

BIG SCIENCE. BIG IMPACT.

14TH ANNUAL

ORPA

RESEARCH

SYMPOSIUM

MAY 6-7, 2026

TENNESSEE ROOMS



U.S. DEPARTMENT OF  
**ENERGY**

 **OAK RIDGE**  
National Laboratory



**ORPA**  
OAK RIDGE POSTDOCTORAL ASSOCIATION

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## Foreword by Laboratory Director



Welcome to the 14th Annual Oak Ridge Postdoctoral Association (ORPA) Research Symposium. Each year, this event brings together the ORNL community to highlight the breadth and impact of research across the laboratory—work that is continually strengthened by the creativity, rigor, and fresh perspectives of our postdoctoral researchers.

Whether our postdocs continue their careers within the national laboratory system or pursue opportunities in academia or industry, their contributions during their time at ORNL are significant. We are committed not only to supporting their immediate research efforts, but also to helping them define the scientific questions and directions that will shape long and

impactful careers.

This year's symposium features an outstanding group of keynote speakers. I'm pleased to welcome Dr. Bob Grove, Chief Operating Officer of the Fusion and Fission Energy and Science Directorate, who will open the program. For nearly seven decades, ORNL has played a central role in advancing fusion and fission science, and these efforts remain critical to meeting global energy needs and enabling future scientific discovery.

Additional keynote speakers include Dr. Jon Taylor, Associate Laboratory Director for Neutron Sciences; Dr. Mitchel Doktycz, Corporate Fellow and Bioimaging and Analytics Section Head; and Dr. Xiao-Ying Yu, Distinguished Scientist and Advanced Nuclear Materials Group Leader. Their expertise—spanning neutron science, bioimaging, and nuclear materials—reflects the multidisciplinary strength that defines research at ORNL and will enrich the discussions throughout the symposium.

I expect our postdoctoral researchers to continue making meaningful contributions across areas that are shaping the future of science and technology, including fusion and fission energy, artificial intelligence, quantum science, biotechnology, and more.

Thank you to all who contribute to and participate in this symposium. Your work fosters a collaborative environment where ideas are exchanged, partnerships are formed, and innovation advances. I look forward to the insights and connections that will emerge from this year's event!

Dr. Stephen Streiffer  
Laboratory Director

## Foreword by Office of Research Education Director



I'm pleased to welcome you to ORNL's annual Oak Ridge Postdoctoral Association (ORPA) Research Symposium.

Now in its 14th year, the symposium has become ORNL's flagship postdoc-led scientific event, providing a high-impact platform for showcasing the depth, breadth, and future direction of ORNL's research portfolio. Over two days, this year's program features 48 oral presentations and 23 posters reflecting both scientific rigor and mission relevance, with topics ranging from fusion materials and quantum simulation to AI for neutron diffraction, environmental microbiology, and critical-minerals recovery.

We are honored to welcome four distinguished keynote speakers, along with senior leaders and external experts who bring perspective across ORNL's mission areas. In addition to technical sessions, the symposium includes a Sponsor Showcase and structured career and networking programming, reinforcing ORPA's role in connecting postdoctoral researchers with industry partners and career pathways beyond the laboratory.

This program is a direct reflection of ORPA's leadership in building a vibrant and connected research community. Their executive committee (ORPEX) continues to deliver a forum that not only elevates postdoctoral research but also strengthens engagement across disciplines, directorates, and external partners. These efforts are essential to maintaining ORNL's position as a premier destination for early-career researchers and to ensuring that our postdocs are well positioned to contribute to the laboratory's long-term scientific leadership.

I thank the ORPEX research committee chairs, Luis Caicedo Torres and Qixing (Jason) Wang, for their outstanding leadership in curating this year's program, and I thank Jana Johnson (Office of Research Education) for her partnership and coordination. I also extend my appreciation to the many postdoc and staff volunteers, judges, and contributors whose efforts make this event possible.

The ORPA Research Symposium remains one of the clearest demonstrations of the talent, innovation, and collaborative spirit that define ORNL's postdoctoral community. I look forward to the insights you will share and the connections that will emerge over the course of the symposium.

Best wishes,  
**Moody Altamimi**

# 2026 Oak Ridge Postdoctoral Association 14th Annual Research Symposium

MAY 6-7, 2026

ORNL Conference Center, Building 5200, Tennessee Rooms (A, B, and C) and 2<sup>nd</sup> Floor

## AGENDA

| Wednesday, May 6 <sup>th</sup> , 2026 (Day 1) |   |                            |
|---|---|----------------------------|
| <b>09:00 – 09:10</b>                          | <b>Research Symposium Overview</b><br><b>Luis Caicedo Torres and Qixing (Jason) Wang</b>                                    | <b>TN Rooms, Bld. 5200</b> |
| <b>09:20 – 09:40</b>                          | <b>Welcome Address</b><br><b>Teja Kuruganti</b> , <i>Director, Computational Sciences and Engineering Division</i>          | <b>TN Rooms, Bld. 5200</b> |
| <b>09:45 – 10:30</b>                          | <b>Keynote Address</b><br><b>Bob Grove</b> , <i>Chief Operating Officer, Fission and Fusion Energy Sciences Directorate</i> | <b>TN Rooms, Bld. 5200</b> |

| Oral Presentation Session I |                                     |   |                                     |
|-----------------------------|-------------------------------------|---|-------------------------------------|
| 10:40 – 11:55               | <b>ML/AI I</b><br>RM 202A           | <b>Biosciences and Ecology</b><br>RM 202B             | <b>Materials Science</b><br>RM 202C |
| Session Chairs              | Jihoon Chung<br>Luis Caicedo Torres | Beant Kapoor<br>Mustapha Abdulmojeed<br>Julian Cosner | Shaofei Wang<br>Ralph Bulanadi      |

|               |  |   |   |
|---------------|--|---|---|
| 10:40 – 10:52 | <b>Timothy Robertson</b><br><i>Operational Machine Learning at the Spallation Neutron Source</i>                             | <b>Kathryn Bazany</b><br><i>Populus trichocarpa selects unique microbial communities under different climate-induced abiotic stress conditions</i>            | <b>Sohee Kwon</b><br><i>Tunable Topological and Magnetic Properties of <math>MnBi_2(Te_{1-x}Se_x)_4</math></i>  |
| 10:52 – 11:04 | <b>Lalit Yadav</b><br><i>Automated Phase Detection and Magnetic Structure Refinement in Neutron Diffraction Data</i>         | <b>Delaney Beals</b><br><i>High-resolution metaproteomics reveals functional redundancy in a defined bacterial community</i>                                  | <b>Brianna Billingsley</b><br><i>Magnetic structure characterization of Shastry-Sutherland material <math>BaRE_2ZnS_5</math> (<math>RE=Nd, Ce</math>)</i> |
| 11:04 – 11:16 | <b>Hunor Csala</b><br><i>MATEY: Open-source Framework for Spatiotemporal Foundation models for Physical Systems</i>          | <b>Dipendra Bhandari</b><br><i>Advancing non-covalent inhibitors against SARS-CoV-2 main protease</i>   | <b>Ralph Bulanadi</b><br><i>Auto-3DPFM: Automating Polarization-Vector Mapping at the Nanoscale</i>   |
| 11:16 – 11:28 | <b>Nasik Muhammad Nafi</b><br><i>Enabling Large-Scale Pressure Prediction for Turbulent Flows using Vision Transformer</i>   | <b>Apurv Mhatre</b><br><i>Unraveling Soil Microbe Establishment: Leveraging Genetic Mapping to Identify Genetic Factors shaping the Soil Microbiome</i>       | <b>Nduka Ogbonna</b><br><i>Hydrophilically Engineered Polyamides for High-Yield Enzymatic Recycling and Critical Minerals Capture</i>                     |
| 11:28 – 11:40 | <b>Emily Herron</b><br><i>CHUNKS: Functional Agents for Functional Materials</i>   | <b>Swetha Suresh Kumar</b><br><i>Systems genetics study of Winter and Summer regulatory networks controlling wood formation in <i>Populus trichocarpa</i></i> | <b>Muchu Zhou</b><br><i>Adsorption of hydroxamic acid ligands for improved extraction of rare earth elements from monazite ores</i>                       |
| 11:40 – 11:52 | <b>Andrew Deas</b><br><i>Beyond Binary Prediction: Interpretable Machine Learning for Risk Stratification in Opioid Care</i> | <b>Shane Franklin</b><br><i>Controlling matric potential in microfluidics to examine microbial dynamics in unsaturated porous media</i>                       | <b>Valentin Pauly</b><br><i>Performance of a Dissimilar Metal Weld for Advanced Ultra-Supercritical Coal Power Plant Applications</i>                     |

|              |  |                        |
|--------------|--|------------------------|
| 12:10 – 1:00 | <p><b>Sponsor Showcase - Working Lunch</b></p> <p><b>Jeffrey Willis</b>, <i>Chairman, United Rare Earths, Inc.</i></p> <p><b>Avery Brown</b>, <i>Senior Mechanical Engineer, Endeavor Composites, Inc.</i></p>   | TN Rooms, Bld. 5200    |
| 1:00 – 1:45  | <p><b>Keynote Address</b></p> <p><i>Xiao-Ying Yu, Distinguished Scientist Group Leader, Advanced Nuclear Materials</i></p>   | TN Rooms, Bld. 5200    |
| 1:45 – 2:00  | <p><b>Group Photo</b></p>  | TN Rooms, Bld. 5200    |
| 2:00 – 5:00  | <p style="text-align: center;"><b>Poster Sessions</b></p> <p style="text-align: center;">[Session 1] 2:15 – 3:15 Odd Numbered Posters</p> <p style="text-align: center;">[Session 2] 3:30 – 4:30 Even Numbered Posters</p> <p style="text-align: center;">Chairs:</p> <p style="text-align: center;">Juhyun Oh</p> <p style="text-align: center;">Hannah Musgrove</p> <p style="text-align: center;">Zechariah Kitzhaber</p> <p style="text-align: center;">Regan McDearis</p> | Main Street, Bld. 5700 |

**Thursday, May 7<sup>th</sup>, 2026 (Day 2)**

|                      |  |                            |
|----------------------|--|----------------------------|
| <b>09:00 – 09:10</b> | <p><b>Research Symposium Overview</b></p> <p><b>Luis Caicedo Torres and Qixing (Jason) Wang</b></p>                      | <b>TN Rooms, Bld. 5200</b> |
| <b>09:10 – 09:25</b> | <p><b>Welcome Address</b></p> <p><i>Moody Altamimi, Director, Office of Research Education</i></p>                       | <b>TN Rooms, Bld. 5200</b> |
| <b>09:30 – 10:15</b> | <p><b>Keynote Address</b></p> <p><i>Mitchel Doktycz, Corporate Fellow and Section Head, Bioimaging and Analytics</i></p> | <b>TN Rooms, Bld. 5200</b> |

**Oral Presentation Session II**

|                |   |   |   |
|----------------|---|---|---|
| 10:25 – 11:40  | <p><b>Building and Transportation Sciences</b></p> <p>RM 202A</p>   | <p><b>Quantum Science and Physics</b></p> <p>RM 202B</p>  | <p><b>Fission and Fusion Energy</b></p> <p>RM 202C</p>  |
| Session Chairs | <p>Saijan Pokhrel</p> <p>Doris Hung</p> <p>Shiwanka Wanasinghe</p>  | <p>Aneesh Ramaswamy</p> <p>Nirjhar Sarkar</p>   | <p>Shaileyee Battacharya</p> <p>Yadu Sasikumar</p>  |
| 10:25 – 10:37  | <p><b>Shrikar Banagiri</b></p> <p><i>Influence of operating conditions on ethanol-fired passive prechamber combustion engines</i></p> | <p><b>Amit Jamadagni Gangapuram</b></p> <p><i>Efficient representation of noisy quantum states at scale</i></p> | <p><b>Gabriel Parker</b></p> <p><i>Chemical, Mechanical, and Thermal Properties Evaluation of Lithium Ceramics as Solid Breeder Materials for Fusion Reactors</i></p> |

|               |   |  |   |
|---------------|---|--|---|
| 10:37 – 10:49 | <p><b>Jihoon Chung</b></p> <p><i>Bridging Advanced Building Control and Scalable Deployment: A Low-Cost, Open-Source Building Energy Management Framework for Small and Medium-Sized Commercial Buildings</i></p> | <p><b>Anshumitra Baul</b></p> <p><i>Entanglement benchmarking in Quantum Simulations of Spin Systems</i></p>   | <p><b>Daniel Schappel</b></p> <p><i>Analysis of Fission Product Release from Furnace-Tested TRISO Particles</i></p>                             |
| 10:49 – 11:01 | <p><b>Chih-Hsuan "Doris" Hung</b></p> <p><i>From Materials to Megawatt-Hours: Modeling Sodium-Ion Batteries for Grid Applications</i></p>   | <p><b>Chiranjit Mondal</b></p> <p><i>Two-band Euler Topology as a Source of Single-Band Quantum Geometry</i></p>   | <p><b>Yuchen Jiang</b></p> <p><i>Transient plasma simulations for interaction with liquid metal in magnetic confinement fusion reactors</i></p> |
| 11:01 – 11:13 | <p><b>Sajjan Pokhrel</b></p> <p><i>Numerical modeling of thermal energy extraction from abandoned mine shafts using closed-loop heat exchangers</i></p>   | <p><b>Deb Mallick</b></p> <p><i>Microstructural-heterogeneity induced macroscopic angular magnetoresistance in conventional and unconventional superconductors</i></p> | <p><b>Zechariah Kitzhaber</b></p> <p><i>Staying in the Loop: Online Monitoring of Molten Salts via Laser-Induced Breakdown Spectroscopy</i></p> |
| 11:13 – 11:25 | <p><b>Huixin Jiang</b></p> <p><i>Multifunctional Metal Organic Framework Composites for Improving Indoor Air Quality</i></p>  | <p><b>DoHoon Kim</b></p> <p><i>Discovery of quantum magnetic delafossites via High-throughput first-principles calculation</i></p>                                     |   |
| 11:25 – 11:37 | <p><b>Karen P. Cortes Guzman</b></p> <p><i>Phosphorous-based Flame Retardants as a Safe and High-performing Solution for Building Technologies</i></p>  |  |   |

|              |  |                     |
|--------------|--|---------------------|
| 11:45 – 1:15 | <p><b>Reflections on Leadership Panel – Working Lunch</b></p> <p><b>Tara Pandya</b>, <i>Section Head, Nuclear Applications, Methods, and Data</i></p> <p><b>Melissa Cregger</b>, <i>Chief Science Officer, Center for Bioenergy Innovation</i></p> <p><b>Sarah Cousineau</b>, <i>Director, Research Reactor Division</i></p> <p><b>Mariam Kiran</b>, <i>Group Leader, Quantum Communications and Network</i></p> | TN Rooms, Bld. 5200 |
| 1:15 – 2:00  | <p><b>Keynote Address</b></p> <p><b>Jon Taylor</b>, <i>Associate Lab Director, Neutron Sciences Directorate</i></p>  | TN Rooms, Bld. 5200 |

### Oral Presentation Session III

|                |  |  |   |
|----------------|--|--|---|
| 2:10 – 3:10    | <p><b>AI/ML II</b><br/>RM 202A</p>   | <p><b>Chemistry and Chemical Ecology</b><br/>RM 202B</p>   | <p><b>Nuclear Materials</b><br/>RM 202C</p>   |
| Session Chairs | <p>Hunor Csala<br/>Yunhan Wu</p>   | <p>Rachel Gaines<br/>Nishu Devi<br/>Mustapha Abdulmojeed</p>   | <p>Jing Lin<br/>Thiago Pinheiro dos Santos</p>  |
| 2:10 – 2:22    | <p><b>Aaron Werth</b><br/><i>Comparison and Analysis of Modern AI-Based Pentesting Tools</i></p> | <p><b>Nishu Devi</b><br/><i>Dopant-Guided Suppression of SO<sub>2</sub> Poisoning in Cu Catalysts for Electrochemical CO<sub>2</sub> Reduction</i></p> | <p><b>Shaileyee Bhattacharya</b><br/><i>Investigation of hydrogen retention and phase stability in neutron-irradiated yttrium hydrides: A synchrotron X-ray diffraction study</i></p> |

|                    |  |   |   |
|--------------------|--|---|---|
| <p>2:22 – 2:34</p> | <p><b>Raymond Borges Hink</b></p> <p><i>From Evidence to Vulnerability Candidates: An Explainable Local Pipeline for Cyber and OT Triage using Large Language Models</i></p> | <p><b>Nicholas Gregorich</b></p> <p><i>Repurposing Lithium Battery Recycling Wastewater for Marine Carbon Dioxide Capture and Storage</i></p>   | <p><b>Matthew deJong</b></p> <p><i>Stability of neutron irradiated yttrium hydride under cyclic heating</i></p>   |
| <p>2:34 – 2:46</p> | <p><b>Yunhan Wu</b></p> <p><i>High-Resolution Modeling of Indoor Radon Exposure with Uncertainty Quantification in Utah</i></p>  | <p><b>Noor Md Shahriar Khan</b></p> <p><i>Theoretical investigation of molecular photoswitch for early detection of Alzheimer's disease</i></p> | <p><b>Yuki Jimba</b></p> <p><i>Effects of High Dose Neutron Irradiation at Light Water Reactor-Relevant Temperatures on the Mechanical Properties of SiC/SiC Composites</i></p> |
| <p>2:46 – 2:58</p> | <p><b>Zhongcan Xiao</b></p> <p><i>Transforming Single Crystal Neutron Diffraction with Agentic AI</i></p>  | <p><b>Molly Paul</b></p> <p><i>Frontiers of particle analysis: an innovative device for single particle ICPMS</i></p>                           | <p><b>Logan Clowers</b></p> <p><i>Fracture Toughness Testing of Nuclear Structural Materials in Extreme Environments Using Miniaturized Test Specimens</i></p>                  |

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|-------------|--|--|---|
| 2:58 – 3:10 | <p align="center"><b>Gomathi Lakshmanan</b></p> <p align="center"><i>Milo: An Intelligent Research CoPilot</i></p> | <p align="center"><b>Jinping Xue</b></p> <p align="center"><i>Sorption-based removal of mercury species from aqueous solutions: Influencing factors and environmental implications</i></p> | <p align="center"><b>Thiago J. Pinheiro dos Santos</b></p> <p align="center"><i>Accurate Prediction of Chemical and Redox Potentials in Molten Salts from DFT-Based Free Energy Simulations</i></p> |
|-------------|--|--|---|

|             |  |  |
|-------------|--|--|
| 3:15 – 4:00 | <p align="center"><i>[previous registration required]</i> <b>Career Pathways Networking Event</b></p>  | <p align="center"><b>TN Rooms Lobby, Bld. 5200</b></p> |
| 4:00 – 4:30 | <p align="center"><b>Career Pathways Panel</b></p> <p align="center"><b>Burak Ozpineci, Corporate Fellow</b></p> <p align="center"><b>Budhu Bhaduri, Chief Data Officer</b></p> <p align="center"><b>Uday Vaidya, Governor’s Chair</b></p> <p align="center"><b>Amanda Thornton, Project Management Specialist</b></p> <p align="center"><b>Ziad Burbar, Siemens Healthineer</b></p> <p align="center"><b>Yadu Sasikumar, R&amp;D Staff Member</b></p> | <p align="center"><b>TN Rooms, Bld. 5200</b></p>       |
| 4:30 – 5:00 | <p align="center"><b>Closing Ceremony</b></p>  | <p align="center"><b>TN Rooms, Bld. 5200</b></p>       |

**Poster Session – May 6<sup>th</sup> 2:00pm – 5:00pm – Main Street, Bld. 5700**

|    |                              |   |
|----|------------------------------|---|
| 1  | Polina Shpilker              | Designing a Metadata Schema and Metadata Tools for Post-Translational Modification Proteomics Workflow Discovery and Interoperability |
| 2  | Owen Johnson                 | Optimization of a Laminar Flow Cell for Shear-Dependent Neutron Reflectometry   |
| 3  | Hannah Musgrove              | Air blown ion plasma treatment of autoxidative inks to reduce setoff  |
| 4  | Regan McDearis               | Interactions Between Warming and Drying Affect Microbial Communities, Activity and Decomposition Processes in Peatland Soil           |
| 5  | Kristyn Ardrey               | Examining EBC Systems on SiC Substrates in Varying High Temperature Steam Environments  |
| 6  | Emily Herron                 | SciEntropy: Calibrated Uncertainty Quantification for Trustworthy Scientific AI Agents  |
| 7  | Qixing (Jason) Wang          | Title: A Game-Theoretic Min-Max Framework for Large-Scale Freight Network Vulnerability Assessment                                    |
| 8  | Preeti Sar                   | Developing a machine learning framework for accurately determining transport fluxes using the quasilinear TGLF model                  |
| 9  | Sanjay Das                   | AI-powered cosmological simulations for dark energy signatures  |
| 10 | Latif Patwary                | Understanding Spatially Varying Determinants of E-Scooter Ridership for Smarter Urban Mobility  |
| 11 | Chandra Sekhar Somayajula    | Cost competitiveness of remanufactured wood products: Techno-economic and macroeconomic analyses                                      |
| 12 | Ernesto Camilo Zuleta Suarez | Evaluation of Anode Designs for Sodium Metal Hybrid Redox Flow Batteries  |
| 13 | Aneesh Ramaswamy             | Characterization of long timescale polarization drifts in aerial-inground fiber using machine learning                                |

|    |                    |   |
|----|--------------------|---|
| 14 | Xinju Dong         | Understanding of Molecular Interactions in Quantum Chemistry on Frontier HPC  |
| 15 | Abdulrasheed Sado  | Physics-Informed Deep Learning for Geometric Deblurring in Hyperspectral Neutron Imaging  |
| 16 | Farhin Farhad Riya | From Gradients to Representations: A Unified View of Privacy Leakage in Federated Learning  |
| 17 | Shalika Meedin     | Water-Ion Correlations and Structural Dynamics in Concentrated Salt Solutions   |
| 18 | Debashish Sur      | Is High Mo Content in Ni based alloys Sufficient to Ensure Corrosion Resistance in Molten Salt Reactor Salts?                                     |
| 19 | Jonas Mart Linge   | Gas Diffusion Electrode Study of Oxygen Reduction on PtNi and PtCo-based Catalyst Layers for High Temperature Proton Exchange Membrane Fuel Cells |
| 20 | Jessica LaFond     | Using High-Throughput Phenotyping to Explore the Genetic Basis of Biological Nitrification Inhibition in Populus                                  |
| 21 | Bal Maharjan       | Plant RNA Vision 2.0  |
| 22 | Shivam Pandit      | Sequence-Encoded Molecular Switches Control Condensate Formation in Plant Stress Proteins   |
| 23 | Adnan Muzaffar     | A Multigene Stacking Approach to Increase Cutin Biopolymer in Poplar  |

## Keynote 1

### Dr. Bob Grove



Bob Grove is a nuclear engineering leader with more than four decades of experience advancing computational methods in reactor physics, radiation transport and shielding, and fusion neutronics applications. His career spans three national laboratories and includes major industry and international collaborations.

He currently serves as Interim Chief Operating Officer for the Fusion and Fission Energy Science Directorate at Oak Ridge National Laboratory. Since joining ORNL in 2010, Bob has held several leadership roles, including Group Leader for Radiation Transport, Section Head for Nuclear Modeling & Simulation, and Chief Scientist within the Nuclear Energy and Fuel Cycle Division.

Bob is an active member of the international fission and fusion communities. He has chaired two OECD Nuclear Energy Agency expert groups – one on Radiation Transport and Shielding and another on the Physics of Reactor Systems – and he has played influential roles in neutronics developments for both ITER and JET. Within the American Nuclear Society, he has served in leadership positions in the Mathematics & Computations Division and the Reactor Physics Division and is an active member in the Radiation Protection and Shielding Division and the Fusion Energy Division.

He holds a Ph.D. in Nuclear Engineering from the University of Michigan and both M.S. and B.S. degrees in Nuclear Engineering from The Pennsylvania State University. Bob has authored numerous technical publications on hybrid Monte Carlo/deterministic methods, fusion neutronics, radiation dose modeling, and advanced radiation transport computational techniques.

## Keynote 2

### Dr. Xiao-Ying Yu



Dr. Xiao-Ying Yu is a distinguished scientist and the group leader of the advanced nuclear materials at the Materials Science and Technology Division of Oak Ridge National Laboratory (ORNL). She obtained her bachelor's degree in Inorganic, Nonmetallic Materials, and her doctoral degree in Physical Chemistry from the University of Michigan.

Dr. Yu did a postdoc at Brookhaven National Laboratory. She then became a staff scientist at Colorado State University. She took the senior scientist position at the Pacific Northwest National Laboratory in 2006 and rose to Chief Engineer in 2020. Dr. Yu joined the Materials Science and Technology Division as a distinguished scientist at ORNL in 2022.

Dr. Yu invented new instrumentation and methodologies to study separation and material interfaces at the micro and nanoscale with diverse applications including biomaterials, system biology, energy storage, decarbonization, and environmental mitigation. She was the principal investigator of the prestigious R&D 100 and FLC Technology Transfer Award of novel analytical instrument based on microfluidics and enabled in situ and operando liquid SIMS and added new solutions in liquid electron microscopy.

Dr. Yu has mentored over eighty students, postdoctoral researchers, and many staff scientists in her tenure in the DOE complex. She is a fellow of the American Vacuum Society. She also serves different roles for American Chemical Society and leads symposia in Microanalysis and Microscopy in North America. Dr. Yu had several US patents and published over 146 peer reviewed articles with an H index of 43.

## Keynote 3

### Dr. Mitchel Doktycz



Mitchel J. Doktycz is a Corporate Fellow and heads the Bioimaging and Analytics Section in the Biosciences Division at the Oak Ridge National Laboratory (ORNL). He is also a member of the Research Staff in the Center for Nanophase Materials Sciences at ORNL and is also a faculty member with the University of Tennessee, Knoxville in the UT-ORNL Bredesen Center. He received his B.S. in Biology and Chemistry in 1985 and his Ph.D. in Chemistry in 1991 from the University of Illinois at Chicago.

His research interests focus on the intersection of natural and synthetic systems. His laboratory is involved in the development of analytical technologies for post-genomics studies with specific emphases on molecular and cellular imaging techniques and the use of nanomaterials to study and mimic biological systems. He has received an R&D 100 Award and National Federal Laboratory Consortium Award for Excellence in Technology Transfer. He is a Fellow of the American Institute for Medical and Biological Engineering and of the American Association for the Advancement of Science.

## Keynote 4

### Dr. Jon Taylor



Dr. Jon Taylor is the Associate Laboratory Director for the Neutron Sciences Directorate at Oak Ridge National Laboratory (ORNL). He earned his bachelor's degree in physics from DeMontfort University in Leicester, England. Upon completion of his Ph.D. in condensed matter physics at Loughborough University in 2000, he became a research scientist at the Rutherford Appleton Laboratory in the United Kingdom. Jon also spent seven years at the European Spallation Source in Lund, Sweden where he was the Head of the Neutron Scattering Systems Division as well as the Data Management and Software Centre.

Jon joined ORNL in 2022 as the Program Manager for Neutron Data and Computing before assuming the role of Neutron Scattering Division Director in June 2023.

## Poster Session Abstracts

### **Designing a Metadata Schema and Metadata Tools for Post-Translational Modification Proteomics Workflow Discovery and Interoperability**

Polina Shpilker\*, Joshua Brown, Patrick Widener

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A lack of metadata causes data to become difficult to discover and reuse. However, creating a novel schema is insufficient: tools need to exist to handle the schema and the development of a novel schema risks creating another difficult-to-use artefact. NW-Brave, a collaborative work funded by DOE BER, aims to de-silo these highly specific data to create powerful predictive models. An example of this is our work to support PTM-Psi, a tool for studying post-translational protein modifications developed at PNNL. We develop a novel JSON-Schema schema for the output of PTM-Psi. We adapt this schema into a LinkML schema to interoperate with the National Microbiome Data Collaborative's (NMDC) existing schema, chosen for its focus on combining and re-using existing standards. As LinkML is a complex schema description language, we also develop upgrades to the data management system used to store PTM-Psi data, DataFed. This involves the creation of a novel schema management service with a focus on modularity and schema and metadata validation capabilities. This process not only extends the capabilities of NMDC's schema but also provides an example for other proteomics pipelines to follow as part of NW-Brave's goal to create powerful cross-domain predictive models.

**Keywords: metadata, schemas, interoperability**

*This initiative is sponsored by: DOE BER*

# Optimization of a Laminar Flow Cell for Shear-Dependent Neutron Reflectometry

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In Situ laminar flow cells at Neutron Reflectometers enable researchers to probe the effects of shear on buried solid/liquid interfaces, with applications ranging from energy storage to lubrications. Historically, these cells have faced a trade-off: they either produce non-uniform shear across the neutron target region, or they rely on diffusing reservoirs requiring prohibitively high fluid volumes, which is costly when using deuterated liquids. A flow cell design that produces laminar flow without resorting to excessive fluidic volumes is desperately needed. In this project analytical fluid mechanics is used to understand the factors that influence flow uniformity in such cells. Based upon these analytical foundations two optimized flow cell designs are developed and rigorously analyzed using computational fluid dynamics across a diverse range of operating conditions. The performance of these optimized cells is compared against that of existing and standard cell designs showing a marked improvement in flow uniformity. Additionally, practical factors such as the effects of thermal expansion and reasonable manufacturing tolerances on the performance of the cells are considered. This work culminates in the successful manufacture and deployment of one of the optimized cell designs to beamline 4B of the Spallation Neutron source.

**Keywords: Neutron Reflectometry, Laminar, Shear**

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## **Air blown ion plasma treatment of autoxidative inks to reduce setoff**

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Air blown ion plasma treatment of autoxidative inks to reduce setoff

Rapid curing of autoxidative inks and coatings is essential for the manufacturing of security products, like banknotes, passports, and microelectronics. However, inadequate ink setting can reduce durability and cause unwanted mass transfer (i.e. setoff) from the printed substrate (donor) to an adjacent (receiver) surface. Air blown plasma treatment is a promising route to accelerate autoxidative setting by driving oxidation and crosslinking of surface-level polymer networks. Despite this potential, application of atmospheric plasma directly to autoxidative inks has yet to be fully explored. Therefore, we evaluated the impacts of air blown plasma on setoff reduction with alkyd-based versus water-based inks. To generate reproducible setoff as a function of plasma parameters and interfacial shear conditions, a reciprocating sliding tribometer was developed to impose controlled contact and shear between donor and receiver substrates. To quantify ink transfer, receiver samples were imaged and analyzed with a trained Weka segmentation. Tribological results were compared with surface characterization via FTIR to track plasma-induced chemical changes and monitor signatures consistent with alkyd resin curing. With this workflow, we determined blown ion plasma can reduce setoff of alkyd-based reagents at industrial time scales, and plan to fine-tune mechanistic guidance to support with scaling plasma-assisted curing.

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**Keywords: Printing Inks, Atmospheric Plasma, Polymer Curing, Rapid Manufacturing**

*This initiative is sponsored by: Bureau of Engraving and Printing Department of Energy Project Number SPPS 2248-Z626-23*

# Interactions Between Warming and Drying Affect Microbial Communities, Activity and Decomposition Processes in Peatland Soil

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Northern peatlands play a vital role in the global carbon cycle due to extensive organic carbon storage, primarily in cold, waterlogged soils. However, these environments are experiencing increasing pressures from warmer temperatures, which may significantly impact carbon cycling processes. Within the ORNL-SPRUCE experiment, warming treatments aimed at understanding these pressures have also resulted in increased surface drying, which complicates efforts to understand their individual effects on soil processes. To address this, we conducted a lab-based study designed to disentangle the effects of temperature and moisture on peat collected from the undisturbed bog adjacent to the SPRUCE plots.

Peat from the 20–30 cm depth layer was incubated for 90 days under controlled conditions, with a factorial design comprising three temperature treatments (14°C, 18.5°C, and 23°C) and three moisture levels (95% VWC, 75% VWC, and 55% VWC) representing the range of observed temperatures and corresponding moisture levels in the field. Carbon dioxide and methane fluxes were continuously monitored throughout the experiment, revealing a significant interactive effect between temperature and moisture treatments. Warmer conditions increased CO<sub>2</sub> respiration rates, but the highest CO<sub>2</sub> flux was in the 75% VWC treatment. Methane flux was also strongly influenced by treatment conditions: samples incubated at higher temperatures initially produced methane, which was subsequently consumed, implying a shift in microbial activity as the moisture in the jars decreased.

To further explore how microbial communities mediate these responses, we are currently performing DNA- and RNA- based amplicon sequencing targeting 16S rRNA genes to profile bacterial and archaeal community composition and to identify the active microbial populations. To complement this, Fourier-Transform Infrared (FTIR) spectroscopy is also being used to assess how warming and drying influence the chemical composition of carbon compounds and metabolites within the peat. These analyses will provide a mechanistic understanding of how temperature and moisture independently and interactively impact peat decomposition processes.

This study elucidates the interplay between warming and drying in shaping the microbial and chemical drivers of carbon cycling in northern peatlands. By resolving the independent effects of temperature and moisture, this work will generate critical information to improve future model predictions of carbon cycling in these ecosystems. **Keywords: peat ecosystem, methane, carbon flux**

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# High Pressure, High Temperature Steam Effects on EBC Systems

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High Pressure, High Temperature Steam Effects on EBC Systems

Kristyn D. Ardrey, Michael J. Lance, Mackenzie J. Ridley

Environmental barrier coatings (EBCs) are engineered to safeguard SiCfiber/SiCmatrix ceramic matrix composites (CMCs) deployed in turbine engines by reducing wear in high-temperature, water vapor-rich environments. EBC failure is frequently linked to accelerated oxidation of the silicon bond coating under elevated-temperature steam, resulting in the development of thickened thermally grown oxide (TGO) layers. Such formation elevates interfacial stress, diminishes adhesion, and leads to coating spallation, thereby exposing the underlying composite to further oxidation. Comprehensive understanding of high-temperature oxidation effects on EBC systems is essential for constructing accurate lifespan models for turbine components. However, it should be noted that the majority of EBC research is performed at atmospheric pressure, whereas actual turbines operate at pressures greater than 20 atm within combustion zones. To more accurately replicate operational conditions, this study conducted experiments on rare earth silicate EBCs applied to SiC substrates under increased pressure settings. The coated samples were evaluated at temperatures of 1100°C, 1200°C, and 1300°C, under both 1 atm and 10 atm pressure, in steam environments. Subsequent analyses focused on the microstructural evolution of the EBC/Si/SiC system. Results from these experiments revealed key dependencies of TGO behavior in relation to elevated pressure conditions.

**Keywords: Environmental Barrier Coatings, Thermally Grown Oxide, High Pressure, High Temperature, Oxidation**

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# SciEntropy: Calibrated Uncertainty Quantification for Trustworthy Scientific AI Agents

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AI agents that autonomously generate hypotheses, design experiments, and interpret data are entering scientific workflows at a rapid pace. Yet these large language model-powered systems are limited by their inevitable tendency to hallucinate, producing plausible but fabricated claims. They provide no built-in measure of output reliability, leaving researchers to manually verify claims at a pace incompatible with the autonomous workflows these agents are designed to accelerate. Independent evaluations of leading scientific AI systems have found high experiment failure rates exceeding and AI evaluators are frequently unable to distinguish correct results from incorrect ones.

We present SciEntropy, a modular uncertainty quantification framework that wraps scientific AI agent outputs with per-claim confidence estimates. SciEntropy combines multiple signals, including semantic entropy over sampled completions, retrieval-grounded verification against source literature, and self-consistency probing, into a single calibrated score. Packaged as middleware for common agent frameworks, SciEntropy provides inline confidence annotations, uncertainty summary cards, and propagation gates that prevent low-confidence claims from cascading through multi-agent pipelines. We evaluate on 500 expert-annotated scientific claims in materials science demonstrating improved hallucination detection and downstream error reduction in multi-step agentic workflows.

**Keywords: Trustworthy AI, Scientific AI Agents, Uncertainty Quantification, Hallucination Detection, Multi-Agent Pipelines**

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# A Game-Theoretic Min-Max Framework for Large-Scale Freight Network Vulnerability Assessment

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This research presents a scalable min-max optimization framework based on game theory for assessing the vulnerability of freight transportation networks under adversarial disruptions. Motivated by increasing threats such as natural disasters, terrorist attacks, and infrastructure failures, we model the vulnerability assessment as a two-player zero-sum game, wherein a strategic disruption agent allocates a limited attack budget to maximize system-wide damage, while a system planner simultaneously optimizes routing and resource allocation to minimize loss. Unlike passive link-removal simulations, this adversarial formulation captures the strategic interdependence between disruption and resilience — modeling an intelligent adversary rather than random failure.

A multi-dimensional loss function unifying economic, logistical, structural, and congestion impacts is optimized via a link-based reformulation that eliminates explicit OD path enumeration, reducing complexity from  $\mathcal{O}(n^2)$  to  $\mathcal{O}(n)$ . The resulting game is solved iteratively using the Method of Successive Averages (MSA), converging to a Nash equilibrium through alternating best-response updates.

Applied to the New York State freight network (~15,000 links, 12,000+ OD flows), the framework completes full vulnerability assessment in under one minute versus over ten days for exhaustive simulation, while achieving ~60% overlap in top-100 critical link identification. This approach offers a scalable, behaviorally grounded tool for national freight resilience planning.

**Keywords: Freight Vulnerability, Game Theory, Min-Max Optimization**

*This initiative is sponsored by: New York State Department of Transportation (NYSDOT)*

# Developing a machine learning framework for accurately determining transport fluxes using the quasilinear TGLF model

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A new neural network model for a quasilinear saturation rule has been developed to map linear gyrokinetic data to nonlinear saturated potential magnitudes to predict the total energy and particle fluxes. The training dataset used is taken from the high-resolution simulation database generated from nonlinear CGYRO for developing the SAT3 model. Overall, SAT3-NN is able to capture the 1D squared potential magnitudes of the dataset more accurately than SAT3, as depicted by lower percentage errors in the peak locations and peak values of the 1D squared potentials. The resulting fluxes also had smaller deviations from the nonlinear CGYRO data as compared to previous saturation models such as SAT0 - SAT2. Consistent with SAT3, SAT3-NN is able to recreate the turbulent flux characteristics such as anti-gyroBohm scaling of fluxes seen for TEM-dominated cases. We further implement integrated modeling to assess the uncertainty of the neural network in practical applications.

## Acknowledgement

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**Keywords: quasilinear models, machine learning, gyrokinetics, saturation rules, plasma fluxes, tokamak core.**

*This initiative is sponsored by: (DOE-FES) Enabling Tokamak Pulse Simulation, ORNL FED*

# Understanding Spatially Varying Determinants of E-Scooter Ridership for Smarter Urban Mobility

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Shared e-scooters have rapidly emerged as a popular choice for short urban trips. However, cities often deploy them without knowing which neighborhoods will actually use them, and why. Poor deployment decisions can waste resources and leave underserved communities without viable mobility options. To this end, we developed a Bayesian spatiotemporal model that estimates daily e-scooter ridership at the neighborhood level. The model includes bike infrastructure, bus service frequency, population density, walkability, and weather as covariates, with spatially varying coefficients that allow each factor's influence to differ by location. We apply this framework to 2022 daily trip records from 80 neighborhoods in Norfolk, Virginia. Results indicate that the effect of infrastructure investments on ridership varies substantially across neighborhoods. The relationship between e-scooter use and public transit also depends on local context: in dense, well-connected areas, e-scooters complement transit as a first-and-last-mile option, while in lower-density settings, the two modes tend to substitute for each other. Weather and day-to-day habits also play a significant role: a high-ridership day tends to carry momentum into the next. These spatially varying patterns can guide transportation planners on where to expand scooter fleets, build infrastructure, and integrate micromobility with transit.

**Keywords: E-scooter Demand, Micromobility, Spatiotemporal Modeling, Bayesian, Urban Transportation**

*This initiative is sponsored by: New York State Department of Transportation (NYSDOT)*

# **Cost competitiveness of remanufactured wood products: Techno-economic and macroeconomic analyses**

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Construction and demolition (C&D) waste often contains materials that remain in good condition and could be reused. Recovering such materials provides an alternative source of raw inputs while simultaneously reducing pressure on increasingly limited landfill capacity. Among reusable materials, wood products, which make up approximately 7% of total C&D debris, are particularly well suited for remanufacturing. Remanufacturing preserves the material's core structure rather than breaking it down into constituent elements.[1] As a result, reclaiming discarded wood products and converting them into engineered wood products (EWP) or mass timber is a promising pathway.

Prior studies have evaluated the structural performance of mass timber produced from reclaimed wood and reported comparable strength to conventional products.[2] However, for broad deployment, remanufactured EWP must also be economically competitive. This work assesses the economic viability of producing EWP from reclaimed wood using technoeconomic and macroeconomic analyses. The technoeconomic analysis compares the remanufacturing pathway with a commercial benchmark process and identifies key cost drivers. It includes estimation of capital and operating expenditures based on raw material inputs, energy use, and the processing equipment required for remanufacture. The macroeconomic analysis quantifies economy-wide ripple effects of this remanufacturing approach across U.S. industries. Key takeaways from the analysis include the final cost of remanufactured EWP produced using the proposed remanufacturing procedure, along with identification of the main cost and energy hotspots to target for further cost reductions.

**Keywords: Scale-up cost analysis, employment creation estimation, mass timber, input-output modeling**

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# Evaluation of Anode Designs for Sodium Metal Hybrid Redox Flow Batteries

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Redox flow batteries (RFBs) are electrochemical energy-storage systems in which power and energy are independently scaled, enabling flexible design, modularity, and straightforward scale-up. A growing variant, the hybrid RFB, pairs a solid redox-active material on one side with a liquid electrolyte on the other. By combining the stability and high capacity of solid electrodes with the compositional tunability of flowing catholytes or anolytes, this approach can increase energy density and improve chemical control. Here, we study a hybrid RFB that uses a sodium metal anode, a liquid sodium thiophosphate catholyte, and a beta-alumina solid electrolyte (BASE) separator. To determine the most effective anode configuration, we tested several Na|Na symmetric cell designs using galvanostatic cycling and electrochemical impedance spectroscopy (EIS): (i) direct Na-BASE contact (no-gap), (ii) a liquid-filled electrolyte gap between the electrodes, and (iii) a porous interlayer at the interface. The results indicate that adding a porous interlayer enhances stability by promoting Na<sup>+</sup> transport, mitigating dendrite growth, and avoiding direct Na-separator contact. Although the no-gap design maintained a steady overpotential, it ultimately failed due to dendrite-driven shorting. Overall, the presentation emphasizes the balance between sodium interfacial stability and ion transport and highlights the importance of engineered interfacial layers for dependable sodium-based hybrid RFB operation.

## Acknowledgements

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**Keywords:** Redox flow batteries, sodium batteries, beta-alumina solid electrolyte.

# Characterization of long timescale polarization drifts in aerial-inground fiber using machine learning

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We collected 11 months of continuous polarization power measurements of a 1550 nm optical signal on a 15 km aerial-inground fiber loop in the QNET quantum network testbed; and analyzed long-timescale (>1 day) polarization drift by computing sub-Hz Fourier magnitudes of the signal. We used non-smooth random forest and smooth support vector machines to estimate the peak temporal statistics of the Fourier magnitudes using current and lagged meteorological conditions (temperature, humidity and wind speed) as predictors. Including 3-day lagged weather features improved test performance by () and reduced test RMSE by ~20% for the peak heights. Feature-importance analysis using SHAP (SHapley Additive exPlanations) values and LOFO (leave-one-feature-out) scores demonstrated temperature to be a stronger predictor, with test SHAP values six times larger than those of humidity/wind, while including humidity and wind yielded a ~10% relative reduction in test RMSE. These results support development of weather-aware monitoring and more robust polarization control for fiber-based quantum networks.

**Keywords: optical fiber polarization, machine learning, optical communications**

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## Understanding of Molecular Interactions in Quantum Chemistry on Frontier HPC

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The couplings among electronic states provide essential clues to reveal details of the electron transfer mechanism within photochemistry processes, such as singlet fission. Singlet fission processes play a significant role in the design of more efficient photoharvesting solar cells. The GronOR1,2 software package renders a computational description of couplings to enable theoretical insight into the singlet fission process, which cannot be obtained directly from experiments. The core methodology of GronOR is non-orthogonal configuration interaction using fragment wave functions (NOCI-F) and allows an intuitive way of interpreting wavefunctions in terms of individually optimized diabatic states. Based on the worker-master execution model, GronOR computes the Hamiltonian matrix in parallel, and scales linearly on modern HPC systems. In this poster, inter-3 and intra-4 molecular singlet fission and performance of GronOR on Frontier will be illustrated.

Uncertainty quantification demonstrates effectiveness in molecular dynamics field of all-atom forms.<sup>5,6</sup> In this poster, coarse-grained martini force field is chosen to allow multiple tropocollagen interactions being simulated spontaneously in fibrils on OLCF Frontier. Within this high-dimensional force-field parameters' space, crucial parameters associated with persistence length of protein helices and protein helix pitch are identified using Deep Active Subspace and kernel-based methods due to their high sensitivity response towards variance.

**Keywords: NOCI-F, GronOR, HPC, UQ, MD**

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# Physics-Informed Deep Learning for Geometric Deblurring in Hyperspectral Neutron Imaging

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## Abstract

Hyperspectral neutron imaging (HSnI) enables simultaneous spatial imaging and wavelength-resolved material characterization. However, experimental geometry at the VENUS beamline imposes a fundamental trade-off when using sample environment such as a furnace, a load frame, gratings and/or polarization equipment: increasing sample-to-detector distance ( $d$ ) increases geometric unsharpness ( $U_g$ ) and thus degrades spatial resolution. Recovering spatial resolution at distances of several tens of cm can be achieved using an artificial intelligence technique called super-resolution. We propose a deep learning approach that integrates measured  $d$ -dependent degradation priors with Squeeze-and-Excitation channel attention to address the ill-posed inverse problem of recovering high-resolution neutron projections from geometrically-blurred observations across the accessible sample-to-detector distance range at VENUS.

Keywords: Hyperspectral neutron imaging, Geometric deblurring, Artificial Intelligence, image reconstruction

Acknowledgement: This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. The beam time was allocated to VENUS on proposals number IPTS-35945

# From Gradients to Representations: A Unified View of Privacy Leakage in Federated Learning

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Abstract:

Federated Learning (FL) is widely adopted to enable collaborative model training while preserving data privacy through local updates and differential privacy (DP). However, emerging evidence shows that privacy leakage persists even under strong DP guarantees, particularly in modern FL systems with heterogeneous privacy budgets, complex model architectures, and increasingly powerful adversaries equipped with advanced analytical capabilities.

In this work, we present a unified perspective on privacy leakage across multiple levels of abstraction in FL, spanning from gradient-space signals to higher-level representations. We first demonstrate that in Heterogeneous Differential Privacy (HDP) settings,  $\epsilon$ -aware aggregation introduces exploitable structure in gradient updates. An honest-but-curious server can leverage denoising and surrogate modeling to perform cross-round linkage and infer client-level attributes, revealing that leakage arises from persistent gradient structure rather than insufficient noise. To mitigate this, we propose IntraShuffler, a lightweight middleware defense framework that combines privacy-aware bucketing with parameter-level shuffling to disrupt structural consistency while preserving aggregation fidelity.

Beyond gradient-level analysis, we show that representation-level signals in modern models introduce additional leakage pathways, even when gradient-level protections are applied. Taken together, these findings expose a broader challenge: privacy leakage in FL is inherently multi-level and can propagate across stages of learning. This perspective highlights the need for defenses that are not only noise-aware but fundamentally structure-aware across the entire learning pipeline.

**Keywords: Federated Learning, Differential Privacy, Privacy Leakage**

*This initiative is sponsored by: DOE ASCR*

# Water-Ion Correlations and Structural Dynamics in Concentrated Salt Solutions

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Ion solvation and water structuring in aqueous salt solutions are fundamental to a wide range of applications, from desalination to energy storage. While many studies address battery salts at low to intermediate concentrations, research on high-salt concentrations, where water behavior changes substantially, is limited. To fill this gap, we probe the local structure and dynamics of water and ion correlations in salt solutions at concentrations ranging from semi-dilute to near-saturation using high-energy X-ray diffraction and molecular dynamics simulations. We find that the addition of alkali and alkali-earth metal halides to water results in a slight increase in the nearest-neighbor distance of water and broadening of the O-O peak in the pair distribution function, which is attributed to the disruption of the water tetrahedral network. Chlorides of Sr<sup>2+</sup>, Zn<sup>2+</sup>, and La<sup>3+</sup> near saturation show a significantly broader peak than those of other chlorides studied, and, interestingly, a well-defined small-angle X-ray pre-peak is observed below 1 Å<sup>-1</sup>. Cation-water interactions dominate over anion-water and water-water correlations for all the salts studied. The M<sup>+</sup>-O peak shifts to a longer distance as the cation charge-to-volume ratio ( $z/r^3$ ) decreases. Stronger cation-water structural correlations lead to slower cation-water cage dynamics and enhanced local O-O relaxation.

**Keywords: Concentrated Salt Solutions, Structural Dynamics, Van Hove Function, High Energy X-Ray Diffraction, Molecular Dynamics Simulation**

*This initiative is sponsored by: U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division*

## **Is High Mo Content in Ni based alloys Sufficient to Ensure Corrosion Resistance in Molten Salt Reactor Salts?**

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Successful development and commercialization of molten-salt reactors will require structural alloys that retain mechanical integrity while resisting aggressive molten chloride corrosion. However, reliable high-temperature corrosion and mechanical performance data remain limited. This study examines the coupled effects of creep deformation under operating stresses and corrosion on candidate Ni- and Fe-based alloys exposed to molten chloride salts at 600–800 °C. Ongoing studies have demonstrated that molten salts significantly reduce creep-rupture resistance of austenitic steels and Ni-base alloys. To complement these performance measurements, a lifetime-prediction framework incorporating physics-based models to describe the corrosion-induced material degradation was applied to assess the environmental impacts of creep behavior in chloride- and relevant fluoride salt systems.

**Keywords: Fission, Corrosion, 244, Molten Salt Reactor**

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# Gas Diffusion Electrode Study of Oxygen Reduction on PtNi and PtCo-based Catalyst Layers for High Temperature Proton Exchange Membrane Fuel Cells

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In HT PEMFC catalysts typically high platinum loadings are used, which makes the catalysts costly and thus economically unsustainable. One way to reduce the cost is to reduce the Pt loading in the catalyst by mixing the Pt with cheaper transition metals like Ni, Co and Fe [1, 2]. In this work, two commercial PtNi/TKK (TECNiE52 Pt 46.5 wt%) and PtCo/TKK (TEC36E52 Pt 45.8 wt%) and an in-house catalyst PtNi-NC (Pt nominally 38.4 wt%) layers with three different binders (Nafion, PTFE and in-house Ionomer X) were tested in high temperature gas diffusion electrode system (GDE, FlexCell™, Gaskatel GmbH) in 85% H<sub>3</sub>PO<sub>4</sub> solution. The in-house catalyst was prepared by dry mixing catalyst precursors using an acoustic mixer and sintering the mixed powder in H<sub>2</sub>/Ar gas mixture to prepare PtNi-alloy nanoparticles. Based on TEM images and EDS analysis, these PtNi-alloy nanoparticles stayed between 2 nm to 7 nm uniformly covering the whole carbon support. At room temperature, Nafion binder containing catalyst layers showed higher activity, however, at 155 °C, catalyst layers with PTFE ionomer showed the best performance and the in-house catalyst the highest mass corrected currents. Catalyst layers with Ionomer X performed on par with the other binders [3].

**Keywords: oxygen reduction reaction, high temperature gas diffusion electrode, 85 wt% phosphoric acid, ionomers**

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# Using High-Throughput Phenotyping to Explore the Genetic Basis of Biological Nitrification Inhibition in Populus

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## Background

Plants can regulate nitrification in the soil microbiome by exuding chemicals that inhibit ammonia oxidizers. This process, known as biological nitrification inhibition (BNI), is emerging as an avenue for increasing nitrogen use efficiency and reducing loss of nitrogen to the atmosphere and waterways. This work evaluates variation in nitrification, measured as gross nitrification rate (GNR), across Populus genotypes. The objective is to determine whether variation in GNR among Populus genotypes has a genetic basis and to identify associated candidate genes.

## Methods

Soil cores (~top 10-15 cm) were collected from two Department of Energy Populus common gardens (Tennessee and Oregon) in summer and spring, respectively. The TN site included 15 genotypes in replicate and 6 background samples (away from trees) while ~320 genotypes were sampled at the OR site. GNR was measured using <sup>15</sup>N isotope dilution methods previously established and modifying the analysis to be compatible with high throughput analysis. Extracted nitrate is reduced via VC13 into nitrite which is then derivatized with 2,3-diaminonaphthalene to form 2,3-naphthatriazole. The sample is then analyzed via immediate drop-on demand technology coupled with an open port sampling interface (I.DOT/OPSI) for rapid high-throughput quantification using a triple-quadrupole mass spectrometer.

## Results

Preliminary results indicate variation in GNRs across genotypes. At the TN site, average GNRs of all genotypes were below the background rate ( $5.29 \pm 0.5$  mg-N kg<sup>-1</sup> d<sup>-1</sup>), with the lowest significant genotype, ILL-101, reducing the GNR by 49%. In a linear mixed model, genotype explained ~17% of GNR variation, suggesting a meaningful genetic contribution. In the larger OR campaign, GWAS linked genotype-specific sequence variation with GNR. Preliminary findings identified single nucleotide polymorphisms (SNPs) exceeding a significance threshold of  $-\log_{10}(p\text{-value}) > 5.0$ , mapping to ~40 genes potentially associated with GNR. These candidate genes include those putatively involved in root modulation, RNA and DNA binding, defense response, and vesicle trafficking.

## Conclusions

Populus genotypes significantly varied in gross nitrification rates across two groves in TN and OR. Initial GWAS results indicate a potential genetic basis for nitrification in Populus and highlight candidate genes for further investigation of related plant-microbe interactions.

**Keywords: Nitrification, Genetics, High-Throughput**

*This initiative is sponsored by: DOE BER early career award*

## Plant RNA Vision 2.0

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RNA abundance provides critical insight into how plants respond to developmental and environmental cues, informing strategies to enhance crop resilience, quality, and productivity. Although a split ribozyme system was recently developed for in vivo RNA imaging in plants, its utility has been limited by low sensitivity and reliance on a single reporter gene. Here, we present an improved ribozyme-based RNA biosensor engineered for enhanced sensitivity and compatibility with multiple reporters. By incorporating translation enhancers (COR47-5'UTR, 3×ARC, and 6×ARC) into both the original split and the modified modular ribozyme systems, we observed increased reporter expression, with the 6×ARC design producing the strongest signal. We further demonstrated system versatility by successfully deploying additional reporters (eYFP, eBFP, and eGFPUV). To boost reporter output, we introduced a complementary peptide (cPEP), resulting in a substantial increase in GFP fluorescence in plant cells. Collectively, these advancements establish a more sensitive, flexible RNA biosensing platform capable of visualizing endogenous gene expression at cellular resolution, enabling more efficient multi-scale RNA imaging in plants.

**Keywords: Biosensor, Ribozyme, UTR, Reporter gene,**

*This initiative is sponsored by: U.S. Department of Energy (DOE) Genomic Science Program, Plant-Microbe Interfaces (PMI) Scientific Focus Area (under FWP ERKP730)*

# Sequence-Encoded Molecular Switches Control Condensate Formation in Plant Stress Proteins

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## Abstract

Biomolecular condensates (droplet-like assemblies) formed via liquid-liquid phase separation (LLPS) play a vital role in cellular stress responses. Yet the sequence “grammar” that regulates LLPS in plant proteins remains poorly understood. To address this gap, we examine how the sequence and structural features of plant intrinsically disordered proteins (IDPs) influence condensate formation. Using the Arabidopsis Companion of Cellulose Synthase proteins (CC1 and CC2) as a model system, we used extensive multichain coarse-grained molecular dynamics (CG-MD) simulations and systematic sequence analyses approach to investigate why highly similar N-terminal domains of these proteins exhibit differential phase behavior under stress conditions. Our computational approach is designed to identify critical sequence signatures and key thermodynamic interactions that could act as molecular switches controlling condensate formation. These findings aim to provide mechanistic insights into how plants regulate condensate formation during environmental stress and to establish a foundation for understanding sequence-encoded phase separation rules in plant systems. More broadly, this work seeks to advance our knowledge of how plant’s cellular organization and stress adaptation are regulated by intrinsically disordered regions.

**Keywords: Biomolecular condensates, liquid-liquid phase separation (LLPS), intrinsically disordered proteins, coarse-grained molecular dynamics, Arabidopsis CC1 protein**

*This initiative is sponsored by: NEAT-LDRD*

# **A Multigene Stacking Approach to Increase Cutin Biopolymer in Poplar**

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Cutin is a complex biopolymer found in plants that serves several vital functions, such as acting as a natural barrier against pathogens, minimizing water loss, protecting plants from various environmental stresses. Importantly, cutin has emerged as a promising sustainable and biodegradable alternative to petroleum-based plastics, offering significant potential for the development of eco-friendly biomaterials. In plants, cutin production starts with the biosynthesis of C16 and C18 fatty acids in plastids. These fatty acids are converted to fatty acyl coenzymes in ER, after oxidation the monomers are formed and exported to cell wall. Several key genes are involved in these steps. A coordinated expression of cutin related genes is required for higher cutin production. Single gene transformation approach is inherently inefficient for engineering multi-step biosynthetic pathways as it requires sequential and time-consuming multiple rounds. Here we overexpress various sets of gene combination to produce higher cutin content. Each gene regulates a critical step in the cutin biosynthetic pathway, and their coordinated expression resulted in enhanced cutin accumulation. To systematically evaluate pathway optimization, we generated 16 distinct multigene combinations by selecting representative genes from each key biosynthetic step. Using these constructs, we produced more than 50 independent transgenic events.

**Keywords: Multi-gene stacking, biopolymer, cutin, pathway engineering**

*This initiative is sponsored by: U.S. Department of Energy, Office of Science, Biological and Environmental Research Program, Genomic Science Program, as part of the Center for Bioenergy Innovation (CBI)*

## Oral Presentation Session I – ML/AI I

### **Automated Phase Detection and Magnetic Structure Refinement in Neutron Diffraction Data**

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Accurate phase identification and magnetic structure determination from neutron diffraction data remain critical yet time-intensive tasks in materials characterization. This work presents an automated pipeline for phase detection and magnetic structure refinement that integrates data-driven inference with physics-based modeling and machine learning . The approach leverages diffraction signal analysis to identify candidate phases and subsequently performs automated Rietveld-style refinement, including magnetic contributions, without manual intervention. This work contributes toward fully autonomous diffraction analysis pipelines, bridging the gap between experimental data acquisition and actionable scientific insight.

**Keywords: powder, diffraction, neutrons, AI, phase, identification, magnetic, refinement**

*This initiative is sponsored by: ILLUMINE*

# **MATEY: Open-source Framework for Spatiotemporal Foundation models for Physical Systems**

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MATEY: Open-source Framework for Spatiotemporal Foundation models for Physical Systems

Hunor Csala, Pei Zhang

We present an open-source framework for spatiotemporal foundation models tailored to fluid dynamics and multiphysical systems. Built on a transformer-based architecture, the model is designed to learn unified representations across a diverse range of partial differential equations (PDEs), capturing shared structure while remaining flexible to system-specific dynamics. The framework is trained on a heterogeneous collection of large-scale datasets, including The Well and PDEBench, alongside application-driven data from fusion energy, combustion, and turbulent flows. By leveraging this diversity, the model aims to learn transferable representations across distinct physical regimes, from reaction–diffusion systems and incompressible and compressible flows to magnetohydrodynamics (MHD) and plasma physics. This work is ongoing, and we focus on the design choices underlying multi-domain training, including variable alignment, multi-task learning, geometry handling, and dataset integration. We discuss early observations, practical challenges, and open questions in building general-purpose models for physical systems.

**Keywords: scientific machine learning, foundation models, partial differential equations**

*This initiative is sponsored by: LDRD AI Initiative*

# Enabling Large-Scale Pressure Prediction for Turbulent Flows using Vision Transformer

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Pressure prediction in turbulent flows is crucial to model and understand the evolution of turbulence, boundary-layer behavior, and energy distribution. Recent advances in deep learning offer compelling alternatives to traditional high-overhead numerical solvers. However, data-driven pressure prediction remains challenging with conventional machine learning architectures for high-resolution pressure fields. To address this, we adopt a Vision Transformer (ViT)-based architecture that explicitly models nonlocal dependencies through self-attention and enables patch-based representations suited for multiscale turbulence data. We propose a pressure-gradient consistency loss to better capture pressure fluctuations. While effective, in ViT the computational cost scales up quadratically as the number of patches grows, hindering scalability to large flow domains. We therefore introduce a physics-guided adaptive patching mechanism that dynamically decides the patch size based on the richness of information and reduces the sequence length. Experimental results with evaluation metrics such as MSE, SSIM, PSNR, and GPU Hours demonstrate the effectiveness of our approach in predictive accuracy and computation cost reduction. These results highlight the potential of physics-guided scalable transformer models for pressure prediction across diverse application domains. Our experiments used resources from Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory, which is a DOE Office of Science User Facility.

**Keywords: Turbulence Modeling, Pressure Prediction, Vision Transformer, Adaptive Patching, Scalability**

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# Beyond Binary Prediction: Interpretable Machine Learning for Risk Stratification in Opioid Care

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Machine learning has shown strong potential for predicting opioid-related outcomes using electronic health record data, with prior research applying a range of approaches, including tree-based and deep learning models. Much of this work has focused on binary overdose prediction, with comparatively less emphasis on how model outputs can be translated into clinically actionable risk assessments. To address this gap, we develop a machine learning framework that estimates patient-level probabilities of experiencing an adverse opioid event (AOE) following opioid therapy initiation. We leverage these model-predicted probabilities to construct ordered risk tiers, enabling structured stratification of patient risk. Data analysis across these risk tiers serves as a second analytic layer that complements model-level feature importance by examining how clinical factors manifest across progressively higher-risk levels. This stratified analysis provides additional insight into associations between clinical features and AOE that may not be captured by model-level summaries alone. Overall, this work builds on prior opioid-related research by connecting patient-level outcome prediction with interpretable, tier-based characterization of risk, supporting more informed and actionable decision-making in real-world clinical settings.

**Keywords: machine learning, opioid crisis, XGBoost, feature importance, data analysis**

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## Oral Presentation Session I – Biosciences and Ecology

### **Populus trichocarpa selects unique microbial communities under different climate-induced abiotic stress conditions**

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Abiotic factors like temperature, water, and nutrients directly influence both plants and their associated microbial communities. Abiotic stress conditions elicit targeted microbial community responses which can have a considerable influence on broader ecosystem processes like nutrient cycling, and on plant fitness, as plants under stress form advantageous partnerships with microbes possessing stress relieving functionality. Using amplicon sequencing, we examined the bacterial and fungal communities of bulk soil, rhizosphere soil, and root endosphere of *Populus trichocarpa* trees from 11 sites along a naturally occurring temperature and rainfall gradient with variable soil conditions over the Cascade Mountains in Washington. We found that climate factors, especially average temperature and rainfall, correlated with both bacterial and fungal community composition in all of the observed niche compartments. We also observed that microbial communities broadly clustered into three main compositional groups driven by climate condition: a high precipitation, warmer group along the lower Cowlitz River on the Western side, a colder high elevation community at the crest of the pass and along the upper Tieton River, and a lower precipitation, hotter condition community along the lower Tieton River on the Eastern side. We are currently investigating the functional potential of *Populus trichocarpa* rhizosphere and endosphere microbial communities under these varying climate and soil conditions using metagenomic approaches. We hypothesize that the host trees will select for microbes with the functional potential to alleviate specific types of abiotic stress and that the functional potential of these communities will cluster based on these same broad climate categories.

**Keywords: Microbiome, Climate, Gradient, Plant, Ecology**

*This initiative is sponsored by: PMI*

## High-resolution metaproteomics reveals functional redundancy in a defined bacterial community

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Microbial communities are often viewed as functionally redundant systems in which overall function persists despite changes in membership. However, most evidence for redundancy is inferred from shared genetic potential rather than direct measurements of realized activity, leaving it unclear whether closely related microorganisms are truly interchangeable.

Here, we test functional interchangeability using a constructed bacterial community as a model system. We assembled a ten-member consortium derived from the *Populus* soil microbiome in which nine members were held constant while the identity of a single *Pseudomonas* strain was systematically varied across closely related isolates. Using ultra-deep, strain-resolved metaproteomics, we quantified proteome-wide activity after communities converged to a stable state.

Despite conserved membership, swapping closely related *Pseudomonas* strains drove reproducible shifts in community structure and global protein allocation. Strains partitioned into distinct functional regimes based on expressed proteomes. These patterns were not predicted by phylogeny or carbon utilization, and the differences propagated across the community.

These results expand how we define functional redundancy in microbiomes by showing that interchangeability is conditional and emerges at the level of realized activity. More broadly, this work demonstrates that ultra-deep metaproteomics enables direct measurement of system-level function, providing a path toward predicting behavior in complex microbiomes.

**Keywords: Functional redundancy, microbial community, metaproteomics, synthetic community**

*This initiative is sponsored by: The Plant-Microbe Interfaces Science Focus Area is supported by the U.S. Department of Energy, Office of Science, through the Genomic Science Program, Office of Biological and Environmental Research under FWP ERKP730.*

## **Unraveling Soil Microbe Establishment: Leveraging Genetic Mapping to Identify Genetic Factors shaping the Soil Microbiome**

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Adapted QTL mapping for *B. velezensis* and explored genome shuffling for generating recombinant progeny populations. Specifically, to construct QTL mapping population we used genome shuffling via protoplast fusion to recombine *B. velezensis* GB03 with *B. velezensis* S4. This approach aims to maximize genetic diversity, enabling mapping of loci associated with microbial fitness and colonization potential.

A crucial factor influencing recombination success in genome shuffling is the restrictionmodification (RMS) system, which acts as a genetic barrier between strains.

Keywords: Microbial establishment, Quantitative trait loci mapping, *Bacillus* spp., Genome shuffling, Restriction-modification systems, Plant-microbe interactions

**Keywords: Quantitative trait loci mapping, *Bacillus* spp., Genome shuffling, Restriction-modification systems, Plant-microbe interactions**

*This initiative is sponsored by: DOE-SEED SFA*

## **Systems genetics study of Winter and Summer regulatory networks controlling wood formation in *Populus trichocarpa***

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Woody biomass from trees is a key renewable resource for future biofuels and biomaterials, yet most knowledge about its molecular basis comes from studies of growth under favorable summer conditions. In reality, the woody stem of temperate deciduous trees remains physiologically active year-round, requiring major adjustments during winter dormancy to protect cells from freezing, desiccation, and membrane or cell-wall damage. This study examined the molecular control of this latent winter state in more than 800 black cottonwood poplars grown in a common garden in the Pacific Northwest. Stem tissues were sampled in summer and winter, and transcriptomes from both seasons were sequenced. Population genomic resources enabled expression quantitative trait nucleotide (eQTN) mapping using over nine million SNPs. The transcriptomic data revealed substantial winter activity in woody tissues and a dramatic seasonal reprogramming of gene expression. eQTN mapping identified distinct regulatory hotspots for each season, including regions specifically influencing winter-biased genes. Integrating eQTNs with co-expression networks and prior biological knowledge uncovered previously uncharacterized transcriptional regulatory networks active in secondary vascular tissues during winter dormancy. Understanding how genetic variation shapes seasonal growth dynamics and winter protection mechanisms offers new targets for improving woody biomass productivity in future bioenergy crops.

**Keywords: Woody Biomass, Winter dormancy, Gene expression regulation, Expression quantitative trait nucleotides (eQTNs),**

*This initiative is sponsored by: DOE BER*

## **Controlling matric potential in microfluidics to examine microbial dynamics in unsaturated porous media**

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The use of microfluidics for the study of soil microbial ecology is an emerging field. Most microfluidic studies of biological systems, however, have been performed under fully saturated conditions that are not representative of natural soil. Therefore, while microfluidics offer many unique capabilities that other methodologies cannot, they are not currently suited to address the effects of matric potential, an important variable defining the microbial moisture niche. Here, a methodology is presented that allows the user to control the aqueous conditions within microfluidic networks by manipulating matric potential using a hanging water column.

**Keywords: microfluidics, soil, matric potential, fungi, bacteria**

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## Oral Presentation Session I – Materials Science

### Tunable Topological and Magnetic Properties of $\text{MnBi}_2(\text{Te}_{1-x}\text{Se}_x)_4$

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The  $\text{MnBi}_2\text{Te}_4$  family has emerged as a class of intrinsic magnetic topological insulators exhibiting exotic transport phenomena such as the quantum anomalous Hall effect. We perform first-principles density functional theory (DFT) calculations combined with maximally localized Wannier functions for  $\text{MnBi}_2(\text{Te}_{1-x}\text{Se}_x)_4$  (MBST), motivated by the most stable stacking configuration identified in recent quantum Monte Carlo simulations. In its antiferromagnetic (AFM) ground state, MBST realizes an AFM topological insulator with gapless surface states protected by the combined time-reversal and translational symmetry. In the ferromagnetic (FM) phase, MBST slabs thicker than five septuple layers exhibit Chern insulating behavior accompanied by a quantized anomalous Hall response. Our calculations confirm that the inverted band structure is preserved under moderate substitutional disorder ( $x \approx 0.5-0.509$ ), demonstrating strong defect tolerance. A systematic analysis of Se alloying in AFM-MBST reveals lattice contraction and a non-monotonic evolution of the band gap, which reaches a minimum near intermediate compositions ( $x \sim 0.5$ ). These findings suggest that MBST is a robust and tunable platform for realizing magnetic topological phases.

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. This work was also supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

**Keywords:** First principle calculations, Magnetic topological insulator, Anomalous Hall conductivity

*This initiative is sponsored by: BES-MSE*

## **Magnetic structure characterization of Shastry-Sutherland material BaRE<sub>2</sub>ZnS<sub>5</sub> (RE=Nd, Ce)**

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*Single Crystal Neutron Scattering*

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The Shastry-Sutherland lattice (SSL) is a two-dimensional geometrically frustrated lattice made up of orthogonal spin dimers. Depending on the strength of intra- and inter-dimer interactions, SSL materials can host exotic properties. Here we characterize two rare-earth SSL compounds, BaRE<sub>2</sub>ZnS<sub>5</sub> (RE=Nd and Ce), through magnetization and neutron scattering techniques. In BaNd<sub>2</sub>ZnS<sub>5</sub>, we observe a 2Q non-collinear magnetic ordering below 2.9 K as well as field-induced partial disorder as a critical phase. Meanwhile in BaCe<sub>2</sub>ZnS<sub>5</sub>, no magnetic order is found down to 70 mK and by modeling neutron scattering data, quantum entanglement of XY-spin-dimers is revealed. In this presentation, I will introduce the unique features of rare-earth spins and their excitations in geometrically frustrated magnetic lattices.

Citations:

[1] Billingsley, B. R., et al. (2022). Single crystal synthesis and magnetic properties of a Shastry-Sutherland lattice compound BaNd<sub>2</sub>ZnS<sub>5</sub>. *Phys. Rev. Mat.*, 6(10), 104403. <https://doi.org/10.1103/PhysRevMaterials.6.104403>

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[3] Ma, Q., et al. (2024). Quantum entanglement of XY-type spin dimers in Shastry-Sutherland lattice. arXiv preprint: arXiv:2412.17913

**Keywords: magnetic frustration, magnetism, Shastry-Sutherland**

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# **Auto-3DPFM: Automating Polarization-Vector Mapping at the Nanoscale**

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Abstract

The functional properties of ferroelectric materials are strongly influenced by ferroelectric polarization orientation; as such, access to consistent and precise characterization of polarization vectors is of substantial importance to ferroelectrics research. Here, we develop a fully automated three-dimensional piezoresponse force microscopy (Auto-3DPFM) technique automating all essential steps in interferometric PFM for 3D polarization vector characterization, including laser alignment, tip calibration and approach, image acquisition, polarization vector reconstruction, and visualization. The automation reduces the experimental burden of ferroelectric polarization vector characterization, while the back-and-forth calibration ensures consistency and reproducibility of 3D polarization reconstruction. An algorithmic workflow is also developed to identify domain walls and calculate their characteristic angles via a spatial vector-angle-difference method, presenting one unique capability enabled by Auto-3DPFM that is not accessible with traditional PFM techniques. Beyond representing a significant step forward in 3D polarization mapping, Auto-3DPFM promises to accelerate discovery via high-throughput and autonomous characterization in ferroelectric materials research. When integrated with machine learning and adaptive sampling strategies in self-driving labs, Auto-3DPFM will serve as a valuable tool for advancing ferroelectric physics and microelectronics development.

Keywords: Automated and Autonomous Experiments; Piezoresponse Force Microscopy; 3D Polarization Mapping; Ferroelectrics; AI/ML

**Keywords: Automated and Autonomous Experiments; Piezoresponse Force Microscopy; 3D Polarization Mapping; Ferroelectrics; AI/ML**

*This initiative is sponsored by: LDRD*

# Hydrophilically Engineered Polyamides for High-Yield Enzymatic Recycling and Critical Minerals Capture

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Enzymatic depolymerization has emerged as an environmentally sustainable approach for recycling of polyamide-based commodity plastics; however, the intrinsic incompatibility between hydrophobic, insoluble substrates and water-soluble enzymes restricts hydrolysis yields to below 5%. Here, we present a materials-design strategy that enhances enzyme accessibility by incorporating ethylene-glycol/sulfonate-containing hydrophilic moieties into Nylon-like polyamides. These structural modifications substantially increase depolymerization efficiency using the Nylon-hydrolyzing enzyme NylC. Notably, even minimal incorporation of hydrophilic groups (as low as 5 mol%) improves hydrolysis performance in insoluble substrates. We further show that the resulting oligomers can be repolymerized and that the polymers exhibit promising utility for rare-earth element extraction. This work highlights how controlled hydrophilic group incorporation can modulate polymer-enzyme interactions, enabling high-yield, circular recycling pathways for polyamides within a sustainable polymer-materials framework.

**Keywords: Recycling, Critical minerals, Enzymes, Polymers.**

*This initiative is sponsored by: Laboratory Directed Research and Development*

## **Adsorption of hydroxamic acid ligands for improved extraction of rare earth elements from monazite ores**

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Efficient separation of rare earth element (REE) ores via froth flotation requires the development of novel ligands with enhanced adsorption capacity and selectivity. To realize these advances, understanding the mechanisms underlying interactions between the ligand and mineral surfaces is essential. This study systematically evaluates the adsorption behavior of alkyl- and aromatic alkyl-substituted hydroxamic acid ligands on monazite surfaces using complementary spectroscopic techniques, including UV–visible (UV–vis) spectroscopy, Raman spectroscopy, infrared spectroscopy, and vibrational sum frequency generation (SFG) spectroscopy, together with the *ab initio* molecular dynamics (AIMD) simulations. Among the studied ligands, octanohydroxamic acid (OHA) and 4-ethoxy-N,2-dihydroxybenzamide (EDHBA) exhibit high adsorption capacity under basic pH (8–10) by forming multilayers on the surface. OHA has a higher equilibrium adsorption capacity compared to EDHBA, but it forms a less stable multilayer susceptible to disruption in the presence of interfering ions. AIMD results show that OHA adopts a single stable chelating geometry, while EDHBA exhibits multiple binding modes involving distinct interactions with La surface atoms and phosphate-bound oxygens, resulting in more complex adsorption kinetics. The variations in surface binding and intermolecular interactions observed between alkyl and aromatic molecules influence the differences in adsorption kinetics, equilibrium adsorption capacities on the mineral surface, and their flotation performance. This work provides valuable insight into the adsorption mechanism of ligands at mineral interfaces, which is crucial for guiding the design of new ligands with enhanced separation performance.

**Keywords:** Rare earth element, adsorption, hydroxamic acid ligand, spectroscopy

*This initiative is sponsored by: CMI*

# Performance of a Dissimilar Metal Weld for Advanced Ultra-Supercritical Coal Power Plant Applications

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Advanced ultra-supercritical (A-USC) coal power plants promise base-load electricity generation with lower fuel consumption and reduced emissions through up to 25% efficiency gains. Realizing these designs hinges on materials capable of sustained operation at high steam temperatures and pressures. Ni-based precipitation-strengthened alloys such as Haynes® 282® and Inconel® 740H® derive their strength from coherent  $\gamma'$  precipitates complemented by grain-boundary and intragranular carbonitrides. They exhibit excellent high-temperature strength up to 760 °C and are prime candidates for these applications. A critical, underexplored link in A-USC architectures is the dissimilar-metal weld (DMW) joining Inconel 740H boiler piping to Haynes 282 turbine casings. This work examines narrow-groove gas tungsten arc welding (GTAW) using Haynes 282 filler to fabricate 740H/282 joints with and without post-weld heat treatment (PWHT). Electron microscopy, microhardness measurements, and tensile testing were conducted to elucidate  $\gamma'$  stability and PWHT-induced changes in hardness and tensile properties in the base metals and weld deposit. Implications for creep-relevant microstructures and component reliability under A-USC steam conditions are discussed, providing guidance for integration of 740H/282 DMW joints in high-efficiency, coal-based power generation and informing qualification protocols for long-term service and assessment.

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**Keywords: Haynes 282, Inconel 740H, advanced ultra-supercritical power plants, gas tungsten arc welding,  $\gamma'$  precipitates**

*This initiative is sponsored by: DoE - Office of Fossil Energy*

## **Oral Presentation Session II – Building and Transportation Sciences**

### **Influence of operating conditions on ethanol-fired passive prechamber combustion engines**

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Cold-start operation in spark-ignition engines is characterized by many drawbacks such as poor fuel vaporization, substantial wall film formation, and weak ignition, which can result in unstable combustion and high concentrations of carbon monoxide (CO), nitrogen oxides (NO<sub>x</sub>), and unburnt hydrocarbons (UHC) prior to catalyst light-off. These challenges are particularly important for ethanol as the fuel's high latent heat of vaporization and low vapor pressure can hinder reliable ignition during cold-start. In this context, passive prechamber ignition systems offer a unique opportunity to improve ignitability by producing hot turbulent jets to promote combustion of lean mixtures but creating challenges associated with establishing robust mixtures at the spark gap. In this study, the influence of operating conditions on jet formation and combustion characteristics in an ethanol-fueled passive prechamber spark-ignition engine is investigated. Results indicate that lower intake pressures lead to delayed and asymmetric turbulent jet formation, and lower peak heat release rates. Lower engine speeds, on the other hand, produced higher peak heat release and faster combustion due to greater residence time in the combustion chamber. These results provide insight into the role of operating strategies on cold-start ramp-up of passive prechamber engines.

**Keywords: Prechamber, Cold-start, Ethanol, Jet Ignition, Computation Fluid Dynamics**

*This initiative is sponsored by: Strategic Partnership Program*

# **Bridging Advanced Building Control and Scalable Deployment: A Low-Cost, Open-Source Building Energy Management Framework for Small and Medium-Sized Commercial Buildings**

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Small and medium-sized commercial buildings represent a vast yet underserved segment of the building stock, accounting for 94% of commercial buildings in the United States while consuming nearly half of total commercial building energy. Although advanced building control strategies have demonstrated significant energy savings and grid-response potential in research settings, their adoption in this sector remains limited due to the high engineering effort, specialized expertise, and fragmented software infrastructure required for deployment. This work presents the integration of advanced control technologies with a scalable, open-source building control platform designed to close this gap. The platform employs a configuration-driven architecture that systematically translates building metadata and control requirements into executable implementations, enabling streamlined deployment across diverse building configurations with minimal manual effort. The platform is validated through high-fidelity simulation-based building environments representing typical office building configurations, confirming its ability to reliably orchestrate advanced control actions while maintaining the scalability and ease of deployment essential for broad adoption. These results establish a practical pathway for enabling advanced energy management with grid-interactive potential in the previously underserved small and medium-sized commercial building sector.

**Keywords: Building Energy Management, Advanced Building Control, Small and Medium-Sized Commercial Buildings, Scalable Deployment**

*This initiative is sponsored by: DOE*

# From Materials to Megawatt-Hours: Modeling Sodium-Ion Batteries for Grid Applications

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Sodium-ion batteries are emerging as a promising alternative to lithium-ion systems, driven by the abundance of sodium resources in the United States and the compatibility of their manufacturing processes with existing battery production infrastructure. Their potential market advantage is particularly compelling for large-scale, megawatt-hour energy storage applications supporting the electric grid.

However, several challenges remain. Owing to the larger ionic radius of sodium, graphite anodes optimized for lithium-ion systems are not suitable for sodium-ion storage. Instead, hard carbon has demonstrated high capacity and power performance. The underlying charge storage mechanisms in hard carbon, however, remain an active area of debate. At least three mechanisms have been experimentally identified — intercalation, surface adsorption, and pore filling — contrasting with the predominantly intercalation-based behavior observed in graphite anodes.

As new sodium-ion materials continue to emerge, there is a growing need for advanced, physics-based electrochemical models to better understand charge storage processes and their interactions with key degradation phenomena, such as sodium plating and solid-electrolyte interphase (SEI) formation. Furthermore, at the system level, where large numbers of cells are connected in series and parallel for grid-scale applications, predicting performance and lifetime under varying load and temperature conditions introduces additional complexity. Understanding how inhomogeneous degradation across individual cells influences overall system behavior is critical for reliable operation. In this talk, I will present our work on modeling these multi-scale problems using physics-based frameworks.

**Keywords: sodium-ion battery, large-scale grid storage system, physics-based electrochemical model, hard carbon anode, battery degradation**

*This initiative is sponsored by: Office of Electricity*

## **Numerical modeling of thermal energy extraction from abandoned mine shafts using closed-loop heat exchangers**

Sajjan Pokhrel\*, Sajjan Pokhrel, Christine Douoghty, Xiaobing Liu

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This talk presents a numerical model for extracting geothermal energy from an abandoned underground mine shaft using closed-loop technology. While energy recovery from abandoned mine water has gained attention in recent years, developing numerical models remains a challenge, especially in closed loop settings where open loops are avoided due to water quality concerns. The model incorporates fluid flow and heat transfer inside the closed-loop heat exchangers, heat and mass transfer in mine shaft driven by natural convection, and heat transfer in the surrounding rock strata. We tested both single and multiple closed-loop heat exchangers and evaluated the effect of thermal interference between them in the shaft. Results show that the water in the shaft mixes well due to natural convection, even when the heat exchangers are installed at shallower depths than the shaft itself. The Coefficient of Performance of heat pump is significantly higher than that of conventional geothermal heat pumps, which rely only on conductive heat transfer at depth. Abandoned underground mines have strong potential to supply thermal demand of surrounding communities and should be studied beyond technical feasibility.

Keywords:

Mine geothermal systems, Abandoned underground mines, Closed-loop geothermal, Numerical modeling, Mine water geothermal

**Keywords: Mine geothermal systems, Abandoned underground mines, Closed-loop geothermal, Numerical modeling, Mine water geothermal**

*This initiative is sponsored by: DOE, Office of Geothermal*

# Multifunctional Metal Organic Framework Composites for Improving Indoor Air Quality

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Indoor air quality (IAQ) is essential for human health, comfort, and productivity, yet its maintenance is hindered by the complex interplay of contaminants including carbon dioxide (CO<sub>2</sub>), moisture, volatile organic compounds (VOCs), and biological pollutants. Traditional IAQ improvement methods typically rely on single-function technologies that are often energy-intensive and narrowly focused. In this study, we report the synthesis of a multifunctional composite material, CuO/HKUST-1, designed to tackle a broad spectrum of indoor pollutants through combined adsorption, photocatalytic, and antimicrobial effects. Synthesized under mild experimental conditions, our work systematically explores the influence of solvent selection and synthesis temperature on the morphology and emergent properties of these composites. The optimized CuO/HKUST-1 exhibits novel structural features that afford enhanced multifunctionality, demonstrating significant potential for simultaneous adsorption of CO<sub>2</sub> and VOCs, effective moisture regulation, and potent biocidal activity. These results not only underscore the promise of metal-organic framework-based composites for next-generation indoor air purification but also provide insights into tailoring synthesis parameters for improved IAQ performance.

**Keywords: Multifunctional Metal Organic Framework, Indoor Air Quality, CO<sub>2</sub>, VOCs, Dehumidification, Photocatalyst**

*This initiative is sponsored by: CMEI*

## **Phosphorous-based Flame Retardants as a Safe and High-performing Solution for Building Technologies**

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Flame retardants (FR) are widely used to reduce ignition and flame spread in polymeric and organic building materials, but many conventional systems—particularly halogenated additives—raise concerns about toxicity and environmental impact. Phosphorus-based flame retardants produced from domestic, biomass-derived feedstocks offer a non-toxic alternative that may also improve supply-chain resilience and reduce exposure to petroleum-driven cost volatility. Here, we report a series of biobased phosphorylated FRs from biobased phenolics using direct phosphorylation to obtain non-volatile, easy-to-handle additives with tunable phosphorus content. Product structures were confirmed by FT-IR and NMR spectroscopy, verifying successful phosphate incorporation. Thermogravimetric analysis showed higher char formation in the synthesized FRs compared to the starting materials with residues increasing from <2 wt% for starting materials to >20 wt% for phosphorylated products. Studies show that phosphate based FRs can help displace flame enhancing radicals, by releasing non-flammable and non-toxic gases, therefore inhibiting the spread of fire in the gas phase. The resulting flame retardants have been incorporated in the wood substrates, insulation foams, wood and hemp fibers where the results show that only 1-5% of loading of biobased flame retardant allows to suppress the flame completely. Overall, these results demonstrate a scalable route to biobased phosphorus flame retardants that provide strong fire performance through combined gas-phase radical quenching and condensed-phase char formation, with potential benefits for cost stability and domestic sourcing in construction and engineered materials.

**Keywords: Flame Retardants, Biobased, Organophosphates, Building Technologies**

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## Oral Presentation Session II – Quantum Science and Physics

### Efficient representation of noisy quantum states at scale

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Tensor network based methods have emerged as effective tools to efficiently represent certain quantum states at scale. However, most of the progress has been limited to the understanding of closed quantum systems with adaptations to open quantum systems gaining traction only recently. This exploration remains important to a broad spectrum of themes ranging from the understanding of many-body noisy quantum dynamics to that of quantifying simulable limits of quantum systems on powerful classical supercomputers. In this talk, I will begin by briefly reviewing the key concepts of matrix product states, leading to the introduction of Locally Purified Density Operators (LPDOs), one of the leading candidates that efficiently represent mixed quantum states. Further, I will present various algorithms that allow for the efficient manipulation of the LPDO under the action of noise channels leading to the simulation of noisy quantum systems at scale. Towards the end, I will briefly discuss different numerical routines that optimize the representation of a LPDO that is maximally mixed.

**Keywords: noisy quantum systems, tensor networks, scalable simulations**

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# Entanglement benchmarking in Quantum Simulations of Spin Systems

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Quantum phase transitions in many-body systems give rise to highly entangled states, and understanding these correlations is crucial for characterizing quantum materials. Traditional entanglement measures such as entanglement entropy are limited to pure states and require full state tomography, making them impractical for near-term quantum devices. Therefore, we explore the Positive Partial Transpose (PPT) criterion as an efficient and scalable entanglement witness in quantum spin models. It detects pairwise entanglement from reduced density matrices, distinguishes quantum from classical correlations, and applies to both pure and mixed states—making it ideal for studying condensed matter systems at finite temperatures. We prepare ground states of one-dimensional spin systems using matrix product states (MPS) and map them to quantum circuits via adiabatic evolution for efficient realization on quantum hardware. The PPT criterion captures clear signatures of phase transitions and is implemented on real hardware using Quantum Overlapping Tomography. This framework provides an efficient way to completely map the two-body entanglement structure in any state, including time-evolved and thermal states, on quantum computers.

**Keywords: Quantum Simulation, Quantum Hardware, Quantum Spin Models.**

*A.B. and P.C.L were supported by the Quantum Science Center (QSC), a National Quantum Science Initiative of the Department Of Energy (DOE), managed by Oak Ridge National Laboratory (ORNL).*

# Two-band Euler Topology as a Source of Single-Band Quantum Geometry

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Quantum geometric quantity, including the quantum metric, Berry curvature play a central role in modern condensed matter phenomena, governing nontrivial topological phenomena, nonlinear transport properties etc.[1,2,3] We uncover a relation between two-band Euler topology and the quantum geometry of individual Bloch bands in spacetime inversion symmetric systems. We show that a nontrivial Euler class enforces a universal lower bound on the quantum metric of the constituent bands, establishing that multi-band topology mandates irreducible singleband geometry. This provides a new two-to-one band correspondence, linking two-band Euler topology to individual bands Fermi-surface transport in space–time inversion symmetric systems with vanishing Berry curvature.

**Keywords: Topological Materials, Quantum Geometry, Parity-Time reversal symmetry, Berry Curvature**

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# **Microstructural-heterogeneity induced macroscopic angular magnetoresistance in conventional and unconventional superconductors**

Deb Mallick\*, Umesh Kumar, Simon Kim, An-hsi Chen, Jacob Cook, Colby Stoddard, Sujoy Ghosh, Qiangsheng Lu, Gyula Eres, Steven J. Randolph, Seongshik Oh, Satoshi Okamoto, Robert G. Moore\*, Matthew Brahlek\*

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Emergent physical phenomena like superconductivity are highly promising for advancements in quantum computing and sensing. Among these, topological superconductivity stands out as a revolutionary solution, as it addresses the long-standing challenge of achieving fault-tolerant quantum computing through the realization of robust and resilient qubits. Symmetry breaking in physics often signals remarkable phenomena. In superconductors, rotational symmetry breaking gives rise to nematic superconductivity, theoretically linked to unconventional Cooper pair pairing. Electrical transport experiments are commonly used to probe rotational symmetry breaking, with Corbino geometry being a widely used tool due to its symmetric device design, enabling azimuthally isotropic electron flow and eliminating geometric artifacts. In this work, using epitaxially grown Fe (Te, Se)/Bi<sub>2</sub>Te<sub>3</sub> thin films, we observe mild six-fold oscillations superposed on dominant two-fold oscillations in the superconducting vortex state. We attribute the two-fold oscillations, surprisingly, to a failure of Corbino geometry in providing truly isotropic electron flow, as confirmed in a polycrystalline s-wave superconductor, MoRe, under similar conditions. By isolating the two-fold background, we uncover intrinsic six-fold oscillations, which we propose originate from interfacial superconductivity contributed by the underlying topological layer, Bi<sub>2</sub>Te<sub>3</sub>. These findings challenge conventional assumptions about Corbino geometry and highlight the interplay between topology and superconductivity. Ongoing experiments aim to unravel the precise origins of these intrinsic observations.

**Keywords: heterogeneity, spatial distributions, superconductor, electrical transport**

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# Discovery of quantum magnetic delafossites via High-throughput first-principles calculation

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Discovering materials with intriguing properties such as quantum spin liquids is challenging because their realization requires a delicate balance among geometrical, electronic, and magnetic conditions. Here, we propose delafossite-based ABX<sub>2</sub> structures that show great potential for realizing quantum spin liquids through chemical substitution. High-throughput calculations systematically investigate geometrical stability, magnetic interactions, spin orders, and strong correlation effects using density functional theory combined with the linear response and magnetic force theory. By screening a wide range of ABX<sub>2</sub> compositions, we identify stable and magnetic delafossites as well as candidates that falling within the phase diagram of quantum spin liquids. Our framework not only identifies promising candidates, including high critical temperature magnets and quantum spin liquids, but also establishes a comprehensive database for the future materials discovery and machine-learning-based studies.

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**Keywords: Materials design, first-principles calculation, high-throughput computation, quantum magnet, delafossites**

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## Oral Presentation – Session II – Fission and Fusion Energy

### Chemical, Mechanical, and Thermal Properties Evaluation of Lithium Ceramics as Solid Breeder Materials for Fusion Reactors

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Fusion breeding blankets will use lithium based materials in either solid or liquid forms. Solid breeder materials, such as lithium titanate ( $\text{Li}_2\text{TiO}_3$ ), lithium zirconate ( $\text{Li}_2\text{ZrO}_3$ ), and lithium silicate ( $\text{Li}_4\text{SiO}_4$ ) are considered candidates for use in fusion pilot plants. We aim to establish baseline mechanical and thermal property measurements based on varying parameters including but not limited to density and porosity to determine tritium retention and release. Here, we examine the production of  $\text{Li}_2\text{TiO}_3$ ,  $\text{Li}_4\text{SiO}_4$ , and  $\text{Li}_2\text{ZrO}_3$  for potential use as solid tritium breeding materials based on chemical characterization and mechanical/thermal properties prior to neutron irradiation. We use x-ray diffraction (XRD), scanning electron microscopy (SEM), and time-of-flight secondary ion mass spectrometry (ToF-SIMS) to evaluate phases, material morphology, and chemical composition of prepared ceramics. Our results indicate essential parameters which can be manipulated to provide consistent chemical phase and morphology. Physical properties were measured using techniques such as pycnometry, dimensional analysis, laser flash analysis, and differential scanning calorimetry to provide the baseline results. We aim to perform neutron irradiations of these ceramics in the High Flux Isotope Reactor (HFIR), which will allow comparisons of the materials chemical, physical, and thermal properties before and after neutron irradiation.

**Keywords: Fusion, Tritium Breeding, Blanket Materials**

*This initiative is sponsored by: FES*

## **Analysis of Fission Product Release from Furnace-Tested TRISO Particles**

Daniel Schappel\*, Martino R. Hooghkirk, Stephen E. Trehitt, Darren J. Skitt, William F. Cureton, and Tyler Gerczak,

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High temperature testing of intact TRISO particles previously irradiated in the AGR-5/6/7 experiment was performed in the Furnace for Irradiated TRISO Testing (FITT) to directly confirm diffusive release of silver and europium from intact TRISO particles. Testing was conducted from 1,100–1,600C for exposure times to 100 h to directly confirm silver through layer release below safety testing temperatures. The FITT analysis showed highest levels of silver release at 1,300–1,400C which confirms athermal release behaviors previous observed in step-wise and transient safety tests. Additionally, release was non-uniform with some particles releasing a majority of their inventory while others did not appear to release silver under identical testing conditions, which was consistent with historic observations. An assessment of the effective silver diffusion coefficient in the SiC layer was conducted and indicated maximum values in the 1,300–1,400C range. The magnitude of the calculated diffusion coefficients also exceeded accepted diffusion coefficients. Wang et al. found localized carbon depletion within about 2 nm of high angle grain boundaries. Additionally, Rollert et al. and Olesinski et al. found that the Ag solubility in Si spikes around 1,300–1,400 C, which when combined with the phase diagram may explain the Ag release behavior.

**Keywords: Silver, Cesium, TRISO, fission product, release, furnace, advanced gas reactor**

*This initiative is sponsored by: DOE-NE*

# Transient plasma simulations for interaction with liquid metal in magnetic confinement fusion reactors

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Understanding the interaction between the plasma in the tokamak core and the liquid metal breeding zone in the blanket is critical for predicting blanket resilience to plasma transients. Rapid plasma events, such as disruptions and edge-localized modes (ELMs), can induce significant electromagnetic perturbations that affect the behavior of electrically conductive liquid metals in the blanket. Although these events occur over short timescales, they can lead to prolonged and complex responses in the liquid metal flow.

To capture these coupled phenomena, recent efforts have focused on integrating plasma simulations with liquid metal magnetohydrodynamic (MHD) modeling. In this framework, time- and space-dependent magnetic fields generated by the plasma are mapped onto the blanket region to evaluate their influence on liquid metal dynamics.

In this study, plasma evolution is simulated using the finite element code M3D-C1. The primary objective is to investigate the effect of isotropic thermal conductivity on key transient plasma events, including the thermal quench, vertical displacement event (VDE), and current quench. Plasma characteristics such as maximum electron temperature, magnetic axis position, and total plasma current are analyzed for different thermal conductivity values.

Most importantly, the time derivatives of the magnetic field are evaluated at locations relevant to the blanket. These results provide essential input for subsequent simulations of liquid metal flow response in transient scenarios.

**Keywords: Fusion Energy, Plasma Physics, Liquid Metal, Magnetohydrodynamics**

*This initiative is sponsored by: U.S. Department of Energy, Office of Science, Fusion Energy Science*

## **Staying in the Loop: Online Monitoring of Molten Salts via Laser-Induced Breakdown Spectroscopy**

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**Abstract:** Molten salts are unique for their high heat capacity and thermal conductivity, making them excellent heat transfer fluids at high temperatures — ideal for applications in concentrated solar power and nuclear fission reactors. Their unique chemistry is also useful in reprocessing spent nuclear fuel and as fusion reactor blankets. To prevent corrosion, the purity of the molten salts must be carefully monitored and controlled. Therefore, measuring the composition and purity of molten salts online and in real time is a critical capability. One suitable technique for this is laser-induced breakdown spectroscopy (LIBS). In LIBS, a high-powered laser pulse is used to vaporize a solid, liquid, or gaseous sample and form a microplasma that emits light at characteristic wavelengths, which can be used to determine the elemental composition of the sample. LIBS is fast and can be performed without any sample preparation. This presentation will discuss recent efforts at Oak Ridge National Laboratory to develop sampling methods and data analysis approaches to establish LIBS as a quantitative technique for online monitoring of molten salts.

**Keywords:** laser-induced breakdown spectroscopy, molten salt, online monitoring, aerosol

*This initiative is sponsored by: DOE NE Molten Salt Reactor Program*

## Oral Presentation Session III – AI/ML II

### Comparison and Analysis of Modern AI-Based Pentesting Tools

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Large language model (LLM)-based pentesting agents have advanced rapidly, but most are built for information technology (IT) rather than operational technology (OT), where validation must stay within safety limits and leave an auditable record. We present UnCLE (Unconventional Cyber LLM Executor), an OT-focused framework for constrained assessment tasks that captures execution traces and device readbacks. UnCLE uses a pipeline architecture in which artifacts obtained through an initial reconnaissance stage drive a planner that maps goals to MITRE ATT&CK for ICS. Furthermore, the planner creates attack trees and dispatches specialist follow-on agents to execute pentesting tasks. The current suite supports Modbus, FTP, Telnet in SEL-451 relay environments through devicemanual retrieval augmentation, and web assessment with Nikto and OWASP ZAP. We compare UnCLE with three other LLM-based pentesting frameworks on a realistic electric utility substation testbed with power-system simulation and real Schweitzer Engineering Laboratories (SEL) protective relays and meters in the loop, examining performance with various metrics on supported tasks and the quality of evidence produced for human review.

**Keywords: AI, Pentesting, LLMs**

*This initiative is sponsored by: ORNL*

# From Evidence to Vulnerability Candidates: An Explainable Local Pipeline for Cyber and OT Triage using Large Language Models

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Security analysts routinely collect large volumes of host, network, and OT/ICS evidence, yet translating that evidence into a prioritized set of relevant vulnerabilities remains labor-intensive and difficult to justify analytically. In this poster, we present a local-first, explainable evidence-to-vulnerability correlation pipeline that we designed and implemented to support analyst-driven triage in privacy-sensitive environments. The system ingests heterogeneous artifacts, including logs, Nmap output, configuration files, JSON/XML/HTML exports, and OT device observations; normalizes them into structured evidence; extracts both explicit identifiers such as CVEs and CPEs and inferred product, package, service, version, model, and firmware clues; and correlates those signals against a local SQLite knowledge base assembled from public vulnerability sources, including NVD, CISA KEV, CWE, and GitHub Security Advisories. Candidate vulnerabilities are ranked using transparent heuristic scoring that prioritizes direct identifier matches, OT-aware model and firmware correlations, package and service evidence, and known exploited vulnerabilities. To support reproducibility and analyst trust, the pipeline preserves provenance through evidence manifests, hashes, timestamps, score breakdowns, and human-readable mapping rationales; an optional local LLM-assisted path improves entity extraction while maintaining offline operation. This work contributes a practical architecture for explainable, privacy-preserving vulnerability triage across enterprise and industrial environments. Rather than acting as a scanner or exploit validator, the system serves as a local correlation layer that converts collected evidence into a ranked, reviewable shortlist of plausible vulnerabilities.

**Keywords: vulnerability management, large language models, industrial control systems, operational technology**

*This initiative is sponsored by: Large Language Models for Pentesting Critical Infrastructure*

# High-Resolution Modeling of Indoor Radon Exposure with Uncertainty Quantification in Utah

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Indoor radon accounts for an estimated 37% of population-level exposure to ionizing radiation in the United States, yet publicly available metrics are typically reported at coarse spatial scales that obscure substantial local variability and limit epidemiologic utility. To support complex health data integration and analysis, we developed a high-resolution, uncertainty-aware machine learning framework to estimate indoor radon concentrations across Utah. A total of 19,497 residential measurements collected between 2006 and 2017 were integrated with environmental and housing covariates and analyzed using a geospatial neural network that captures spatial dependence and nonlinear effects. Predictions were generated on a uniform H3 hexagonal grid at 0.73 km<sup>2</sup> resolution (level 8). Household-level out-of-sample performance showed moderate correlation with observed concentrations (Pearson  $r = 0.44$ ), reflecting considerable household-specific variability. Predictive uncertainty was well calibrated: 24.3% of held-out observations exceeded the predicted 75th-percentile threshold, close to the nominal 25%. Spatial maps of predicted concentrations and exceedance probabilities above 4 pCi/L revealed pronounced fine-scale heterogeneity not evident in conventional summaries. These findings demonstrate how uncertainty-aware machine learning framework can integrate complex environmental and health-related data to enable fine-scale, decision-relevant exposure assessment.

**Keywords: Indoor radon, Exposure modeling, Geospatial machine learning, Uncertainty quantification**

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# Transforming Single Crystal Neutron Diffraction with Agentic AI

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Single-crystal neutron diffraction is an indispensable, yet highly specialized technique for accurate molecular and magnetic structure determination. This work introduces an agentic system designed to fundamentally transform the specialized and labor-intensive workflow of single-crystal neutron diffraction experiments. The core of the application is an AI agent powered by a Large Language Model, which interprets natural language goals and generates optimized strategy and instructions for experiment execution, effectively assisting experiment steering. This system employs a client-server architecture to provide real-time guidance across various experiment stages, integrating with instrument control, live data streaming, and data reduction to ensure optimized data coverage, continuous quality checks, adaptive control, and efficient use of neutron beam time. These are realized via a real-time adaptive control engine that utilizes regression models for live data analysis and prioritizes measurements in regions of interest, coupled with machine learning algorithms for robust data quality enhancement and treatment of background noises with quantified error estimates.

**Keywords: Agentic AI, Single Crystal Neutron Diffraction, Integrated Experiment Workflow**

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# Milo: An Intelligent Research CoPilot

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**Keywords: Retrieval-augmented Generation, Knowledge Graph, Large Language Model, Literature Synthesis, Semantic Clustering**

*This initiative is sponsored by: WINTR: Winter Transcriptome Regulation in Poplar*

## Oral Presentation Session III – Chemistry and Chemical Ecology

### Dopant-Guided Suppression of SO<sub>2</sub> Poisoning in Cu Catalysts for Electrochemical CO<sub>2</sub> Reduction

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**Abstract:** Electrochemical CO<sub>2</sub> reduction (eCO<sub>2</sub>RR) on Cu-based catalysts can produce value-added C<sub>2</sub>+ products, yet practical deployment is hindered by poor tolerance to gas-phase impurities such as SO<sub>2</sub>. We examine impurity-driven performance loss and dopant-enabled mitigation using undoped and transition-metal-doped copper hydroxy nitrate (Cu<sub>2</sub>(OH)<sub>3</sub>NO<sub>3</sub>, CHN; dopants: Ni, Co, Zn) synthesized by solution precipitation. Catalysts were tested in an H-cell (Pt/Ti anode, anion-exchange membrane, 0.1 M KHCO<sub>3</sub>) at -10 mA for 1 h under either pure CO<sub>2</sub> or CO<sub>2</sub> containing ~20 ppm SO<sub>2</sub>.

XRD confirmed CHN as the dominant phase (basal (001) reflection), and STEM-EDS mapping indicated uniform dopant distribution within brucite-like nanosheets (~200-500 nm) with intercalated nitrate. Product analysis by gas chromatography showed H<sub>2</sub>, CO, CH<sub>4</sub>, and C<sub>2</sub>H<sub>4</sub>. Under pure CO<sub>2</sub>, undoped CHN favored H<sub>2</sub> (Faradaic efficiency (FE) ~75%) with C<sub>2</sub>H<sub>4</sub> as the main carbon product (FE ~25%). SO<sub>2</sub> contamination decreased H<sub>2</sub> selectivity to ~48%, introduced substantial CH<sub>4</sub> formation (FE ~21%), and reduced C<sub>2</sub>H<sub>4</sub> to ~19%. Notably, Zn-doped CHN maintained higher C<sub>2</sub>H<sub>4</sub> selectivity under SO<sub>2</sub> (FE ~24%), indicating improved sulfur tolerance.

Ex situ XRD after eCO<sub>2</sub>RR revealed strong catalyst reconstruction, including attenuation of CHN (001) features and emergence of metallic Cu (111)/(200) peaks, consistent with Cu<sup>2+</sup> → Cu<sup>0</sup> reduction; Zn-doped CHN best preserved residual layered signatures. Ex situ SEM showed nanosheet-to-nanocluster restructuring (~50-100 nm) and SO<sub>2</sub>-enhanced dendritic growth. ICP-OES further indicated minimized Cu leaching for Zn-doped CHN. We hypothesize that the enhanced SO<sub>2</sub> resistance to Zn-induced modification of Cu's local electronic/structural environment that suppresses sulfur-species adsorption while sustaining C<sub>2</sub>H<sub>4</sub> selectivity which is under investigation.

**Keywords:** eCO<sub>2</sub>RR; copper hydroxy nitrate; SO<sub>2</sub> contamination; layered hydroxides; ethylene, dopants, selectivity; phase reconstruction, Faradaic efficiency

**Keywords:** eCO<sub>2</sub>RR; copper hydroxy nitrate; SO<sub>2</sub> contamination; layered hydroxides; ethylene, dopants, selectivity; phase reconstruction, Faradaic efficiency

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## **Repurposing Lithium Battery Recycling Wastewater for Marine Carbon Dioxide Capture and Storage**

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While climate change continues to evolve, the ocean acts as a natural sink for carbon dioxide (CO<sub>2</sub>) and has absorbed 30% of all CO<sub>2</sub> emissions since the Industrial Revolution. This has lowered the pH of the ocean by 0.1, a 26% increase in acidity that is detrimental to marine wildlife. The ocean's ability to sequester CO<sub>2</sub> can be leveraged with alkaline materials via Ocean Alkalinity Enhancement (OAE). Interestingly, waste generated during the extraction of end-of-life lithium-ion batteries (LIBs) is highly alkaline in the form of aqueous sodium hydroxide (NaOH) and can be used to perform OAE. A techno-economic analysis was performed for a proposed mixing facility that will process 50M gallons of LIB waste and 150M gallons of seawater in a closed loop process of capture and storage. The proposed facility will capture 55 tons of CO<sub>2</sub> annually at a processing cost of \$324 per ton of CO<sub>2</sub> and an energy requirement of 1.7 GJ per ton of captured CO<sub>2</sub>. This energy requirement is lower than electrochemical methods that dominate the ocean-based CO<sub>2</sub> removal space. Results from this study underscore the importance of identifying cost-effective sources of alkaline waste materials to perform OAE and advance carbon capture.

Keywords: Carbon capture, sustainability, battery recycling

**Keywords: Carbon capture, sustainability, battery recycling**

*This initiative is sponsored by: LDRD*

# Theoretical investigation of molecular photoswitch for early detection of Alzheimer's disease

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Molecular photoswitches based on the norbornadiene/quadricyclane (NBD/QC) system have emerged as promising platforms for both solar energy storage and fluorescence-based biomedical imaging. In this work, we present a theoretical investigation of two pyrenefunctionalized NBD derivatives (NBD-1PY and NBD-2PY) and their corresponding QC isomers, with the aim of evaluating their potential as photoswitchable probes for early detection of Alzheimer's disease. Using time-dependent density functional theory (TD-DFT) at the CAM-B3LYP-D4/def2-TZVP level, complemented by third-order cluster perturbation theory CPS(D-3), we systematically analyze excitation and emission properties in vacuum, implicit solvent, and explicit dichloromethane environments. The results demonstrate that NBD derivatives exhibit consistently lower excitation energies than their QC counterparts, with solvent effects inducing modest red shifts due to dielectric stabilization. Explicit solvation further enhances these effects, highlighting the role of short-range polarization in stabilizing excited states. Substituent positioning is found to significantly influence photophysical behavior: NBD-1PY displays strong fluorescence, while NBD-2PY enables efficient and reversible photoswitching without excimer formation. These differences are attributed to variations in conjugation and orbital coupling between the pyrene moiety and the NBD/QC scaffold. Overall, the photophysical properties remain robust across environments, suggesting suitability for biological applications. The observed tunability of absorption and emission characteristics, combined with favorable switching behavior, supports the potential of pyrene-substituted NBD/QC systems as next-generation fluorescent probes for high-contrast imaging of amyloid- $\beta$  aggregates. This study provides key structure-property insights to guide the rational design of photoswitchable molecules for diagnostic and energy-related applications.

**Keywords:** Quantum Chemistry, Electronic Structure Theory

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## **Frontiers of particle analysis: an innovative device for single particle ICPMS**

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Nanotechnology plays a significant role in today's scientific landscape, prompting rapid advances in analytical methods for particle-scale composition analysis. However, many current approaches are resource-intensive, can mask population-level trends, or recover only a small fraction of particles from solid substrates. Here, we describe a device for sonication-induced (SI) single-particle (SP) inductively coupled plasma mass spectrometry (ICP-MS) and evaluate its performance using natural and synthetic particles spanning a range of sizes. This method improves throughput by eliminating the need for pre-extraction of particles prior to analysis. Our results demonstrate the effectiveness of the SI-SP approach for particles deposited on Si wafers and J-swipes. The impact of this invention extends to nuclear forensics, particle synthesis, environmental monitoring, and semiconductor fabrication.

**Keywords: particles, nuclear forensics, sample introduction, ICPMS**

*This initiative is sponsored by: National Nuclear Security Administration*

## **Sorption-based removal of mercury species from aqueous solutions: Influencing factors and environmental implications**

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Mercury (Hg) is a pervasive global contaminant that poses significant risks to human and ecosystem health. Freshwater systems impacted by legacy Hg contamination are particularly vulnerable because inorganic Hg (iHg) persists and can be transformed into highly toxic methylmercury (MeHg). In-situ sorbent amendments offer a low-cost, low-impact approach to reducing Hg mobility and bioavailability in sediments, yet their large-scale implementation remains limited. We are conducting ongoing evaluations of Hg species adsorption by several sorbents, including sulfur-impregnated and brominated activated carbon, biochar, FerroBlack H40-coated vermiculite (FeS/polysulfide), and cryptomelane (a manganese oxide). Preliminary results show that, with the exception of FerroBlack-coated vermiculite, iHg adsorption onto the other sorbents in phosphate buffer (pH 7.4) follows Freundlich isotherm behavior. Similar adsorption patterns are expected for MeHg. We are also examining the influence of factors such as pH, ionic strength, and dissolved organic matter (DOM) on iHg and MeHg uptake by these five sorbents. Current findings indicate strong potential for these materials to support Hg remediation at contaminated sites such as East Fork Poplar Creek (EFPC), historically influenced by the Y-12 National Security Complex. Incorporating realistic water and sediment matrices into ongoing laboratory studies will further clarify sorbent performance under environmentally relevant conditions.

**Keywords: Mercury remediation, novel sorbents, water-sediment ecosystems**

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## Oral Presentation Session III - Nuclear Materials

### Investigation of hydrogen retention and phase stability in neutron-irradiated yttrium hydrides: A synchrotron X-ray diffraction study

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Yttrium hydride (YH<sub>x</sub>) is a promising moderator material for nuclear microreactors due to its high hydrogen density [1], radiation resistance [2], and thermal stability [3] under compact, high-temperature operating conditions [4]. A critical concern, however, is hydrogen redistribution and potential loss under fast neutron flux, which can degrade moderation performance [5]. In this study, high-energy synchrotron X-ray diffraction (XRD) was employed to investigate phase evolution and hydrogen retention in sub-stoichiometric YH<sub>x</sub> (H/Y = 1.69–1.87) following neutron irradiation up to 2.0 dpa at ~600 °C.

Transmission-mode synchrotron-XRD revealed strong persistence of hydride-phase peaks across all irradiated specimens, accompanied by suppression of metallic yttrium reflections, indicating substantial hydrogen retention despite elevated temperature exposure. Micro-focused diffraction measurements showed only minor spatial variations in hydride-to-metal peak intensity ratios, suggesting limited local stoichiometric heterogeneity and absence of large-scale hydrogen depletion. Comparative analysis further demonstrated that initial hydrogen stoichiometry exerted a stronger influence on phase fractions than irradiation dose within the examined range. Notably, the invariant hydride-phase peak position corresponded to a constant lattice parameter, confirming structural stability under irradiation.

These results establish that hydrogen redistribution in YH<sub>x</sub> is governed by localized, diffusion-limited processes, whereas the hydride lattice remains stable under reactor-relevant conditions, supporting its viability for microreactor moderator applications.

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

*This initiative is sponsored by: -*

## **Stability of neutron irradiated yttrium hydride under cyclic heating**

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Metal hydrides are considered for solid moderator applications in compact thermal microreactor designs. Among them, yttrium hydrides are promising due to their comparatively high thermal stability. To qualify yttrium hydride for long-term operation, it is critical to understand degradation mechanisms during heating. Here, we track microstructural evolution in neutron-irradiated YH<sub>1.87</sub> during thermal cycling. Thermal cycling was performed using differential scanning calorimetry measurements and transmission electron microscopy was used to characterize changes in the bulk and near-surface regions. Heating promoted crystallization and epitaxial growth of surface oxidation as well as slight hydrogen desorption. In contrast, the bulk matrix crystal structure, irradiation-induced cavities, and matrix precipitation remained unchanged. These results provide insight into thermally driven degradation in yttrium hydride, enabling informed decisions on future hydride processing to improve stability under reactor-relevant conditions.

**Keywords: Yttrium Hydride, Heat Treatment, Transmission Electron Microscopy**

*This initiative is sponsored by: Microreactor Program*

# Effects of High Dose Neutron Irradiation at Light Water Reactor-Relevant Temperatures on the Mechanical Properties of SiC/SiC Composites

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Neutron irradiation effects on thermomechanical properties of SiC/SiC composites are critical for assessing their feasibility and lifetime in accident-tolerant core structures of light water reactors (LWRs). A knowledge gap currently exists regarding the transitional processes in radiation-induced thermomechanical degradation at high neutron doses. To capture the processes and identify the underlying mechanisms, grades of nuclear grade chemical vapor-infiltrated SiC/SiC composites with different interface microstructures were irradiated up to 30 displacements per atom (dpa) at the High Flux Isotope Reactor at Oak Ridge National Laboratory.

Flexural testing, dimensional measurement, and thermal diffusivity analysis showed irradiation-induced changes saturated over the dose range of 2–30 dpa for certain composite materials. However, the retention of mechanical properties differed from degradation behavior reported in the literature for similar SiC/SiC composites. The discrepancy is discussed based on numerical analysis on irradiation-induced stress evolution informed by Raman spectroscopy analysis of carbon interphase in the as-fabricated composites. Finally, radiation-resistance interphase microstructure will be discussed.

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**Keywords: Silicon Carbide, Ceramic Matrix Composite, Neutron Irradiation, Interphase**

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# Fracture Toughness Testing of Nuclear Structural Materials in Extreme Environments Using Miniaturized Test Specimens

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Fracture toughness testing is essential for down-selection and code qualification/licensing of structural materials for nuclear reactor applications. Neutron irradiation drives microstructural evolution that leads to hardening and embrittlement, expressed macroscopically as a degradation of fracture toughness and ductile-to-brittle transition temperature (DBTT). Miniaturization of fracture toughness test specimens is often necessary to utilize small heats of engineering materials, reduce space occupied during test reactor irradiation and minimize the total activated material needed for post-irradiation testing and examination. Testing of these irradiated miniature test specimens is difficult and must often be performed in hot-cells, at either cryogenic or elevated temperatures, and even in inert environments, all of which drive the need for specialized test fixtures and accounting for specimen size effects.

In this work, a variety of unique testing fixtures were designed to test miniature specimens emphasizing compliance with ASTM Standards and utility in a hot-cell environment. A series of test campaigns were performed across sample geometries, e.g., compact-tension (C(T)) and single-edge bend (SE(B)), and materials systems including reduced activation ferritic/martensitic steels, low-alloy steels, and refractory tungsten alloys. Results contribute to current understanding of specimen size effects and highlight the efficacy of specimen miniaturization for evaluation of fracture toughness of irradiated materials.

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**Keywords: Nuclear, Materials, Testing, Fission, Fusion**

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# Accurate Prediction of Chemical and Redox Potentials in Molten Salts from DFT-Based Free Energy Simulations

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Accurate prediction of condensed-phase free energies remains a major challenge for chemically complex liquids such as molten salts, even when employing state-of-the-art machine learning interatomic potentials (MLIPs) trained on density functional theory (DFT) data. In this work, we present a computational framework for free energy calculations in molten salts that addresses key thermodynamic and numerical limitations. In particular, we incorporate finite-size standard-state corrections to ensure thermodynamic consistency and introduce soft-core repulsive potentials within thermodynamic integration to mitigate numerical artifacts. These soft-core formulations are shown to be critical for stabilizing simulations and enabling robust error estimation, especially at small alchemical coupling parameters. We further outline the construction of consistent thermodynamic cycles by explicitly including standard-state corrections appropriate for finite simulation cells, thereby allowing direct comparison with experimental thermodynamic quantities. The approach is applied to determine redox potentials in pure molten LiCl, NaCl, and KCl, as well as the formal redox potentials of AgCl relative to the  $\text{Cl}_2/\text{Cl}^-$  couple at infinite dilution in these media. In addition, we demonstrate an efficient strategy for improving MLIP accuracy through  $\Delta$ -learning using higher-level quantum chemical calculations. Together, these advances establish a robust and transferable foundation for predictive, quantitatively accurate thermochemical modeling of molten salts.

**Keywords: Molten Salts, Machine Learning Potentials, DFT, Redox potential, MD simulations**

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