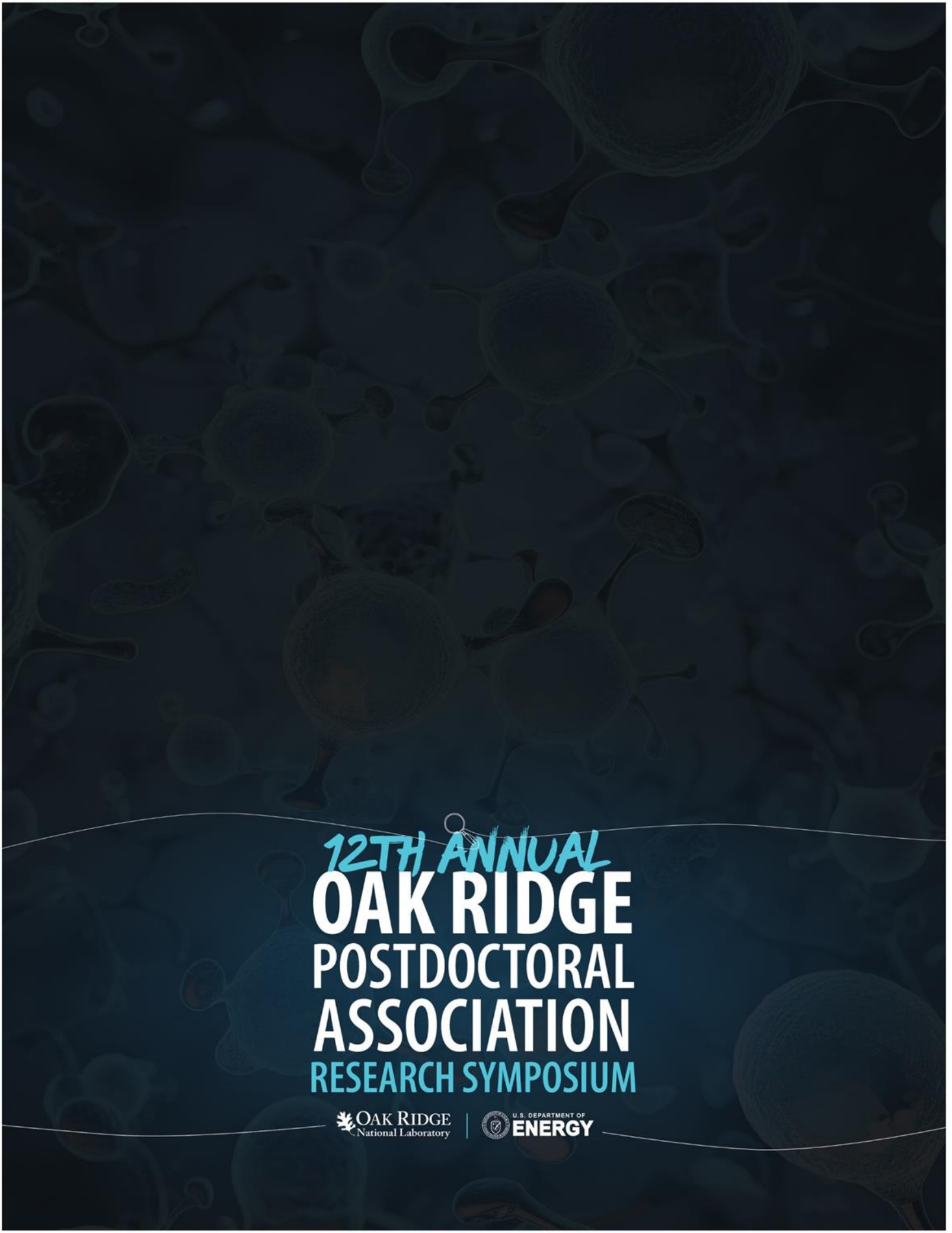
Mixed-matrix membranes (MMMs) combine the inherent advantages of polymeric support and microporous fillers. MMMs have become a focus for novel gas purification membranes. Although MMMs provide an opportunity to combine numerous porous fillers and polymeric support, the chemical incompatibility of prospective materials results in non-uniform dispersion, voids, or pockets. This affects the performance of MMMs. Porous liquids combine the porosity of microporous solids and the fluidity of liquids (including polymers). These materials with strong particle-fluid/polymer interactions have recently been proposed as an excellent precursor for the synthesis of MMMs. In this work, we present a novel generalized strategy for the synthesis of MMMs from porous liquids. We demonstrate the synthesis of a representative porous liquid with prototypical zeolite and tethered polymeric ionic liquids. The polymeric cation tethers to the surface silanol groups of the zeolite to provide uniform distribution and prevent agglomeration. The anion acts as a fluid medium for stable dispersion of zeolite particles of ~ 60 nm. The fluidity enables the transfer and coating of these porous liquids over support membranes via spin coating. In this case, the ether bonds in the anion were utilized as a precursor for e-beam cross-linking and polymerization. Such proof-of-concept studies can be extended to several porous fillers such as metal-organic frameworks, covalent organic frameworks, etc., and polymeric matrix materials.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