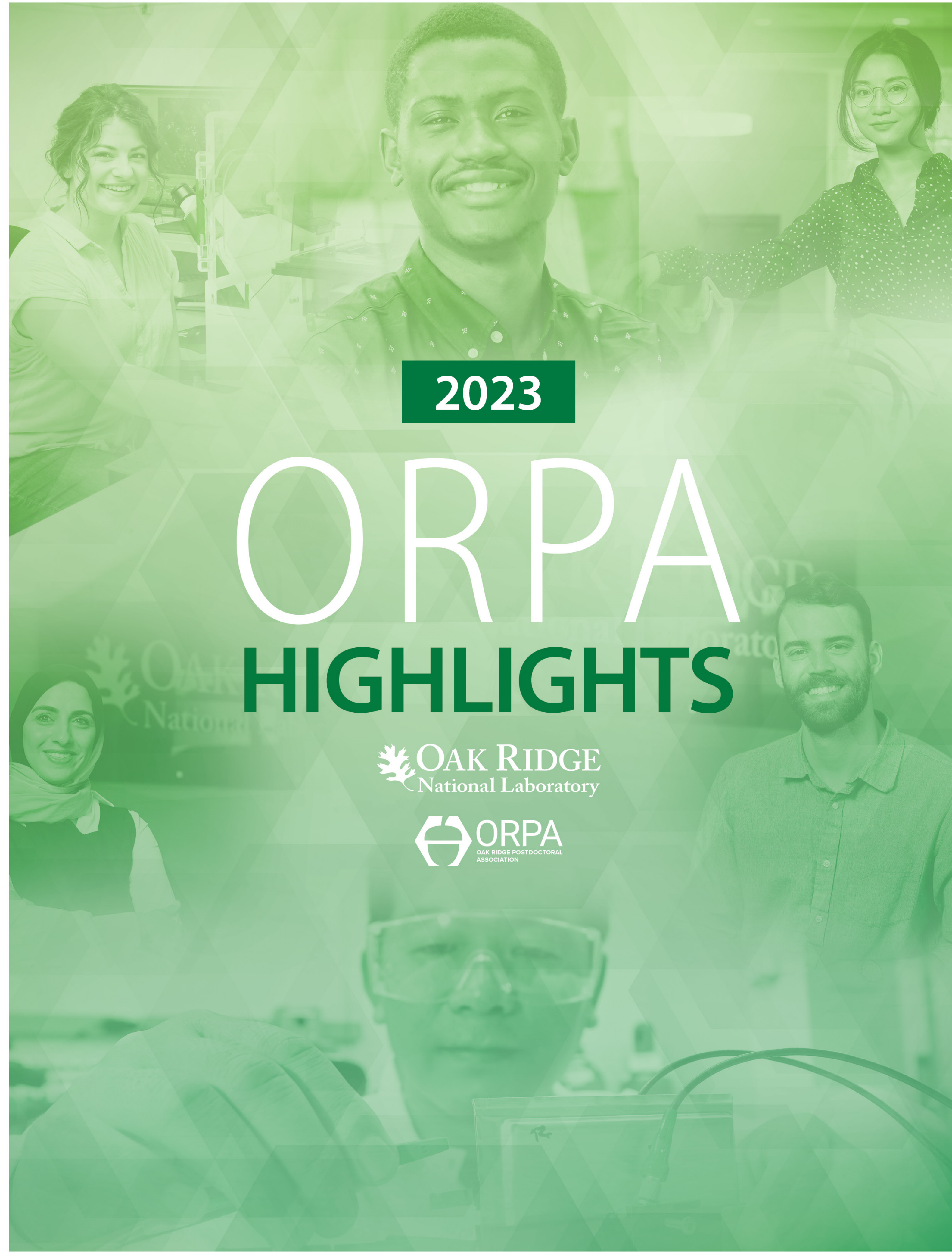
2023

ORPA HIGHLIGHTS

Oak Ridge National Laboratory

ORPA
Oak Ridge Postdoctoral Association



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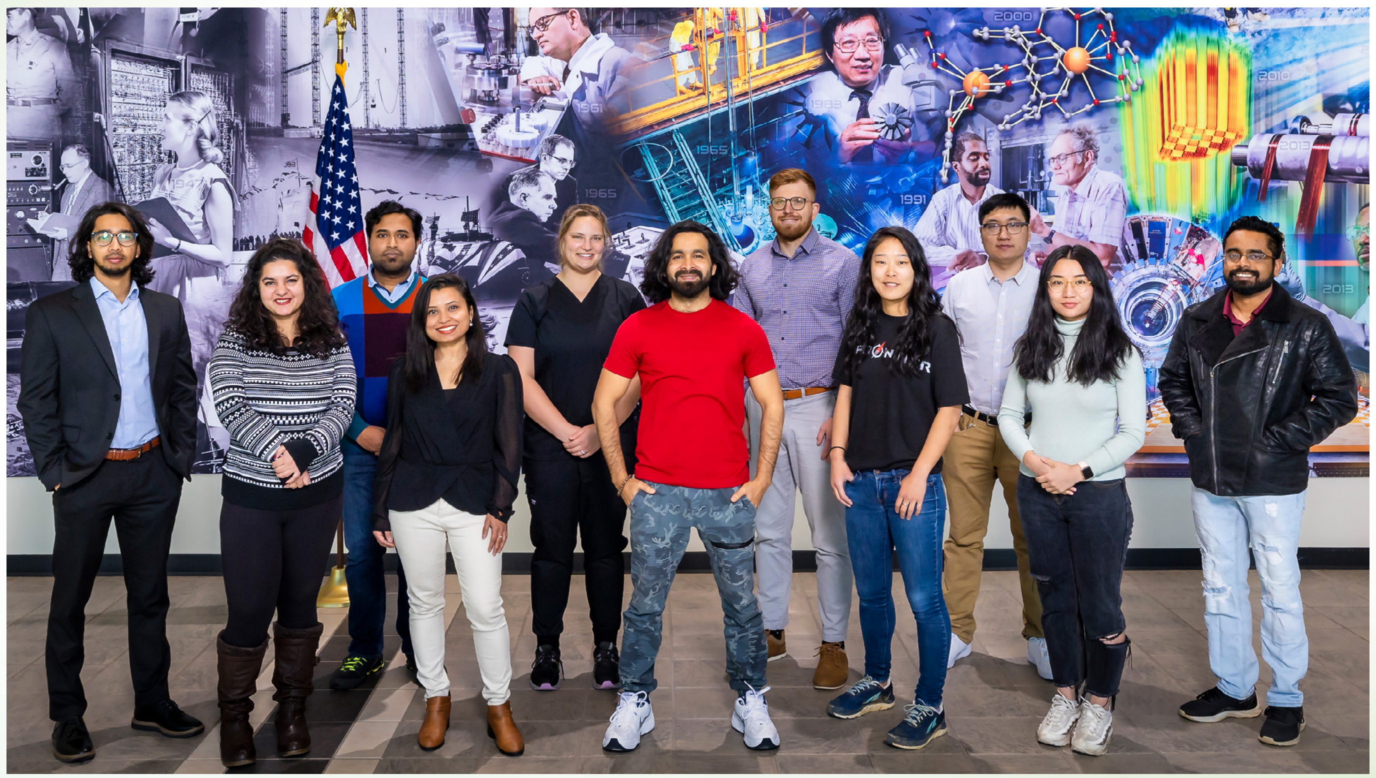
Introduction

Welcome to the first issue of *ORPA Highlights Magazine*! The Oak Ridge Postdoctoral Association (ORPA) launched this annual magazine to serve as a means to highlight postdoctoral research at Oak Ridge National Laboratory (ORNL) and to summarize the accomplishments of the Oak Ridge Postdoctoral Executive Committee (ORPEX), ORPA's governing body. The magazine, released during National Postdoc Appreciation Week (September 18–22, 2023), is being made available in digital form on ORPA's internal website and in a limited run of hard copies.

About ORPA

ORPA is dedicated to fostering a sense of community and social well-being for the members of the postdoctoral community at ORNL, to facilitate their professional development, and to advocate on their behalf. ORPA activities are coordinated by ORPEX, whose members head the New Hire, Social, Outreach, and Research committees. ORPEX members also lead communication, advocacy, and cross-lab networking and collaboration initiatives. ORNL encourages all postdocs to be active in ORPA. To reach the current executive committee, email ORPEX@ornl.gov.



Oak Ridge Postdoctoral Executive Committee , 2023. Left to right: Indranil Roy, Pratishtha Shukla, Subhamay Pramanik, Biva Talukdar, Briana Schrage, Torik Islam, Tomas Grejtak, Emily Mazeau, Johnson Lu, Athena Chen, and Shuvo De.

ORPA's committees introduce postdocs to opportunities to develop professionally and to serve others while at ORNL.

- The New Hire Committee reaches out to postdocs during the onboarding process to establish a connection to ORPA and the postdoc community.
- The Social Committee creates and hosts events for postdocs to interact and build relationships.
- The Outreach Committee motivates and facilitates opportunities for postdocs to give back to the community through service opportunities.
- The Research Committee focuses on facilitating professional development by encouraging postdocs to attend monthly seminars and to present their work to other ORNL researchers at the annual Postdoctoral Research Symposium.

Fostering a Sense of Community and Social Well-Being

ORPA is here to support you during your time as a postdoctoral researcher at ORNL. We look forward to getting to know you and serving you. Please feel encouraged to participate in our activities advertised in the quarterly newsletter, or send us an email (ORPEX@ornl.gov) if you would like to be added to our listserv.

Professional Development

Membership in ORPA and ORPEX offers ORNL postdocs a wide range of professional development opportunities. Board members learn many new skills, including leadership, organization, communication, and event planning and budgeting that they use to impact their research divisions and future employers.

Advocacy

ORPEX President Indranil Roy (royi@ornl.gov) and Vice-President Subhamay Pramanik (pramaniks@ornl.gov) address advocacy issues for postdocs in collaboration with ORNL management. Please email them if you have an issue. They will be happy to discuss it.

New Initiatives

Annual ORPA Highlights

ORPEX collaborated with Creative Services to design *ORPA Highlights Magazine* and to begin its publication in 2023. Be sure to submit your research for inclusion in future issues. ORPEX will issue a call in the summer.

Postdoc Offboarding Guide

ORPA developed the *Postdoc Offboarding Guide* in response to frequent questions received regarding the process at ORNL and options for the postdocs, including extending their position, transitioning to staff, and finding an external position. The document is available on ORPA's internal website under the "Resources" tab.

Cross-Lab Elevator Pitch Competition

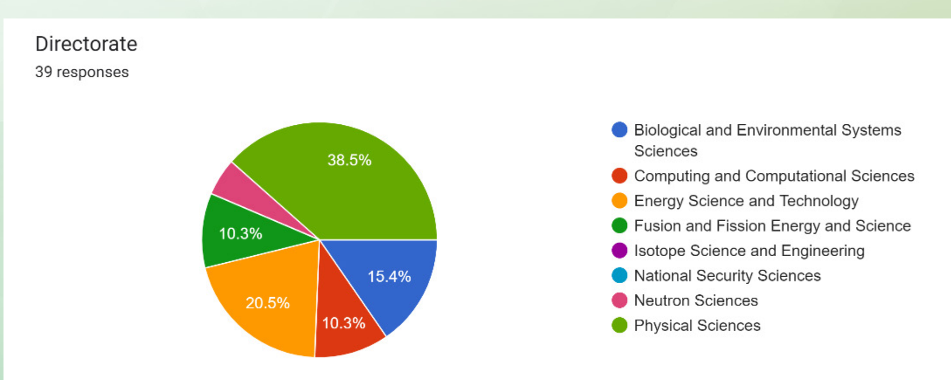
In FY 2023, ORPEX initiated a cross-lab collaboration with Argonne and Los Alamos National Laboratories. ORPEX members championed a virtual lightning talk competition in collaboration with the three national laboratories and with the University of Tennessee, Knoxville, as the organizer and host. The first competition is scheduled to take place during Postdoc Appreciation Week (September 18–22, 2023). Postdocs representing all three labs will participate, and senior researchers have been recruited from all three labs to serve as judges. Three winners, one from each lab, will be invited to deliver a virtual seminar at the lab of their choosing.

ORPA Collaborates with the APAC ERG on a Carpooling Initiative

ORPEX collaborated with the Asian Pacific American Club, an ORNL employee resource group, to develop the APAC Carpool Volunteer List, a database to connect staff looking for a carpooling option with staff willing to share rides to work. For more information, contact Pratishtha Shukla (shuklap@ornl.gov) or Yashika Ghai (ghaiy@ornl.gov).

Postdoc Research Skills Database

ORPEX initiated an effort to build the Postdoc Research Skills Database, a catalog of postdoc scientific and technical skills that is searchable by any ORNL staff member looking for specific support. Postdoc entries were collected with the goal of benefiting the hiring process across all ORNL directorates. This voluntary, user-friendly database will be hosted on the internal website to help identify specific project openings or suitable candidates for staff positions. This newly launched initiative has received almost 40 responses to date from participants representing almost all of the research directorates in ORNL.



Response to the FY23 initiative—Postdoc Research Skills Database by directorate

ARPA-E Seminar

ORPA hosted Advanced Research Projects Agency-Energy (ARPA-E) Fellows Dr. Anil Ganti and Dr. Julia Greenwald on January 19, 2023. The presentation featured opportunities for obtaining funding and for becoming an ARPA-E Fellow. The speakers provided a brief introduction to the funding model at ARPA-E and the Fellows program inviting eligible early career scientists and postdocs to become ARPA-E Fellows.

ORPEX Vice President Subhamay Pramanik, New Hire Chair Pratishtha Shukla, and President Indranil Roy welcomed ARPA-E Fellows Julia Greenwald and Anil Ganti (left to right) for a presentation on opportunities at ARPA-E.

Research Events

Research Seminar Series. ORPA organizes research seminars throughout each fiscal year. In FY 2023, we hosted three research seminars. On December 14, 2022, we hosted Dr. Bryan Chakoumakos, Corporate Fellow and Single-Crystal Neutron Diffraction group leader in the Neutron Scattering Division. On January 18, 2023, we hosted Dr. Stephen Nagler, Corporate Fellow in the Neutron Scattering Division. On April 27, 2023, we hosted Prof. Peter Heaney, from Pennsylvania State University's Department of Geosciences. All the invited speakers delivered very informative talks in their research domains and provided valuable suggestions for collaborating effectively with scientists in very diverse research fields, keeping oneself open to learning new knowledge and skills, and maintaining high productivity and work-life balance.

Eleventh Annual ORPA Research Symposium. The eleventh annual ORPA Research Symposium, held on May 18 and 19, 2023, gave postdocs the opportunity to deliver talks and poster sessions on their research, hear from well-respected keynote speakers, and network with other postdocs and ORNL research staff. Eighteen ORNL postdocs volunteered to organize the symposium and to plan sessions, judge talks, collect audience votes for people's choice of best presentations and posters, and prepare an abstract booklet.

ORPEX officers and postdocs organized the 2023 Research Symposium.

Deputy for Science and Technology Susan Hubbard delivered welcome remarks at the 2023 Research Symposium.

Scenes for this year's Research Symposium: (left) The audience listens to a presentation and (right) attendees had two rooms of posters to discuss.

National Postdoc Appreciation Week: ORPEX organized a full week of activities for the National Postdoc Appreciation Week, held from September 18 to September 22, 2023. The activities included:

- guided tours of the Graphite Reactor and Advanced Plant Phenotyping Laboratory;
- panel sessions with early-career and senior scientists from academia, industry, and other national labs;
- a panel session with staff members who had recently transitioned from a postdoc position at ORNL;
- a presentation by a DOE Early Career Research Program awardee;
- a lightning talk competition among the postdocs from ORNL, ANL, and LANL;
- the opportunity to have head shots taken by a professional photographer;
- a working lunch with the Postdoctoral Engagement Committee members; and
- an off-site social.

Your Science in a Nutshell: Eight postdocs participated in this year's Your Science in a Nutshell competition on June 22. They delivered exciting two-minute talks that were judged by leaders at ORNL, DOE Oak Ridge Site Office, and University of Tennessee. The judges chose the first-, second-, and third-place winners, and the in-person audience voted to select the winner of the People's Choice award. The first-place winner was Janet Meier, a postdoc in the Materials Science and Technology Division. The second-place winner and People's Choice winner was Sandeep Kaur, a postdoc in the Chemical Sciences Division. Third place went to Daniel Adams, a geospatial scientist in the Geospatial Science and Human Security Division. Finalists attended presentation skills training and worked one-on-one with researcher-mentors from across the lab. The three winners had lunch with Interim Lab Director Jeff Smith and Deputy for Science and Technology Susan Hubbard in August. Our first-place winner will compete with winners from across the national lab complex in the first national Research SLAM! competition, which is scheduled for November 15, 2023, in Washington, DC.

Social and Wellness Events

During FY 2023, ORPA held social events, including eighteen Friday happy hours around Knoxville, seventeen midweek trivia nights, weekend hikes in the Smokies, at Abrams Falls and Elmont Campground, and a frisbee golf tournament at Admiral Farragut Park. ORPEX also organized "R U Feeling OK?" activities in conjunction with ORNL's Mental Health Awareness Month in May, handing out themed T-shirts for a group photo and hosting a meditation session and virtual presentation on stress in the workplace. ORPA Vice President Subhamay Pramanik led R U Feeling OK? activities.

Happy hour gathering of ORPEX officers, postdocs, and allies, February 2023.

ORPEX officers (left) and postdoc allies (right) on R U Feeling OK? day, May 24, 2023.

Outreach and Volunteering Events

The Outreach Committee connected ORNL postdocs with several service opportunities during FY 2023. ORNL postdocs participated in community events such as coding activities for local K–12 students to encourage them to consider STEM careers. During Engineering Week, ORNL postdocs discussed the science conducted at ORNL with a local fifth-grade class and explained how they can pursue a career in engineering. ORNL postdocs volunteered for several other outreach events, including SAGE Camp, Linden Elementary STEM Day, Next-Generation Pathways to Computing, YO-STEM!, and Oak Ridge Computer Science Girls.

Outreach Committee chair Tomas Grejtak met with local students during Engineers Week, February 2023.

Postdoc Experience Questionnaire

In FY 2023, ORPEX developed a questionnaire to gather information about how the postdoctoral program and work experience are meeting the needs of ORNL postdocs. Questions addressed professional development opportunities, the relationship with the postdoc's supervisor, and the postdoc experience in general. Responses will help ORPEX boards to better advocate for the postdoctoral community. The questionnaire closes at the end of FY 2023, specifically, September 22. ORPEX will publish the results of the postdoc experience questionnaire in early FY 2024.

Archana Ghodeswar

Quantifying the Economic Costs of Power Outages Owing to Extreme Events

Archana Ghodeswar, Manufacturing Energy Efficiency Research and Analysis Group, Energy and Industrial Decarbonization Section, Manufacturing Science Division

Big Science Problem
What are the best methods and tools for quantifying costs of power outages owing to natural disasters?

Motivation
In the face of increasing natural disasters and the need for sustainable energy solutions, stakeholders may need help identifying the most suitable model(s) or methodologies and understand the differences between different candidate models to estimate the cost-effectiveness of increasing resiliency and reliability.

Tools
- CDF Calculator (National Renewable Energy Laboratory [NREL]): Estimates the cost of power outages by quantifying the economic impact on customers, aiding disaster preparedness
- ICE Calculator (NREL): Assesses economic consequences of power interruptions, informing resilient energy systems

Results, Conclusions, and Future Work
The review of power outage–related economic costs owing to extreme events revealed methodological inconsistencies in assessing power outage costs and reliance on outdated data, impacting comparability and accuracy. Sectoral variations in costs were observed, with commercial and industrial sectors bearing higher burdens. Larger customers experience greater expenses, and longer outages lead to increased economic losses. The study also evaluates method strengths and tools and suggests potential paths for future research.
Power outage costs vary based on sector, customer type, and duration. Standard quantifying units, updated surveys, and granular outage data are required. The interruption cost estimate calculator is better suited for macroeconomic costs. A customer damage function calculator is better suited for individual consumers. Quantifying outage costs helps justify investments in renewable and sustainable power.

More accurate methodologies should be developed for quantifying individual consumer-level power outage costs, including understanding specific costs for different types of consumers, such as commercial and industrial customers. Data collection and analysis methods should be standardized across regions and sectors to improve accuracy and comparability of power outage cost assessments. Inclusion of cost-related questions in annual surveys by the US Energy Information Administration is recommended to capture macroeconomic impacts on industrial, commercial, and residential sectors. The effectiveness of various strategies and investments should be investigated for enhancing electric power system reliability and resilience, including backup power systems, microgrids, combined heat and power, and demand response programs.

Current research includes the following:
- What are the energy needs and best energy policies for rural and remote places such as parts of Alaska, Puerto Rico, and Hawaii?
- What are the best tools, metrics, and methods to serve energy and environmental justice in weatherization programs, state and community energy programs, repurposing of abandoned coal mines, and shutting down of coal power plants?
- What are the best metrics for quantifying non-energy benefits of weatherization programs?

Arpan Biswas

Toward Improved Guided Experimentation through Human–AI Collaborative Adaptive Learning

Arpan Biswas, Data NanoAnalytics Group, Theory and Computation Section, Center for Nanophase Materials Sciences

Big Science Problem
Optimization for tasks such as material characterization, synthesis, and determination of functional properties for desired applications within multidimensional control parameter and function spaces requires rapid, strategic searching through active learning. However, in all cases, before optimization, the target structure–material property relationships to be explored are assumed to be known; and the ability to shift the trajectory of an optimization based on human-identified findings during an experiment is lacking. This issue can be critical in conducting expensive experiments on new materials in which the experimental results are likely not aligned to any appropriate scientific outcomes because of improper target setting, ultimately wasting time and money. The failure rate and cost are even higher when multitarget spaces are being explored to learn the interactions among multiple properties to find the optimal trade-offs during material synthesis for desired applications.

Motivation
This research aims to highlight the best of both machine learning (ML) or artificial intelligence (AI) and domain experts' knowledge with the focus on the appropriate balance between accelerated and meaningful scientific discoveries. The research introduces the human-AI–collaborative active recommender system, which aims to design and shape a target property to be explored "on the fly" with real-time visual assessment during Bayesian optimized sequential experiments, ultimately bypassing the need to define any target scalarizer before the optimization process. The proposed approach allows researchers to seamlessly combine the human input with the policy of the ML agent during early explorations (when prior knowledge is minimal) to refine the selection of

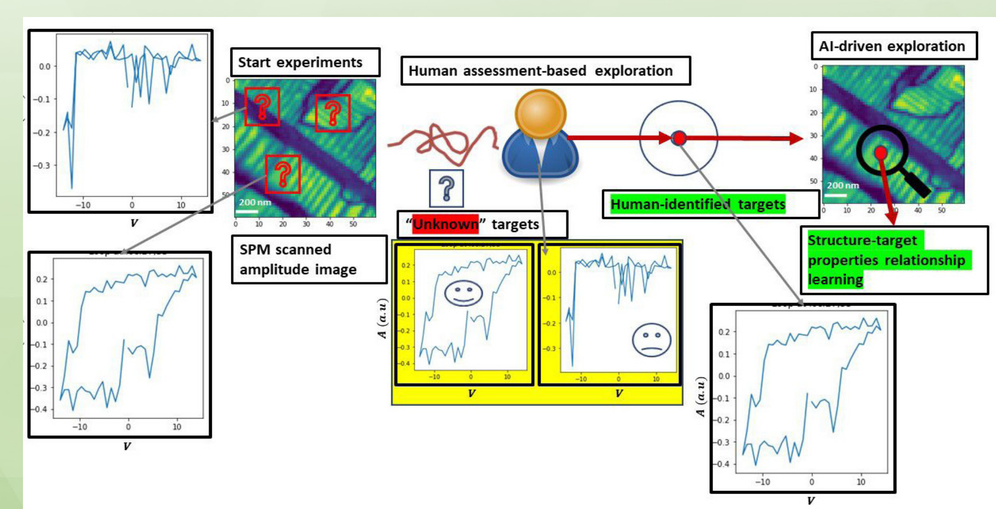


Figure 1. Workflow of the proposed human–AI collaborative autonomous material characterization. *SPM*: scanning probe microscopy. (Credit: A. Biswas)

targets to explore. With future adaptive explorations (when prior knowledge is sufficient), the preferences shift completely toward AI to accelerate the learning with human-assessed goals.

Tools

The approach has been integrated with a scanning probe microscope located in the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) for autonomous characterization of a ferroelectric thin film, aiming for rapid exploration over multifunctional space of "on the fly" human-assessed targets.

Publications

A. Biswas, Y. Liu, N. Creange, Y.-C. Liu, S. Jesse, J.-C. Yang, S.V. Kalinin, M. A. Ziatdinov, and R. K. Vasudevan "A Dynamic Bayesian Optimized Active Recommender System for Curiosity-Driven 'Human-in-the-Loop' Automated Experiments," https://doi.org/10.48550/arXiv.2304.02484.

This article has been published in arXiv and is currently being reviewed by *npj Computational Materials*. The authors and contributors and their affiliations are as follows: Y. Liu (CNMS, ORNL), N. Creange (ex-ORNL), Y.-C. Liu (National Cheng Kung University, Taiwan), S. Jesse (CNMS, ORNL), J.-C. Yang (National Cheng Kung University, Taiwan), S. V. Kalinin (University of Tennessee, Knoxville), M. A. Ziatdinov (Computational Sciences and Engineering Division, ORNL), and R. K. Vasudevan (CNMS, ORNL).

Results, Conclusions, and Future Work

In this analysis, efficient structure-property learning was achieved with less than 10% exploration (characterization) of a material image space (scanned by the microscope). The total run time of this automated-experiment analysis was less than 30 min, whereas the computational cost to run the experiment exhaustively for all grid points (in a 128 × 128 pixel image) was about 15–24 h. This partially combined human-in-the-loop AI workflow enables researchers to use the microscope to perform new types of experiments that previously were out of reach (e.g., analysis with higher-resolution images). This work shows an advancement toward human–AI collaborative automated experiments in which big data is likely unavailable, but a higher quality of data is required (e.g., material synthesis with expensive experiments). This advancement required intelligent sampling through simultaneous steering of optimization trajectories and acceleration of the path to optimal learning with human guidance and AI-driven experimentation. In future work, an open-source website application will be developed for broad groups of designers, experimentalists, and materials scientists.

Acknowledgment

The experiments, autonomous workflows, and deep kernel learning were supported by the Center for Nanophase Materials Sciences, which is a US Department of Energy Office of Science user facility at Oak Ridge National Laboratory.

Hsuan-Hao Lu

Exposing Quantum Frequency's Secrets: Bayesian Tomography in High-Dimensional On-Chip Biphoton Systems

Hsuan-Hao Lu, Quantum Communication and Networking Group, Quantum Information Science Section, Computational Sciences and Engineering Division

Big Science Problem

Photonic qubits form the cornerstone of quantum communication and networking. Qudits, lesser-known counterparts of qubits, offer higher information capacities and improved noise tolerance. However, characterizing these states has traditionally been challenging. This study focused on frequency-bin qudits, which are single particles of light in a quantum superposition of multiple colors, and successfully developed an effective measurement technique for their characterization.

Motivation

Quantum state tomography is essential for precise characterization of quantum systems, but traditional techniques encounter difficulties in scaling to higher dimensions, especially in photonic systems. Through a quantum analog of Galton's board, known as a *quantum walk experiment*, distinct probability distributions at the output for varying input states were observed. This approach served as the inspiration to devise an elegant method, utilizing both experimental and numerical approaches, to reconstruct the input states from such experiments.

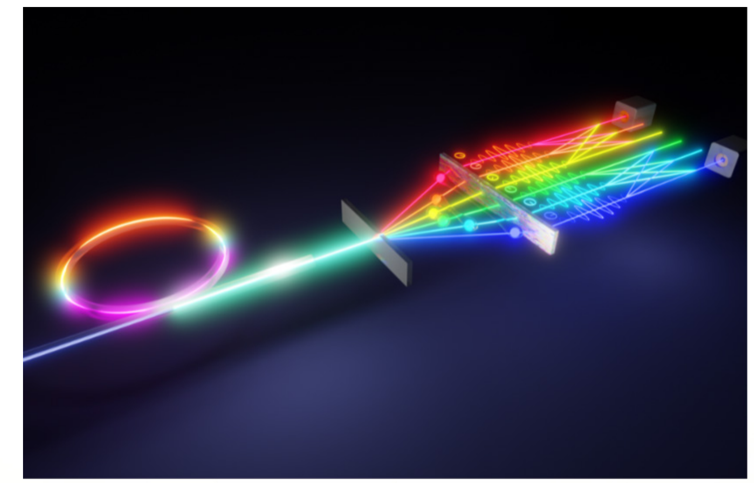


Figure 1. Entangled photons generated from a microring resonator undergo dynamic spectral transformations through random mixing using a pulse shaper and a phase modulator. (Credit: Y.-Y. Pai)

Tools

The experiment commenced by illuminating a laser into a silicon nitride microring resonator, producing entangled photons in the form of two qudits with correlated frequencies. With the use of an electro-optic phase modulator and a Fourier transform pulse shaper in the setup, the various light frequencies could be mixed and their spectral phases could be manipulated. By applying these operations randomly, a diverse range of frequency correlations was effectively captured. Employing Bayesian inference as a data analysis tool, advanced computing resources were harnessed to conduct simulations. These simulations enabled inference of the quantum states responsible for the observed frequency correlations.

Publications and Related Link

H. H. Lu, K. V. Myilswamy, R. S. Bennink, S. Seshadri, M. S. Alshaykh, J. Liu, T. J. Kippenberg, D. E. Leaird, A. M. Weiner, and J. M. Lukens, "Bayesian Tomography of High-dimensional On-chip Biphoton Frequency Combs with Randomized Measurements." *Nat. Commun*. 13, 4338 (2022). https://www.osti.gov/biblio/1879134

"New measurements quantifying qudits provide glimpse of quantum future," Oak Ridge National Laboratory News , October 13, 2022,
https://www.ornl.gov/news/new-measurements-quantifying-qudits-provide-glimpse-quantum-future.

Results, Conclusions, and Future Work

Entanglement was successfully verified, and the density matrix of quantum frequency combs in an 8 × 8 dimensional two-qudit Hilbert space—the highest dimension achieved for frequency bins—was reconstructed. The next focus is deploying these entangled photon sources within Oak Ridge National Laboratory's quantum local area network to implement diverse quantum communication protocols. Additionally, parallelizing Bayesian computation methods are being actively explored to expedite data analysis in this research.

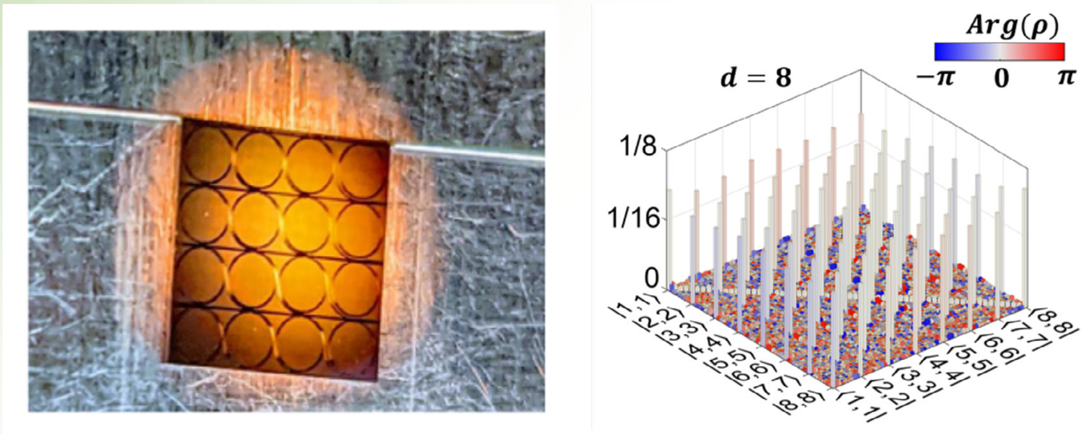


Figure 2. (Left) Microscope image of the silicon nitride microring resonators. (Right) Retrieved mean density matrices for dimensions $d = 8$. Figure is from H.-H. Lu et al. (2022) and is covered by Creative Commons BY license.

Jane Chen

Tunable Superconductivity in Hybrid Interface $FeTe_{1-x}Se_x/Bi_2Te_3$

An-Hsi (Jane) Chen, Quantum Heterostructures Group, Foundational Materials Science Section, Materials Science and Technology Division

Big Science Problem
Superconductivity in a heteroepitaxial thin film was tailored.

Motivation
The hybrid interfaces of topological insulators and s-wave superconductors are considered great candidates for realizing Majorana bound states in the context of quantum computing. Much material combination is reported, such as iron-based superconductor/topological insulator $FeTe_{1-x}Se_x/Bi_2Te_3$.

Tools
Molecular beam epitaxy (MBE), x-ray diffraction (XRD), a physical properties measurement system, and the Spallation Neutron Source were used.

Results, Conclusions, and Future Work
Superconductor-topological insulator hetero thin films were systematically investigated. Changing the Te/Se flux ratio in MBE enabled the critical temperature (T_c) of $FeTe_{1-x}Se_x/Bi_2Te_3$ thin films to be tuned. The ultrahigh vacuum system (<10^{-9} torr) of MBE protects thin film growth from most contamination, resulting in epitaxial hybrid interfaces. Figure 1 shows the crystalline structure and transport properties studies of $FeTe_{1-x}Se_x/Bi_2Te_3$ thin films. In Figure 1(a), the out-of-plane XRD shows that (00L)$FeTe_{1-x}Se_x$ grows epitaxially on (00L)Bi_2Te_3 (red dashed lines). The (00L)$FeTe_{1-x}Se_x$ peaks shift toward the right as the Se concentration increases (from $x = 0.00$ to 0.25). Figure 1(b) shows low-temperature transport measurements on thin films with different Se concentrations. Figure 1(c) shows that as X% increases, the T_c increases and then decreases, similar to the results expected in a bulk $FeTe_{1-x}Se_x$ crystal. The maximum $T_{c,max}$ = 13 K appears around X% ~ 40. This work will reveal the role of the Se and $FeTe_{1-x}Se_x/Bi_2Te_3$ interface in this hetero thin film, which may become a robust platform for realizing advanced quantum devices.

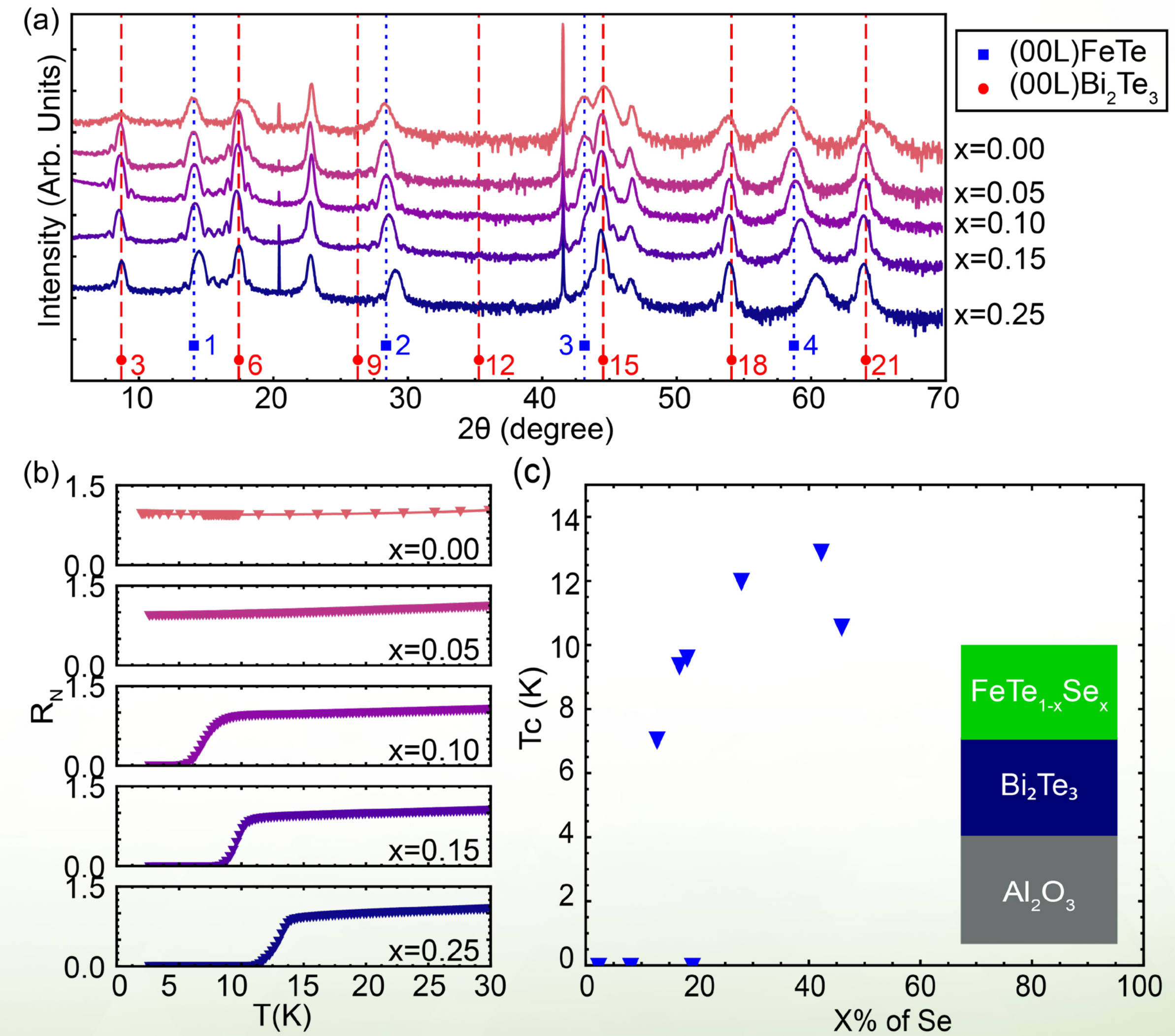


Figure 1. (a) Out-of-plane XRD scanning of $FeTe_{1-x}Se_x/Bi_2Te_3$ thin films. **(b)** Normalized resistance R_N versus temperature. **(c)** T_c versus X% of Se in hybrid-thin films. T_c is defined with 50% of R_{max}. Inset is sample stacking, Al_2O_3(substrate)/Bi_2Te_3/ $FeTe_{1-x}Se_x$ from bottom to top. (Credit: J. Chen)

Jayanthi Kumar

A Thermodynamic Exploration of the Impact of Anions on Delithiation in Layered Double Hydroxides

Jayanthi Kumar, Nanomaterials Chemistry Group, Separations and Polymer Chemistry Section, Chemical Sciences Division

Big Science Problem

This study investigated the effect of anions on the delithiation of (Li-Al) layered double hydroxides (LDHs) and provided thermodynamic insights.

Motivation

LDHs have recently been demonstrated to be promising sorbent materials for selective lithium extraction and recovery from geothermal brine. Based on the choice of the anion and the amount of water in the interlayer, the delithiation behavior varies. The thermodynamic stability of LDHs depends on the strength of the bond between the metal hydroxide layer and the anion in the interlayer. Therefore, it is important to determine the thermodynamic stability of a given LDH and compare it with that of different anions in the interlayer.

Tools

This study used an Empyrean x-ray diffractometer from Pan Analytical, PerkinElmer Frontier Fourier transform infrared spectroscopy, a Q-50-1665 TA analyzer (TA Instruments), and an iCAP PRO (Thermo Scientific) inductively coupled plasma optical emission spectrometer.

Publications

K. Jayanthi, M. P. Paranthaman, B. T. Manard, and A. Navrotsky, "Effect of Anions on the Delithiation of (Li-Al) Layered Double Hydroxides: Thermodynamic Insights," *J. Phys. Chem. C* (2023) (manuscript submitted).

Results, Conclusions, and Future Work

The findings of this research illustrate that the anions that form strong hydrogen bonds with the interlayer water and the hydroxyl group of the layer are a crucial factor underlying the stability of a given LDH. Significant work in this direction can potentially serve in tailoring LDH structures with specific compositions that have implications for their lithium extraction capabilities and subsequent recovery.

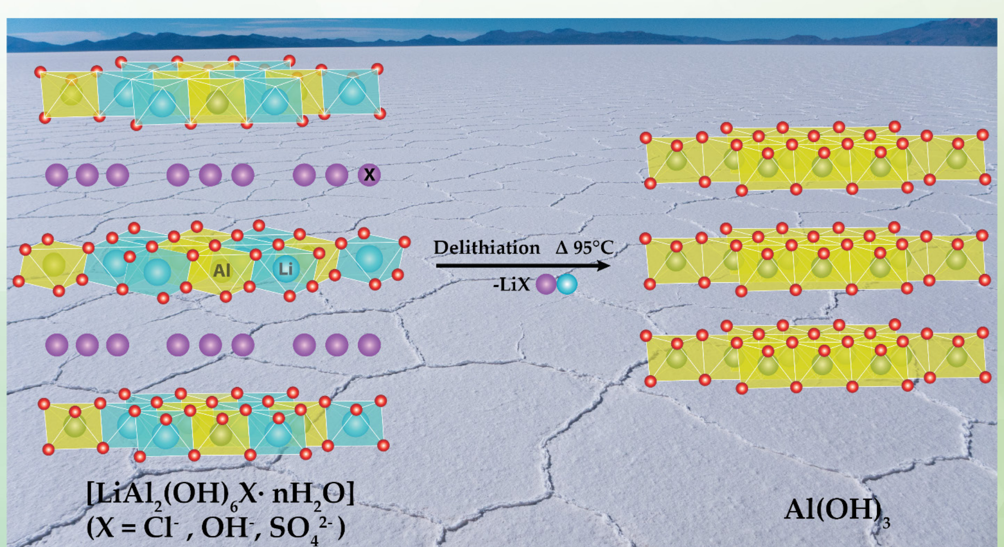


Figure 1. Structural transformation of gibbsite-based (Li-Al) LDH to parent gibbsite phase on delithiation. (Credit: J. Kumar)

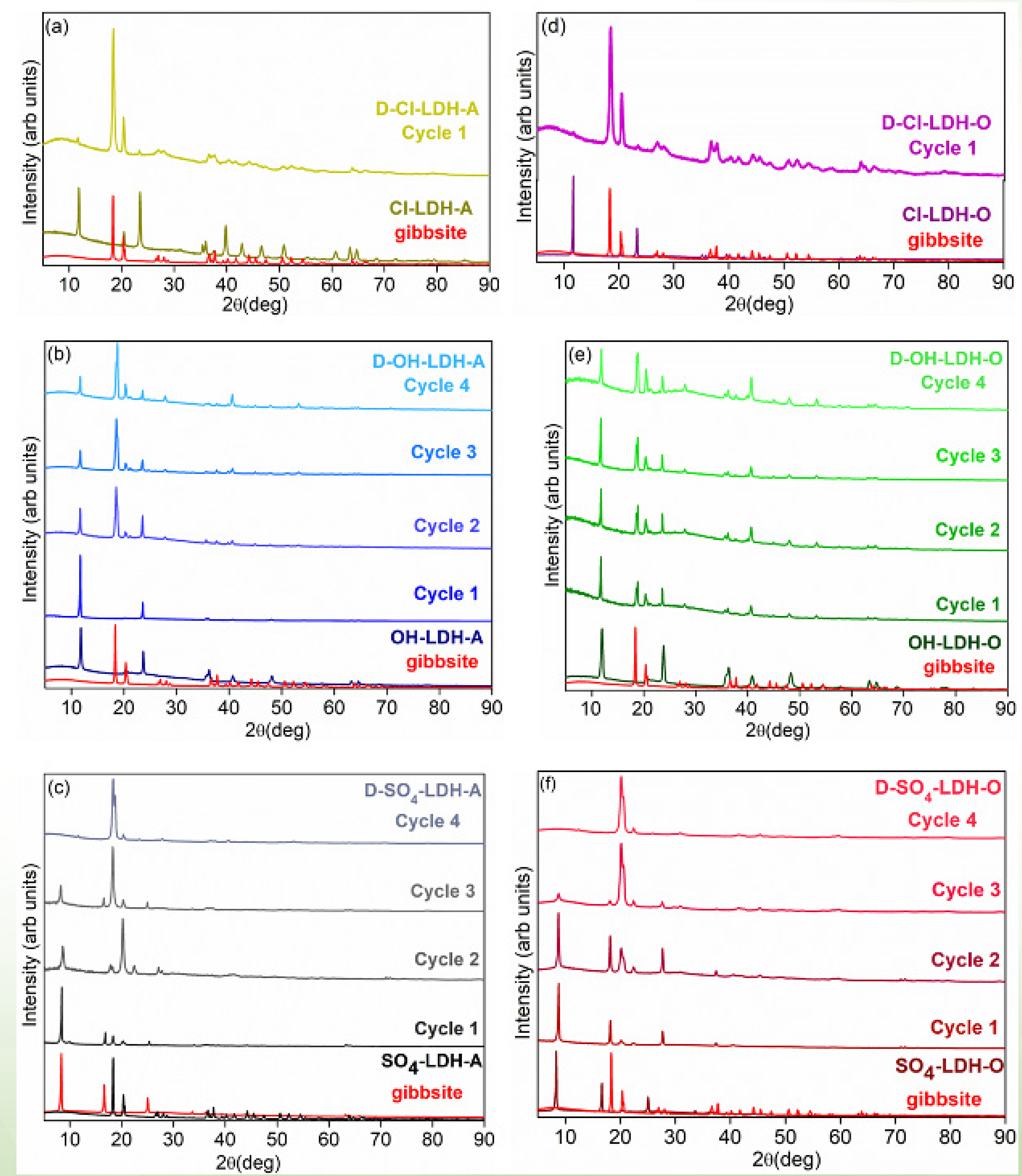


Figure 2. Powder x-ray diffraction patterns for the delithiation cycles: (a) Cl-LDH-A, (b) OH-LDH-A, (c) SO_4-LDH-A, (d) Cl-LDH-O, (e) OH-LDH-O, and (f) SO_4-LDH-O. (Credit: J. Kumar)

Jopaul Mathew

Toward Maximizing Uranium Recovery: Extractants for Amplified Separation of U and Pu

Jopaul Mathew, Chemical Separations Group, Separation and Polymer Chemistry Section, Chemical Sciences Division

Big Science Problem

Spent nuclear fuel (SNF) reprocessing is vital for nuclear waste management and expanding nuclear power to produce electricity. The Material Recovery and Waste Form Development initiative within the US Department of Energy's Office of Nuclear Energy aims to simplify and reduce costs for future recycling. They are working on developing an efficient U recycling method, like the PUREX process, which uses tri-n-butyl phosphate (TBP) to recover U/Pu from SNF. TBP's drawbacks include not following the CHON principle and being prone to radiation-induced degradation.

Motivation

Some of these difficulties have been resolved by using monoamides in the Group Actinide Extraction (GANEX-I) process (Figure 1). Nitric acid is commonly and significantly consumed in these two processes. Among different monoamides, *N,N*-bis(2-ethylhexyl)isobutyramide (DEHiBA) yields efficient U/Pu separation. The structure of the monoamide, specifically the size of the alkyl R groups, plays a significant role. Research aims to determine ideal alkyl size through structure–activity relationships. This study focuses on developing novel monoamide ligands, optimizing R group lengths and branches for enhanced U/Pu separation performance.

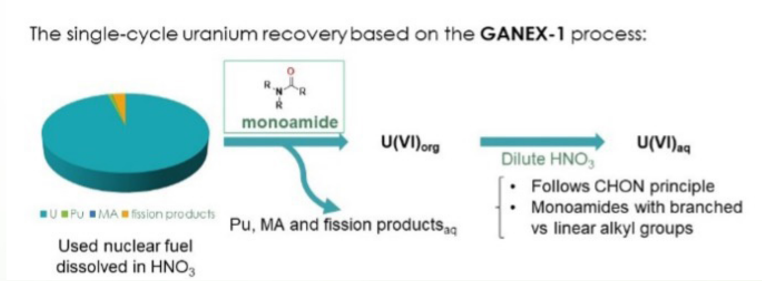


Figure 1. GANEX-I process. (Credit: S. Jansone-Popova)

Tools

The synthesis, purification, and characterization were accomplished in wet laboratories at Oak Ridge National Laboratory (Figure 2). Extraction studies were conducted at Idaho National Laboratory.

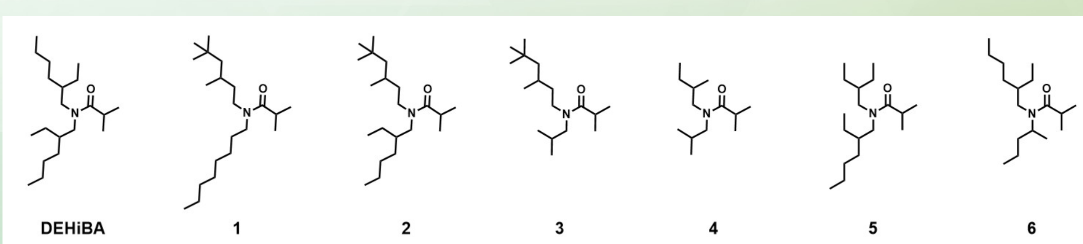


Figure 2. DEHiBA and monoamides synthesized. (Credit: J. Mathew)

Results, Conclusions, and Future Work

Of all the monoamides synthesized, 1–4 showed higher extraction of U(VI) than did DEHiBA. But the reduced steric hindrance around the metal ion binding site led to more Pu(IV) being extracted as well. Third-phase formation was observed for ligands 3 and 4 because of the reduced lipophilicity of the ligand-metal complexes. The purity of the ligands affects U(VI)/Pu(IV) separation. For example, even trace amounts of impurities—such as the secondary amine, which is used as a starting material—result in increased extraction of Pu(IV). Ligands 5 and 6 showed improved or comparable selectivity compared with DEHiBA. In the future, the extraction of U(VI) by monoamides will be quantified using spectroscopic methods such as ultraviolet-visible spectroscopy. Structure–activity relationship studies to uncover monoamides with optimal properties to maximize U separation will continue.

Małgorzata Makoś

Reaction Pathways Search Using Global Optimization and Machine Learning Algorithms

Małgorzata Z. Makoś, Nanomaterials Chemistry Group, Separations and Polymer Chemistry Section, Chemical Sciences Division

Big Science Problem

Computational simulations have become essential for understanding reaction mechanisms, identifying optimal catalysts, and designing materials. However, even with existing capabilities, reaction pathways are explored manually based on known experimental and theoretical facts, often in a trial-and-error fashion. The problem grows exponentially with system size because of the increasing number of low-energy isomers and intermediates. Additionally, locating transition states along reaction paths constitutes a computational challenge on its own. Exploring the kinetics associated with real chemical problems also depends on knowing the reaction paths and transition states, not only of one set of reactions but also of ensembles of many that may occur at experimentally relevant conditions.

Motivation

To overcome these limitations, this research aims to develop advanced computational methods that can efficiently and comprehensively explore chemical reactions.

Tools

This research has been made possible and advanced in large part by computational resources like CADES at Oak Ridge National Laboratory and the National Energy Research Scientific Computing Center (NERSC), which have played an essential part in enabling and advancing this project.

Publications

M.Z. Makoś, N. Verma, E.C. Larson, M. Freindorf, and E. Kraka, "Generative Adversarial Networks for Transition State Geometry Prediction," *J. Chem. Phys.* 155(2) (2021). doi.org/10.1063/5.0055094.

Results, Conclusions, and Future Work

This work primarily focused on developing an automated method integrating a global optimizer and a machine learning algorithm that enabled efficient exploration of a given potential energy surface and identification of possible reaction pathways. The global optimizer used in this research was highly beneficial for identifying low-energy minima in large systems containing around 10^2–10^3 atoms. The algorithm facilitates the generation of initial structures, determines the most favorable global minimum, and provides a comprehensive set of reactants and products. The global optimization procedure was leveraged with the power of generative adversarial networks (GANs) to predict transition states. GANs have demonstrated remarkable success in predicting the transition states and determining complex networks across possible reaction pathways. Utilizing GANs enables effective navigation of the intricate landscape of reaction mechanisms and enables insights into the various possible routes.

The approach has been highly successful in identifying the mechanisms of various chemical reactions, particularly those involving heavy elements and surface reactions. Notable results have been achieved in several cases, such as O_2 adsorption on graphene, in which the method used accurately determines the starting materials that result in specific products and provides reliable energy barriers for 12 viable reactions. This method also showed promise in studying the UO_2 insertion reaction in a Pt-crown complex for selective uranyl separations.

This research has potential for discovering new reactions, predicting novel structures, and extracting generalized system descriptors, which are crucial for enhanced sampling and free-energy methods.

Meijia Li

Mechanochemistry-Induced Strong Metal–Support Interactions Construction Toward Enhanced Catalysis

Meijia Li, Nanomaterials Chemistry Group, Separations and Polymer Chemistry Section, Chemical Sciences Division

Big Science Problem

Noble-metal catalysts on transition metal oxide supports face deactivation issues during long-term service.

Motivation

The development of approaches capable of inducing strong metal–support interaction (SMSI) constructions under ambient conditions is still at the preliminary stage and facing the limitations on support materials, fabrication methods, and complex experimental procedures. The goals of this research are to (1) develop facile approaches capable of controllable construction of SMSI overlayers, particularly under ambient and neat conditions, and (2) customize the overlayer structures and the degree of encapsulation to enhance catalysis over diverse support structures.

Approach

A facile and efficient mechanochemistry-driven approach was undertaken to address obstacles to producing stable catalysts. The approach enables strong metal-support interaction (SMSI) constructions to be fabricated over heterogeneous catalysts by a neat process under ambient conditions.

Tools

Diffuse reflectance infrared Fourier transform spectroscopy and gas-phase hydrogenation tests were conducted as part of a user project at the Center for Nanophase Materials Sciences, which is a US Department of Energy Office of Science user facility at Oak Ridge National Laboratory.

Publications

M. Li, T. Zhang, S. Yang, Y. Sun, J. Zhang, F. Polo-Garzon, K. M. Siniard, X. Yu, Z. Wu, D. M. Driscoll, A. S. Ivanov, H. Chen, Z. Yang, and S. Dai, "Mechanochemistry-Induced Strong Metal-Support Interactions Construction toward Enhanced Hydrogenation," *ACS Catal*. 13, 6114–6125 (2023).

Results, Conclusions, and Future Work

A facile and efficient mechanochemistry-driven approach was developed for SMSI construction under neat and ambient conditions to enable modification of structural and electronic properties of supported metal nanocatalysts and thus to improve stability and enhance catalysis (Figure 1). The initial study on the $NaBH_4$-assisted mechanochemical treatment of Pd/TiO_2 (anatase) revealed that the combined benefits from reducibility of the additive and the high interaction efficiency endowed by the mechanochemical treatment could rapidly afford abundant active intermediates, Ti^{3+}, and oxygen vacancies within the scaffolds to induce the formation of an SMSI overlayer. The degree of encapsulation can be tuned and controlled by varying the reducibility of the additives and the mechanochemical treatment parameters. This approach could be further extended to supported Pd nanoparticles on TiO_2 with diverse phases (anatase, rutile, and mixed counterpart), diverse reducible metal oxide–involved nanocatalysts (ZnO, CeO_2, Fe_3O_4, and Nb_2O_5), and different supported noble metal nanoparticles (Pd, Ru, and Pt). The enhanced hydrogenation activity of the nanocatalysts was achieved upon SMSI overlayer construction by tuning the electronic properties of the cores of the noble metal nanoparticles, which, conversely, could be further regulated by applying a mechanochemical treatment to control the degree of encapsulation.

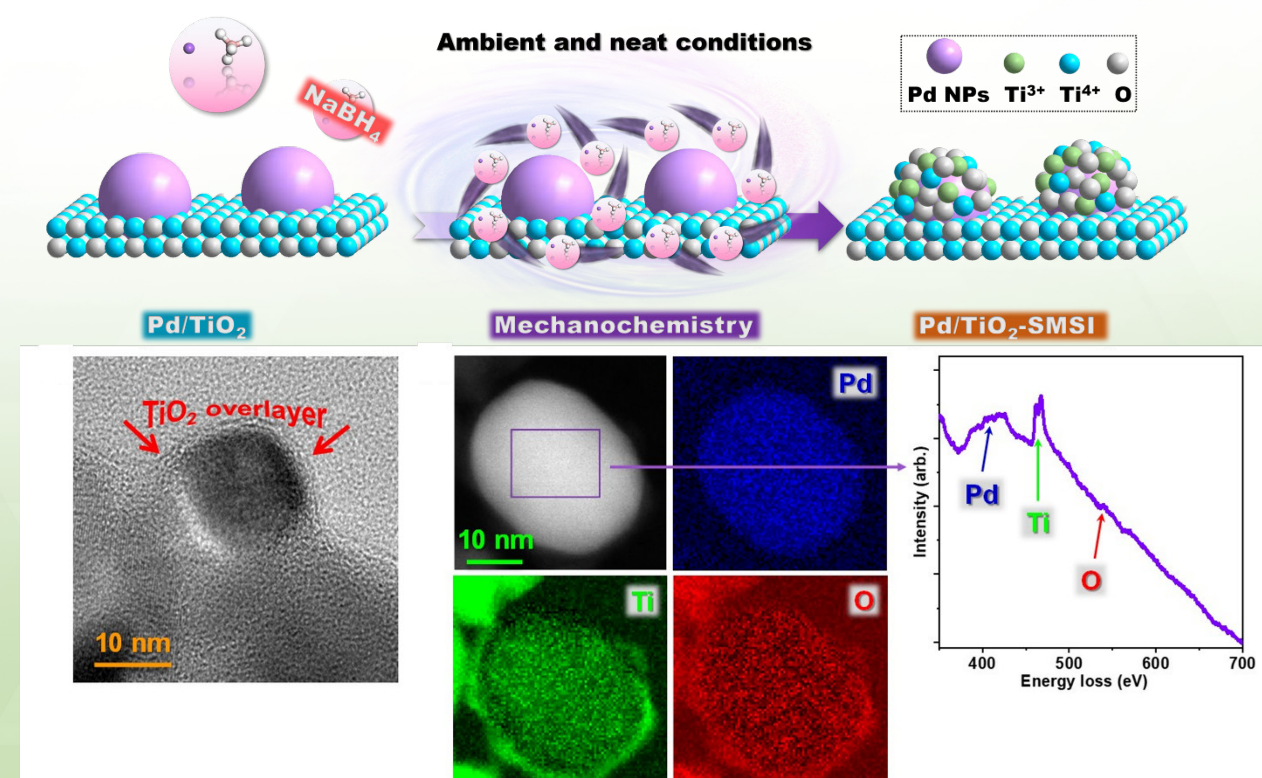


Figure 1. Top: Schematic illustration of mechanochemistry-induced strong metal-support interaction (SMSI) construction of Pd/TiO_2 in the presence of $NaBH_4$. **Bottom**: Spectroscopic characterizations of a Pd/TiO_2-SMSI construction. **Bottom left**: High-resolution transmission electron microscopy image. Bottom center: Scanning transmission electron microscopy annular dark-field images featuring an encapsulated Pd nanoparticle. **Bottom right**: A corresponding electron energy loss spectroscopy curve. Figure is from Li et al. (2023) and used by permission of the American Chemical Society.

Ritin Mathews

Prediction and Mitigation of Distortion during Machining of Aerospace Components

Ritin Mathews, Intelligent Machine Tools Group, Precision Manufacturing and Machining Section, Manufacturing Science Division

Big Science Problem

Was the wheel an invention out of necessity? Or was it a serendipitous discovery? As the most intelligent beings on planet Earth, humans' endeavor to satisfy curiosity and enhance convenience gave rise to a world in which creations are approaching intelligence levels of the creators. However, the technological journey that led to these achievements was challenging and had unintended consequences. Following the industrial revolution, the development of weaponized automobiles, tanks, and ships in the early twentieth century, fueled by human greed, gave rise to the first world war. Shortly after, the proliferation of weaponized aircrafts and advanced destructive technologies initiated World War II, which saw the greatest death toll of any human conflict in history. If the trend had continued, then even deadlier wars, greater casualties, and possibly a lifeless planet would have resulted. But experience triggered the epiphany that perhaps there is no winner in conflict. Proponents of pacifism, nonproliferation of weapons of mass destruction, and unity soon prevailed. At present, science and engineering strive to improve global security, safety, and lifestyle. However, despite global efforts, a disconnect between advanced prototypical designs and practically manufacturable components still exists.

Motivation

The manufacturing science research performed at the Manufacturing Demonstration Facility (MDF) aims to develop new technologies, improve existing technology, and build stability in manufacturing in the United States. The various collaborative and consolidated teams at MDF conduct experimental and computational research on conventional and emerging manufacturing technologies involving metallic, plastic, and ceramic materials.

Tools

This research consists of computationally modeling manufacturing techniques to elucidate fundamental material behavior, assist experimental analyses, and design practical concepts for the next generation of manufacturing machines. Specifically, finite element technique is employed to investigate the influence of mechanically and thermally induced stresses during machining (milling) of monolithic aerospace components. Measurement and reconstruction of material-inherent residual stress, high-fidelity modeling of end-milling process, and their experimental counterparts are involved in this work. This effort can be extended to other subtractive manufacturing processes (e.g., drilling, turning), additive manufacturing techniques (powder/wire based), hybrid (combination of additive and subtractive), and forming (shaping, forging, etc.) techniques. A wide range of equipment at the MDF, machine tools at the Oak Ridge National Laboratory main campus, the VULCAN neutron scattering instrument at the Spallation Neutron Source, and several other resources are used to assist the work.

Publications

R. Mathews, S. Sunny, A. Malik, and J. Halley, "Coupling between Inherent and Machining-Induced Residual Stresses in Aluminum Components," *Int. J. Mech. Sci.* 213, 106865 (2022).

R. Mathews, K. M. Nagaraja, R. Zhang, S. Sunny, H. Yu, D. Marais, A. Venter, W. Li, H. Lu, and A. Malik, "Temporally Continuous Thermofluidic–Thermomechanical Modeling Framework for Metal Additive Manufacturing," *Int. J. Mech. Sci.* 254, 108424 (2023).

Contributions include more than 15 journal papers pertinent to manufacturing technology and innovation. Stand-out published works include development of a computational reconstruction and modeling technique of residual stress in wrought and additively manufactured metals, a high-fidelity machining model elucidating the coupling of inherent and machining-induced stresses, and a thermomechanical-thermofluidic model for directed energy deposition additive manufacturing. Contributions also include modeling of laser impact welding, metal rolling mill dynamics, roller burnishing, selective laser melting/sintering additive manufacturing, and microstructure evolution.

Results, Conclusions, and Future Work

Existing research suggests that conventional processes can be improved by further study of influential factors affecting production rate, material wastage, part quality, and energy consumption. Results show that inherent residual stress plays a role in distortion of machined components, albeit not as significant as machining-induced stress. The nonlinear coupling between the two, which depends on the process conditions, parameters, tool, and tool path used, is a challenge to model and predict. Work is now underway to mitigate the net adverse effects of stresses in components. Developing improved manufacturing techniques and machines, exploiting the strengths of various existing processes, and addressing their limitations would significantly enhance the state of manufacturing. This research also supports the national interest of increasing domestic manufacturing and self-reliability to improve national defense, space transportation, and general quality of life in the United States. Furthermore, the next generation of the manufacturing industry is committed to environmental sustainability and reduced emissions, thus assisting in averting a climate crisis.

Technological advances in recent years have propelled the development of previously unimaginable digital equipment, medicines, and human-like artificial counterparts. Twenty-first century technology, contrary to prior times, generates a sense of unity and protection among the human population. Consensus now holds that there exists no logical rationale for conflict and destruction; rather survival of the human species depends on cooperation and persistence. Perhaps the wheel was in fact an invention—one that set the ball rolling toward serendipity.

Sandeep Kaur

Can We Capture Forever Chemicals?

Sandeep Kaur, Chemical Separations Group, Chemical Sciences Division, Physical Science Directorate

Big Science Problem

This research effort, supported by the DOE Basic Energy Sciences program, focused on anion sequestration in aqueous media using ionic covalent organic frameworks (iCOFs). The challenging and novel part of the research involved the development of materials that can selectively capture anions that belong to the family of forever chemicals, or polyfluoroalkyl substances (PFAS). These persistent chemicals are commonly found in household items—for instance, nonstick cookware, firefighting foams, and even water.

Motivation

The Environmental Protection Agency has ranked PFAS as a possible human carcinogen. Once they enter the human body through air, water, or food, it is impossible to remove them. This is why they are called *forever chemicals*. Reducing PFAS contamination in the environment is the grand challenge.

Tools

To pursue the experiments, an AVANT ultra-high performance liquid chromatography ([U])HPLC) instrument was used, which provided simple, high-performance liquid chromatography with an Advion compact mass spectrometer (LC/CMS).

Results, Conclusions, and Future Work

A method was developed that uses (U)HPLC mass spectrometry to quantify the uptake capacity of PFAS within the pores of iCOFs. Through the incorporation of extended lipophilic regions in iCOFs, these networks exhibited enhanced sequestration efficiency for these harmful pollutants. The newly synthesized iCOFs are porous and incorporate functional groups that show strong affinity such as hydrogen bond as well as ionic interactions for PFAS. These materials hold great promise for effectively removing hazardous contamination from water sources. The iCOFs were able to trap PFAS even at very low concentrations, so nearly all the toxic chemicals could be removed from water. See Figures 1 and 2. The success of this project will have a profound impact on both the environment and health by removing forever chemicals.

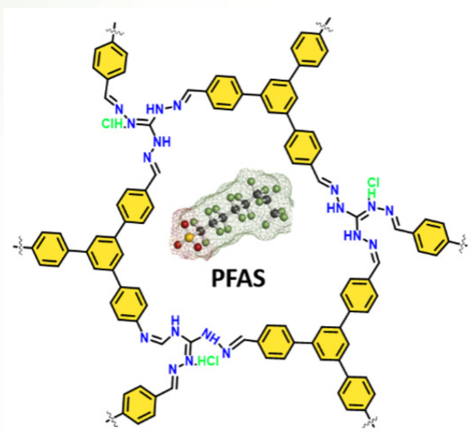
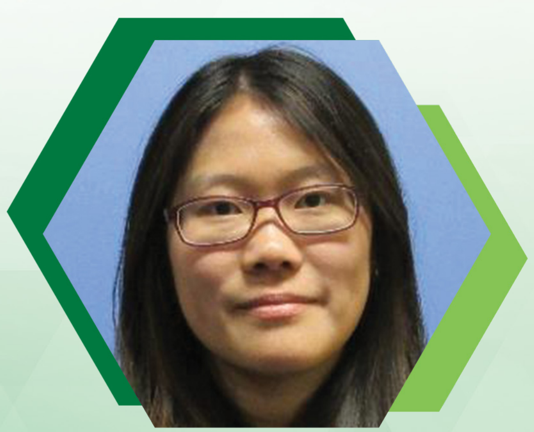


Figure 1. Porous adsorbent (i-COF) filters out nanosized contaminants (PFAS) to clean drinking water. (Credit: S. Kaur)

Figure 2. The AVANT (U)HPLC with the expression compact mass spectrometer for a seamlessly integrated, complete LC/CMS solution. (Credit: S. Kaur)



Su-Ann Chong

Microchannel Plates with Quad Timepix3 Detector (MCP/TPX3) for Time-of-Flight Neutron Imaging

Su-Ann Chong, Detectors Group, Neutron Instrument Technologies Section, Neutron Technologies Division

Big Science Problem

The Versatile Neutron Imaging Instrument (VENUS) under construction at the Spallation Neutron Source (SNS) will feature time-of-flight (TOF) neutron imaging enabled by the 60 Hz pulsed beam accelerator of the SNS. Compared with traditional neutron imaging, TOF neutron imaging provides additional information about the energy of the neutrons that interact with the sample. Utilizing the energy-dependence behavior of neutrons, more advanced neutron imaging techniques such as Bragg-edge imaging, resonance imaging, and stroboscopic imaging are possible. TOF-capable neutron imaging enables mappings of compositional and structural (phase, strain, and texture) variation and imaging of phase transformation and dynamic processes in materials.

Motivation

To enable TOF neutron imaging, synchronization of the imaging instrument with the pulse generation is necessary. A TOF-capable neutron imaging camera is a crucial component in time-tagging the arrival times of neutrons from source to detector. The primary focus of this work is on developing a TOF-capable neutron imaging camera with a high spatial resolution and rate capability. The detector developed for VENUS to perform TOF neutron imaging consists of a pair of chevron-stacked microchannel plates (MCPs) coupled to a quad Timepix3 (TPX3) readout in a vacuum enclosure. It follows the principle developed by A. Tremsin [1] but replaces the previous generation frame–based Timepix chips with the latest data-driven TPX3 chips (Figure 1).

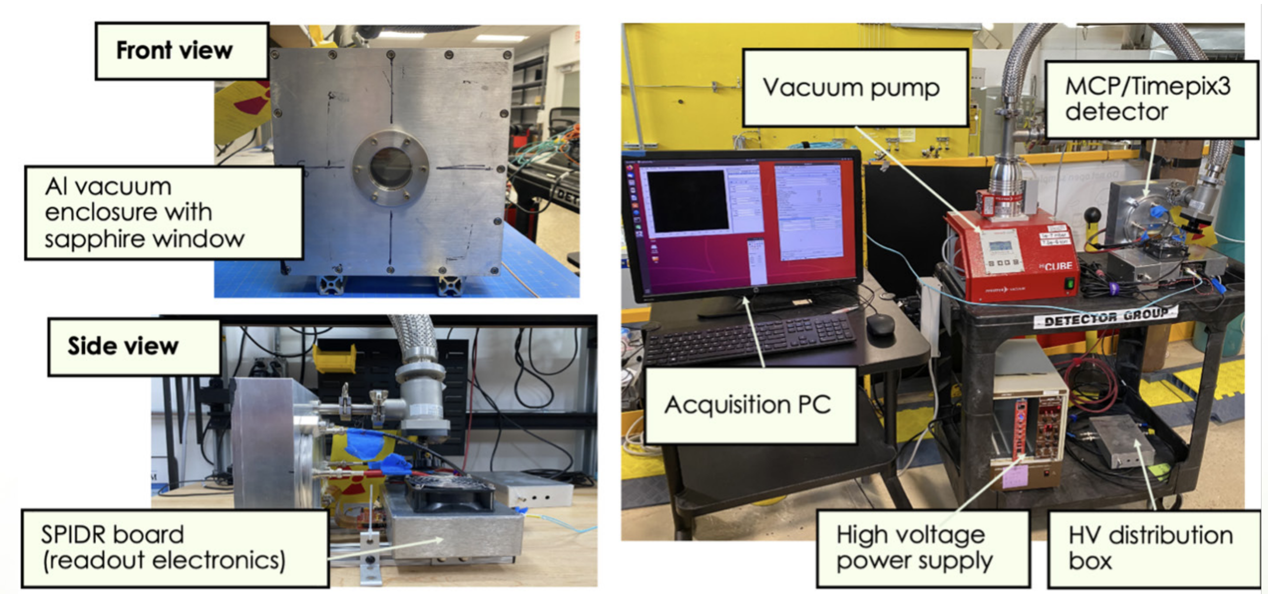


Figure 1. The chevron-stacked MCPs and quad TPX3 chips are inside the aluminum vacuum enclosure with a sapphire window. The TPX3 readout comes with its associated readout electronic and acquisition software. The vacuum pressure is constantly kept around ≤ 1×10^{-6} torr. (Credit: S.-A. Chong)

Tools and Results

The MCP/TPX3 detector was used to perform Bragg-edge imaging at the Spallation Neutrons and Pressure Diffractometer (SNAP) at the SNS to test its TOF capability. A nickel powder sample was placed in front of the MCP/TPX3 detector. Figure 2 shows the Bragg edges featuring the crystallographic planes hkl of nickel. By analyzing the Bragg edges in the spectrum, the crystal structure and defects in the material being imaged can be studied. In the same experiment, a spatial resolution mask was used to quantify the spatial resolution of the detector, as shown in Figure 3.

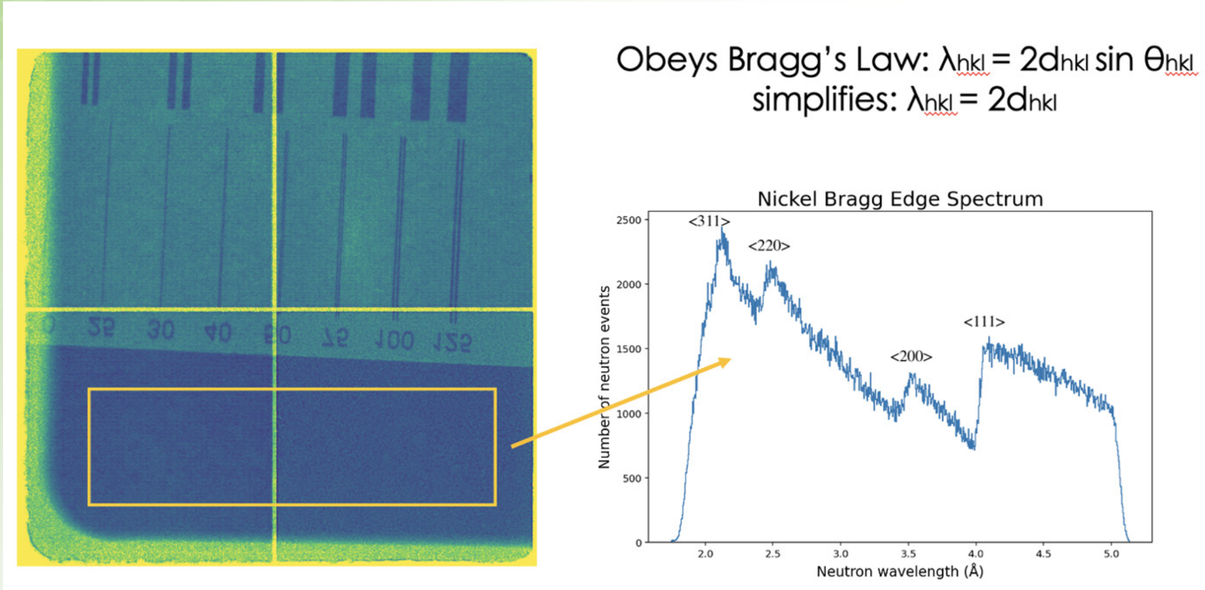


Figure 2. Bragg-edge spectrum shows the crystallographic planes hkl of nickel within the range of neutron wavelength from 1.842Å to 5.139Å. The wavelength resolution corresponds to a time resolution of ≤1 µs. (Credit: S.-A. Chong)

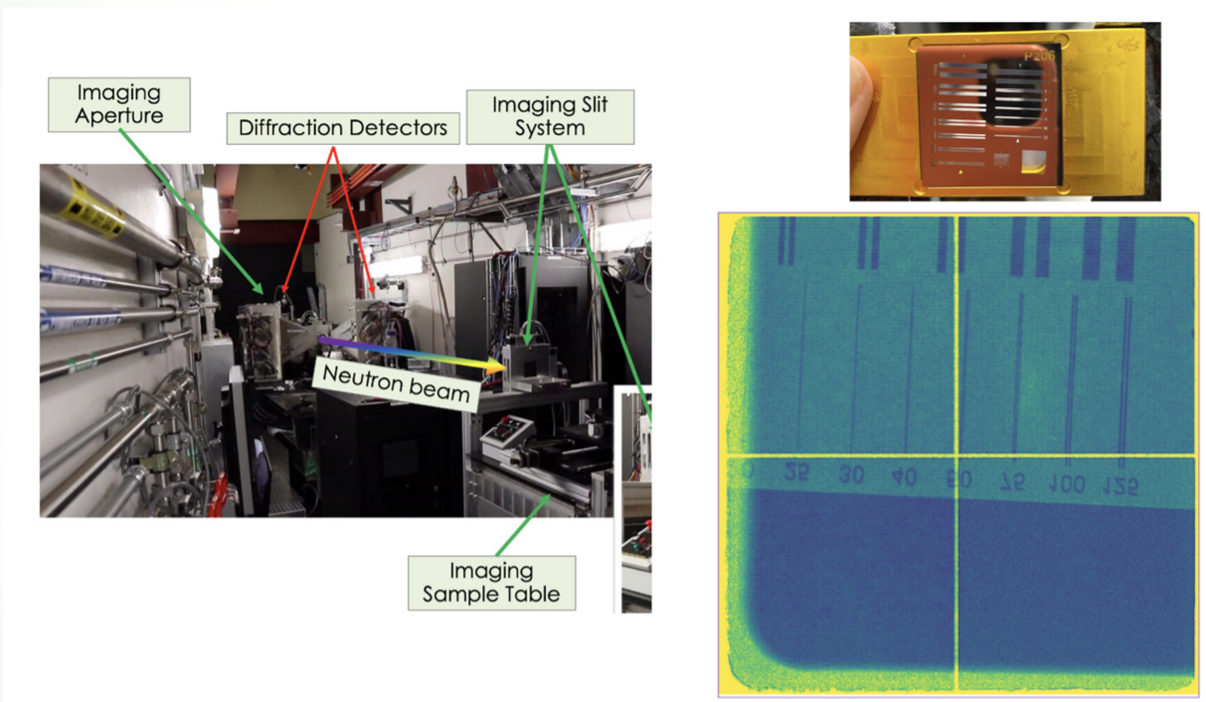


Figure 3. The detector also demonstrated a spatial resolution of sub-75 µm using an Inconel linepair mask (shown top right) at the SNAP (shown at left). (Credit: S.-A. Chong)

Conclusion and Future Work

The MCP/TPX3 detector is a promising detector candidate for VENUS because it has demonstrated TOF imaging with a time resolution of ≤1 µs, sub-75 µm spatial resolution and a rate capability of ≤120 Mhits/s. Future work will include exploring and benchmarking different clustering algorithms to improve the neutron-gamma discrimination of the detector.

Publications

Tremsin, Anton S., W. Bruce Feller, and R. Gregory Downing. "Efficiency optimization of microchannel plate (MCP) neutron imaging detectors. I. Square channels with 10B doping." *Nucl. Instrum. Meth. A* 539.1-2 (2005): 278–311.

Subhamay Pramanik

Electrifying Rare Earth Elements Separation

Subhamay Pramanik, Nanomaterials Chemistry Group, Separations and Polymer Chemistry Section, Chemical Sciences Division

Big Science Problem

How can rare earth elements (REEs) be selectively separated using an environmentally friendly approach?

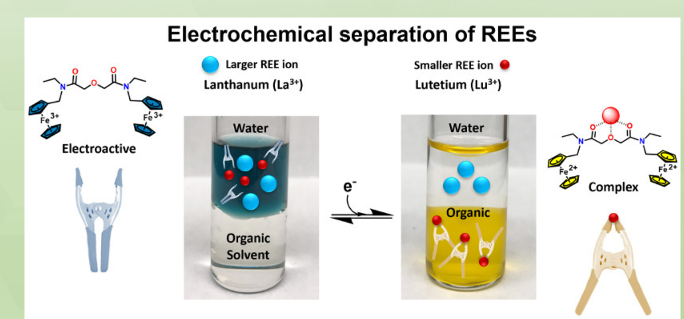
This research mostly involved working on the Transforming Critical Materials Separation Using Precision Control project supported by the Basic Energy Sciences program. The overarching goal was to develop novel organic materials for the environmentally friendly separation of REEs. Conventional acid extractions increase the cost of separation and resources, and the corrosive waste produced damages the environment. Because of these challenges, no environmentally friendly separation strategy exists at the industrial scale. Thus, to establish domestic production, an eco-friendly and sustainable separation method is being developed at Oak Ridge National Laboratory using an electrochemical separation strategy.

Motivation

The REEs considered include yttrium, scandium, and 4f-block elements (lanthanides from lanthanum to lutetium). These are crucial to modern life and technological advancement. They have been widely used in wind turbines, permanent magnets, electric vehicles, radiopharmaceutical therapy, cell phones, and other renewable energy resources. Because the ionic radii of REEs are very similar—having differences between La^{3+} and Lu^{3+} of less than 0.2 Å—separating individual elements in the pure stream is extremely challenging (Figure 1a). Conventional industries implement liquid–liquid extraction techniques that produce thousands of tons of corrosive acid waste along with environmentally harmful waste, and these extractions must be repeated hundreds of times to produce high-purity REEs. Liquid–liquid extractions also release tons of radioactive waste, hazardous dust, and water pollutants.

	Light REEs						Medium REEs				Heavy REEs				
REEs	Lan-thanum 57 La 138.91	Cerium 58 Ce 140.12	Praseo-dymium 59 Pr 140.91	Neo-dymium 60 Nd 144.24	Prome-thium 61 Pm [145]	Sama-rium 62 Sm 150.36	Europ-ium 63 Eu 151.96	Gadolin-ium 64 Gd 157.25	Ter-bium 65 Tb 158.93	Dyspro-sium 66 Dy 162.50	Hol-mium 67 Ho 164.93	Erbium 68 Er 167.26	Thulium 69 Tm 168.93	Ytter-bium 70 Yb 173.05	Lute-tium 71 Lu 174.97
Ionic radii (Ln^{3+}), Å	1.16	1.14	1.13	1.11	1.09	1.08	1.07	1.05	1.04	1.03	1.02	1.00	0.99	0.99	0.98

a.



b.

Figure 1. (a) Series of REEs (lanthanides) with ionic radii; **(b)** electrochemical separation method. (Credit: Adapted from Wikipedia, "Lanthanide," https://en.wikipedia.org/wiki/Lanthanide)

Tools

Flash column chromatography was used for purification of organic compounds. Additionally, an Advion mass spectrometer, a Bruker Avance III 400 MHz nuclear magnetic resonance spectrometer, a ThermoFisher Scientific iCAP triple quadrupole inductively coupled plasma mass spectrometer, a PerkinElmer Frontier Fourier transform infrared spectrometer, and an AVANT ultra-high performance liquid chromatography instrument were used.

Results, Conclusions, and Future Work

The technology being developed in this research could become the first green separation technology using colorimetric and phase-switchable electroactive material for the separation of REEs (Figure 1b).

Tomas Grejtak

Enhancing Performance and Durability of Biomass Preprocessing Equipment by Applying Advanced Blade Materials

Tomas Grejtak, Surface Engineering and Tribology Group, Materials Structure and Processing Science Section, Materials Science and Technology Division

Big Science Problem

Advanced blade materials were used to improve the efficiency and durability of biomass preprocessing tools.

Motivation

Biomass is a renewable source of energy that has the potential to positively impact environmental sustainability and reduce dependency on fossil fuels. Mechanical preprocessing of biomass, including size reduction, is an important step in converting biomass into biofuel. One of the biggest challenges facing the mechanical preprocessing of biomass is excessive damage and wear of the cutting tools caused by hard inorganic contaminants contained in biomass feedstocks, which negatively impacts the cost of the milling and quality of the biomass product. Improving the performance of biomass size-reduction equipment is critical to the overall bioenergy economics and in line with the mission of the US Department of Energy.

Tools

The multiscale mechanical characterization involved tribological (wear and friction) and hardness testing, and the morphological analysis involved scanning electron microscopy and energy-dispersive x-ray spectroscopy.

Publications

T. Grejtak, J. A. Lacey, M. W. Kuns, D. S. Hartley, D. N. Thompson, G. Fenske, O. O. Ajayi, J. Qu, "Improving Knife Milling Performance for Biomass Preprocessing by Using Advanced Blade Materials," *Wear* 522, 204714 (2023).

Results, Conclusions, and Future Work

The collaborative research efforts demonstrated that applying wear-resistant blade materials improves the durability and performance of a knife mill. Tungsten carbide and iron-borided candidate materials were selected through bench-scale testing and tribo-analysis. These materials were then used to fabricate cutting knives that were mounted on a knife mill. Experimental knife milling revealed that tungsten carbide and iron-borided blades improved the durability of the knife mill by 8× and 3×, respectively, in comparison with the traditionally used steel blades. The improvement in the durability of the knife mill also resulted in higher milling throughput and reduction in power consumption. The experimental results were used as inputs in a technoeconomic analysis, which demonstrated that tungsten carbide and iron-borided blades could reduce the knife milling cost by \$2–\$3 per ton of biomass processed, with downtime reduced by 65%–85%. The knowledge gained from this research is now being applied in a variety of biomass preprocessing applications. The ongoing collaborations with industry partners are focused on improving the milling efficiency of rotary shear tools and small-scale shredders. See Figure 1.

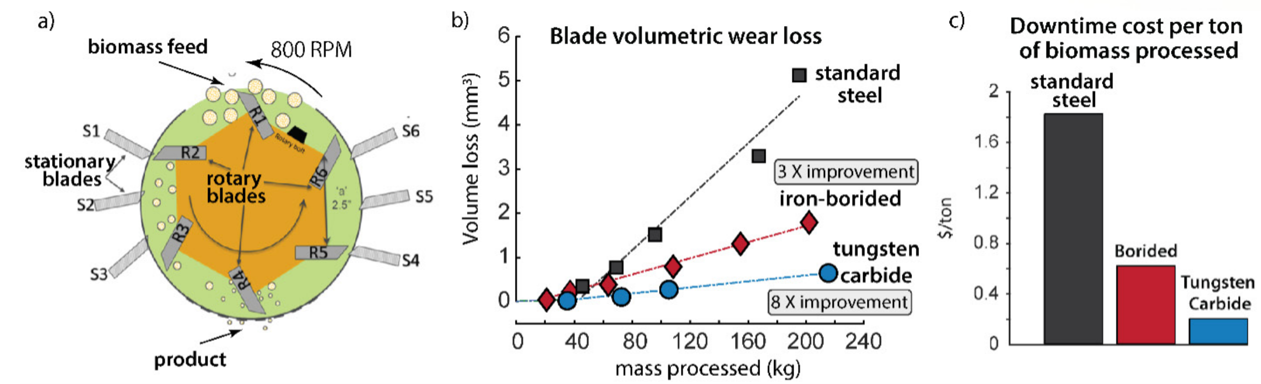


Figure 1. (a) Schematic of a milling procedure (Grejtak et al. 2023), **(b)** wear performance of different sets of blades in the knife mill tests (Grejtak et al. 2023), and **(c)** downtime cost of the milling using different blade materials. Figure 1c is used by permission of Tomas Grejtak.

Wenbo Wang

Marine Turbine Lubrication Additives: Ionic Liquids with High Lubricity and Eco-Friendliness

Wenbo Wang, Surface Engineering and Tribology Group, Materials Structure and Processing Science Section, Materials Science and Technology Division

Big Science Problem

This research focused on developing eco-friendly, high-lubricity ionic liquids (ILs) as novel additives for marine turbine lubrication.

Motivation

Tidal energy capable of generating clean and sustainable electricity through specially designed generators (e.g., turbomachinery) is a promising addition to the renewable energy portfolio. However, essential components in the tidal turbine, such as the gearbox and bearings, are susceptible to rolling contact fatigue and wear and are difficult to maintain because of the undersea environment. The conventional lubricants currently used in marine turbomachinery are toxic and exhibit low biodegradability, potentially resulting in a serious threat to marine ecosystems in the case of a leak or spill. Therefore, it is crucial to develop environmentally acceptable lubricants with high performance in wear protection.

Tools
This research used different types of tribometers, a 3D optical profiler, advanced materials characterization (e.g., scanning electron microscopy, energy-dispersive x-ray spectroscopy, focused ion beam, transmission electron microscopy, x-ray photoelectron spectroscopy), toxicity testing, and other resources.

Results, Conclusions, and Future Work
Recently, eco-friendly, high-lubricity ILs were invented at Oak Ridge National Laboratory and are being further developed for tidal turbine gearbox lubrication. Compared with commercial baseline additives, the "not toxic" and "readily biodegradable" IL-additized lubricants performed more effectively in mitigating friction, rolling contact fatigue, and wear loss, based on initial bench-scale tribological testing results.

For future work, the protection mechanisms will be investigated through surface and tribofilm characterization. Meanwhile, considering the actual working conditions of tidal turbines, the effects of marine water (including oil viscosity variation, corrosion problems) and lubricant aging on the performance of IL-additized lubricants will be studied.

ORPA Executive Committee Members

President: Indranil Roy
(October 2022–August 2023)
Indranil Roy was until recently a postdoctoral researcher in the Microstructural Evolution Modeling Group within ORNL's Materials Science and Technology Division. Indranil joined GE Global Research in September 2023. His work is primarily focused on understanding microstructure during solidification, especially in additive manufacturing. Indranil completed his PhD at Lehigh University, where he explored multiscale computational techniques to understand oxidation of compositionally complex alloys.

Vice President: Subhamay Pramanik
Subhamay Pramanik is working as a postdoctoral research associate in the Nanomaterials Chemistry Group within ORNL's Chemical Sciences Division. After receiving his PhD from Guru Nanak Dev University, in India, he spent four years as postdoctoral researcher at Kansas University. His current research focuses on the synthesis of novel and stimuli-responsive organic materials to be applied in the separation and crystallization of lanthanides.

Secretary: Briana Schrage
(October 2022–August 2023)
Briana Schrage joined the Chemical Separations Group in ORNL's Radioisotope Science and Technology Division as a postdoc in 2022, after completing her PhD in inorganic chemistry at the University of Akron and spending a year as a postdoctoral research associate at the University of Tennessee, working on the design and application of functional dyes. Her research currently focuses on the development of new chelators for targeted radionuclide therapy. She transitioned to an ORNL staff position in August 2023.

Secretary: Belen Cueva Sola
(August–September 2023)
Belen Cueva Sola received her bachelor's degree in chemical engineering from Universidad San Francisco de Quito, Ecuador. She received her master's degree and PhD in Korea in KAIST and UST, respectively. Her research focuses on hydrometallurgy for the recovery of primary and secondary metal resources. She currently works in the Chemical Separations Group in ORNL's Chemical Sciences Division in the development of ligands for selective leaching and separation of rare earth metals.

ORPA Executive Committee Members (cont.)

Treasurer: Aparna Annamraju

(October 2022–February 2023)

Aparna Annamraju graduated with a PhD from the University of Tennessee in 2021. She is a chemist by training with degrees in both organic and inorganic chemistry. After completing her graduate studies, she joined the Carbon and Composites Group in ORNL's Chemical Sciences Division as a postdoctoral research associate. Her main research interest is to decipher the architecture of complex systems by understanding their fundamental chemical structures. While at ORNL she served as treasurer for ORPA and social chair for Women in Physical Sciences. She transitioned to the role of development scientist at Y-12 National Security Complex.

Treasurer: Torikul Islam

(February–September 2023)

Torikul Islam is a postdoctoral research associate in the Synthetic Biology Group within ORNL's Bioscience Division. His work is mainly focuses on multiple gene stacking, traits improvement, and single-cell RNA-sequencing in poplar. He received his PhD in biotechnology from Academia Sinica and National Chung Hsing University, Taiwan. Before joining ORNL, he worked as a research scientist at the University of Florida.

New Hire Chair: Pratishtha Shukla

Pratishtha Shukla joined ORNL in November 2021 after completing her PhD in electrical engineering at North Carolina State University. She is a member of the Computational Systems Engineering and Cybernetics Group in ORNL's Computational Sciences and Engineering Division, where she works on edge computing for smart grids with specific focus on control algorithms in power distribution systems. Her research interests include optimization, game theory, stochastic modeling, power, control, and energy systems.

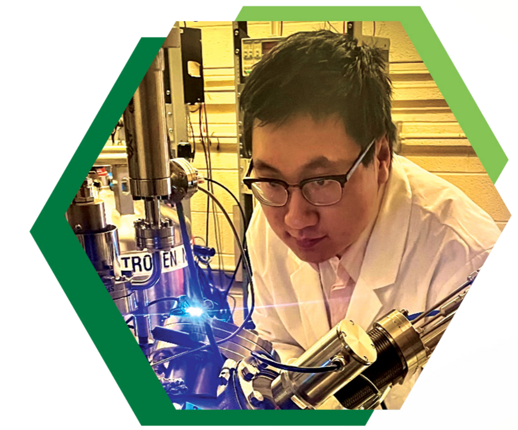
Research Chair: Hao Ma

(October 2022–February 2023)

Hao Ma joined ORNL as a postdoctoral research associate in the Neutron and X-Ray Scattering Group within the Materials Science and Technology Division. He received a bachelor's degree in material physics from the University of Science and Technology of China in 2014 and a PhD in mechanical engineering from Cornell University. Hao's research interests include micro- and nanoscale heat transfer, thermal functional materials and devices, thermal management, thermal insulation, thermoelectric energy conversion, carbon neutrality, and energy sustainability. Hao left ORNL in February 2023 for a job opportunity in China.

Research Chair: Si (Athena) Chen

Si (Athena) Chen joined ORNL as a postdoctoral research associate in the Geochemistry and Interfacial Science Group within the Chemical Sciences Division in January 2022. She received a dual-title PhD degree in Geosciences and Biogeochemistry at Pennsylvania State University in 2021. At ORNL, she performs DOE-funded research in which in situ x-ray/neutron diffraction and high-resolution chemical imaging techniques are used to understand the role of impurity ions in the crystallization of minerals.



Research Chair: Qiangsheng (Johnson) Lu

(February–September 2023)

Qiangsheng (Johnson) Lu is a postdoctoral research associate in the Materials Science and Technology Division's Quantum Heterostructure Group. He got his PhD in condensed matter physics at the University of Missouri, Columbia. His research focuses on the precise fabrication and spectroscopic characterization of low-dimensional quantum systems and novel topological/superconducting materials. He has more than 8 years of experience in angle-resolved photoemission spectroscopy, molecular beam epitaxy, scanning tunneling microscopy, and density functional theory.

Social and Well-Being Chair: Ajay Yadav

(October 2022–February 2023)

Ajay P. Yadav works in the Computational Systems Engineering and Cybernetics Group within ORNL's Computational Sciences and Engineering Division. Ajay received his PhD in 2021 in Electrical Engineering from the University of Texas at Arlington, where his research was funded by the National Science Foundation. His PhD research focused on electric machine characterization, convex optimization, and hardware acceleration based on field-programmable gate arrays. Apart from his primary research, he has also been involved in multiple projects on ac/dc microgrids. He completed his bachelor's and master's degrees at the Indian Institute of Technology.

Social and Well-Being Chair: Shuvo De

(October 2022–August 2023)

Shuvo De is a postdoctoral research associate in the Multiscale Materials Group in ORNL's Computational Sciences and Engineering Division. He received his bachelor's degree in mechanical engineering from Jadavpur University, India. He completed his doctoral degree at Virginia Tech, in engineering science and mechanics with a focus on finite element modeling and multidisciplinary design optimization. He then worked as a postdoctoral fellow in the Department of Chemical and Biological Engineering at the University of Alabama, Tuscaloosa, where his research focused on multiphysics simulation of the electrodeposition process. Shuvo also worked briefly at the Translational Genomics Research Institute.

ORPA Executive Committee Members (cont.)

Social and Well-Being Chair: Emily Mazeau
(March–August 2023)
Emily J. Mazeau received her bachelor's degree in chemical engineering from Rensselaer Polytechnic Institute, where her research focused on engineering co-culture systems for cellulose degradation. She earned her PhD in chemical engineering from Northeastern University, where her research focused on software development for generating microkinetic models for heterogeneous catalysis. She currently works on computational chemistry in the Materials and Chemistry Group within ORNL's Nuclear Nonproliferation Division.

Social and Well-Being Chair: Deng Dong
(August–September 2023)
Dengpan (Deng) Dong received his PhD degree in materials science and engineering in 2018. His research focuses on using molecular simulations to investigate multicomplex materials and interfaces. He is also an active developer of polarizable and nonpolarizable potentials. Currently, he is working in the Chemical Group within the Chemical Sciences Division to obtain a molecular-level fundamental understanding for the development of a polymer antiscalant and for the behavior of liquid-air interfaces. His research interests also include monovalent and multivalent ion battery systems.

Social and Well-Being Chair: Ernesto Zuleta Suarez
(August–September 2023)
Ernesto Camilo Zuleta Suarez holds a PhD in energy science and engineering from the University of Tennessee. Originally from northern Colombia, he has resided in Tennessee for the past 10 years. He is currently working as a postdoctoral research associate in the Energy Storage and Conversion Group within ORNL's Chemical Sciences Division. His research focuses on electrochemical energy storage applications.

Outreach Chair: Tomas Grejtak
Tomas Grejtak is a postdoctoral research associate in the Surface Engineering Tribology Group within ORNL's Materials Science and Technology Division. He earned his PhD (2022) in mechanical engineering at Lehigh University. Before joining ORNL, Tomas spent two years at Florida State University studying wear-resistant thin films for space applications and structure-property relationships of dinosaur dentitions. His research focuses on analyzing and developing wear- and friction-reducing surfaces and bioinspired damage-tolerant materials.

Communications Chair: Biva Talukdar
(October 2022–August 2023)
Biva Talukdar was until recently a postdoctoral research associate in the Materials MicroAnalysis Group and at ORNL's Center for Nanophase Materials Sciences. Her research focuses on the use of advanced microscopic techniques such as S/TEM, EELS, and Cryo-EM to characterize catalysts. She received her PhD in sustainable chemical science and technology from National Yang-Ming Chiao Tung university in 2021. She is an expert in synthesizing novel architectures of bimetallic and trimetallic core-shell alloy nanocatalysts, microscopic techniques, electrochemical carbon dioxide reduction to useful chemicals, nitrogen reduction to ammonia, and fuel cell applications. Biva joined Pacific Northwest National Laboratory in August 2023.

ORPA Advisory and Support Staff

Office of Research Education Director: Moody E. Altamimi
Moody E. Altamimi is the founding director for the Office of Research Education at ORNL. Her diverse skills and expertise in research development and management, strategy development and implementation, and technology translation support organizational efforts to advance ORNL's science and innovation culture. She works with students, postdoctoral researchers, and early-career scientists in hopes of inspiring them to excel as they navigate their career paths by encouraging collaboration and team science that will produce world-changing outcomes. Moody earned her master's and doctoral degrees in computer science from George Washington University.

Advisor: Laurie Varma
Laurie Varma serves as the early career programs specialist in the Office of Research Education. She supports the Oak Ridge Postdoctoral Association Executive Committee in their efforts to make an impact on the ORNL campus, providing guidance related to projects, events, planning, reporting, and budget.

Administrative/Project Support: Caitlyn Wakefield
Caitlyn Wakefield provides project and administrative support for ORE. Caitlyn supports ORPA through the coordination of projects, ensuring alignment with the laboratory mission. She is engaged in event and process planning and provides expertise on the parameters of ORNL policies and procedures.