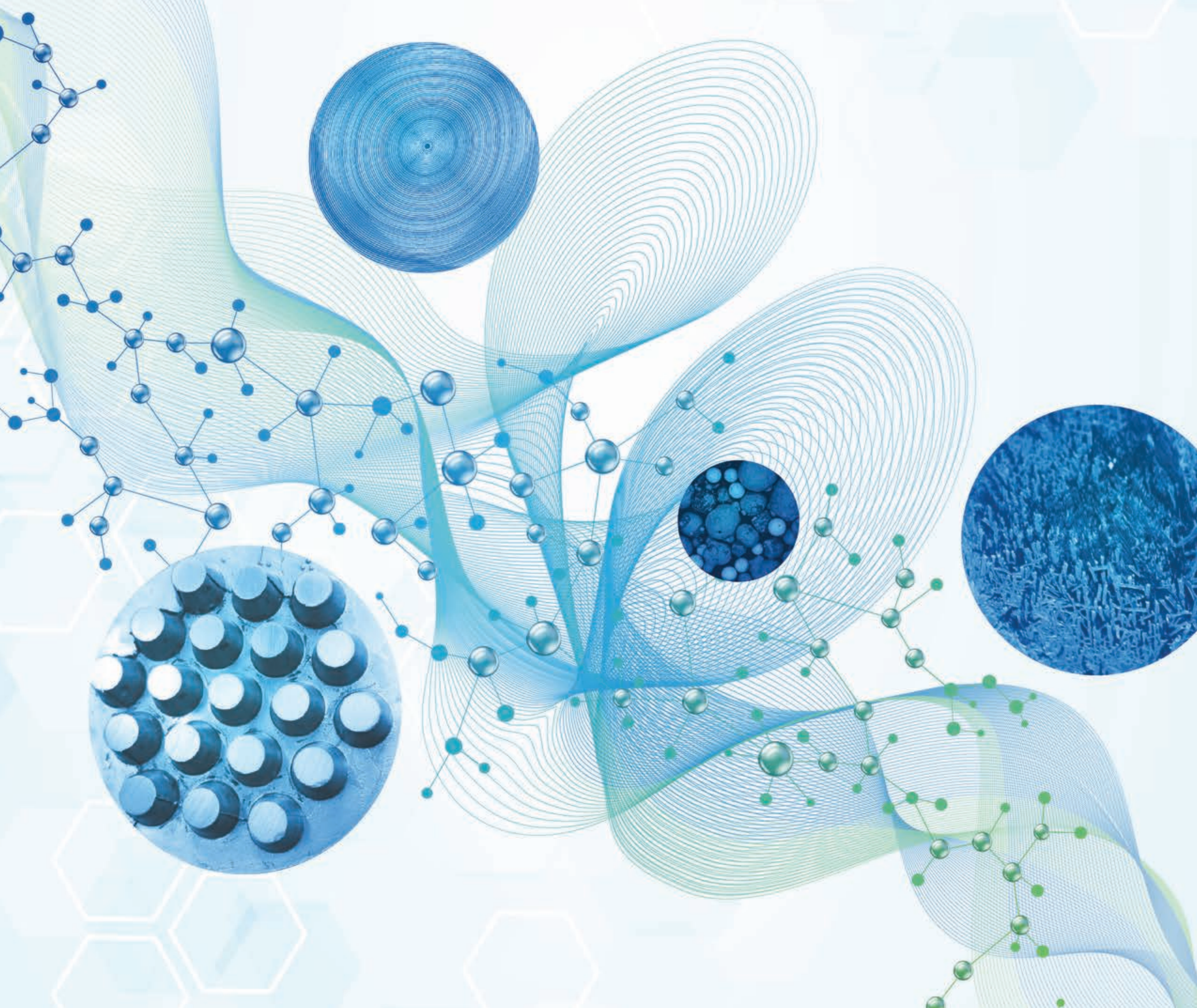
INL/RPT-26-90181

IDAHO NATIONAL LABORATORY

2025
ANNUAL REPORT
Laboratory Directed Research & Development



FROM INL'S CHIEF RESEARCH OFFICER

DR. TODD COMBS
Deputy Laboratory Director for Science and Technology, Chief Research Officer Idaho National Laboratory

I am inspired by the breadth and depth of scientific achievement in the Laboratory Directed Research and Development (LDRD) projects. The work showcased here represents more than individual research projects—it embodies Idaho National Laboratory's (INL's) unwavering commitment to scientific excellence and our role in addressing the nation's most critical energy and security challenges.

The LDRD program continues to fulfill its essential mission: maintaining the scientific vitality that makes INL a world-class research institution. By empowering researchers to explore bold, high-risk ideas beyond the constraints of existing programs, we lay the groundwork for transformative breakthroughs. This year's portfolio clearly illustrates how such early-stage investments can evolve into impactful, programmatically supported initiatives.

Our strategic focus on emerging core capabilities—chemical and molecular science, computational science, and condensed matter physics and materials science—has enabled discoveries from understanding radiation chemistry at the molecular level to engineering materials with unprecedented properties for extreme environments.

The scope of innovation represented in this report is remarkable. Our researchers are reimagining materials design through biomimicry, developing artificial intelligence-powered tools that secure critical infrastructure against sophisticated cyber threats, advancing critical materials recovery, and unlocking the fundamental physics of quantum materials. Each project pushes the boundaries of what we can achieve.

Looking ahead, the challenges facing our energy production, infrastructure, and national security demand the kind of bold, innovative thinking that the LDRD program enables. The research we are advancing today shapes the solutions that will define tomorrow.

I want to express my deep appreciation to everyone who makes this program successful: the principal investigators, researchers, technicians, administrative staff, and our external partners. Your collective efforts embody the spirit of scientific inquiry and excellence that defines INL.

Thank you for your interest in our LDRD program. I hope this report conveys the excitement and significance of the work being conducted and inspires continued support for the fundamental and applied research that is shaping our energy future.

With warmest regards,
Todd Combs

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JEREMY HARTVIGSEN

LDRD OVERVIEW

DOE LDRD OBJECTIVES

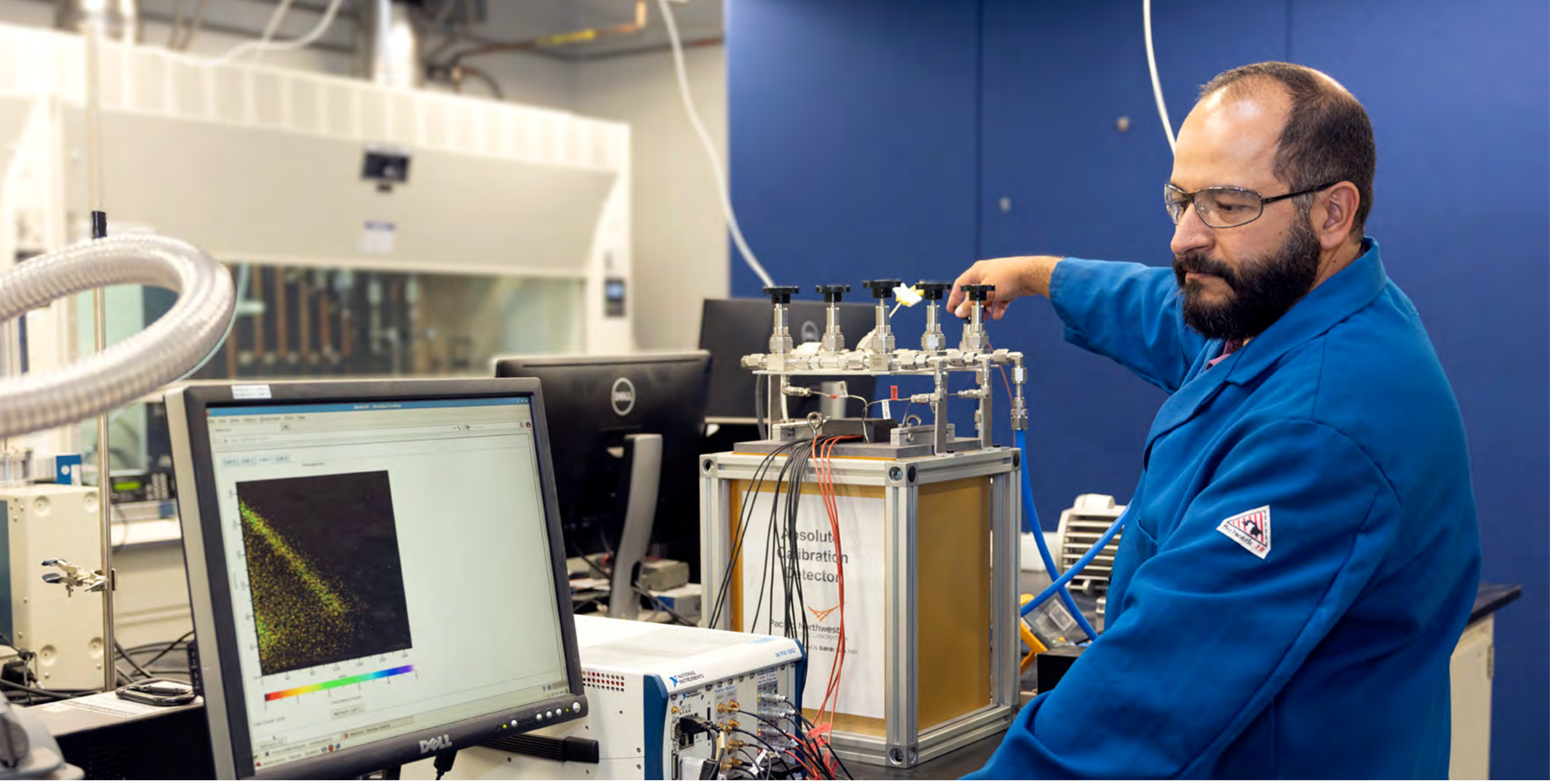
MISSION AGILITY
Enable agile responses to national security, energy, and environmental challenges.

SCIENTIFIC AND TECHNICAL VITALITY
Advance the frontiers of science, technology, and engineering.

WORKFORCE DEVELOPMENT
Attract, retain, and develop tomorrow's scientific and technical workforce.

INL's LDRD program empowers high-risk, high-reward research that positions the laboratory to respond quickly to evolving national energy and security challenges. The Department of Energy (DOE) allows the national laboratories to devote up to 6% of their research effort to creative and innovative work that 1) maintains their scientific and technical vitality, 2) enhances their ability to address current and future DOE missions, 3) fosters creativity and stimulates exploration of forefront areas of science and technology, 4) serves as a proving ground for new research and development concepts, and 5) supports high-risk, high-value research and development.

Throughout fiscal year 2025 (FY-25), the United States (US) government significantly elevated the urgency of increasing our nuclear energy capability, critical minerals and materials independence, and cyber-physical resilience. INL has strong capabilities in all these areas and sharpened its research focus to support the national priorities. These efforts included prioritizing funding for new LDRD projects that, for example, enable the quadrupling of nuclear power by 2050, deliver critical national security technology, transform critical and strategic materials research, and utilize artificial intelligence to advance research.



Alonzo Martinez showcasing advanced Noble Gas Detection technology in action.

INL's LDRD Portfolio

INL's diverse LDRD portfolio explores a range of scientific and engineering concepts through technically sound, innovative, and novel research projects. The LDRD program stimulates exploration in basic and applied science and engineering with a portfolio composed of five investment components that are continually aligned with INL's vision, mission, and science and technology initiatives:

- The strategic research and development fund supports research that advances INL's science and technology initiatives.
- The seed fund supports high impact, innovative research that is aligned with INL's mission. The fourth quarter seed call focused on projects that utilize artificial intelligence to advance research.
- The distinguished postdoc fund supports early career researchers in INL's three distinguished postdoctoral fellowships, providing them leadership opportunities while they conduct leading edge research that supports INL's mission.
- The strategic hire fund grows INL science and technology capabilities by providing new hires opportunities to conduct research aligned with our mission.
- The early career researcher fund promotes the careers and future opportunities available to INL's early career research staff working in areas of interest to DOE Office of Science. Each principal investigator has a mentor who helps the researcher navigate an Office of Science early career award submittal following the LDRD project.

$58 MILLION TOTAL PROJECT BUDGET UP FROM $53M MILLION IN FY-25.

The INL LDRD program budget increased from $53 million in FY-24 to $58 million in FY-25. Of the 156 active projects in FY-25, 63 concluded and are highlighted in this report. To increase their value and impact, the program expects researchers to publish at least one peer reviewed paper for each $200,000 of LDRD project funding. This is part of INL's overall strategy to continue strengthening its basic and applied research excellence culture. Intellectual property generation is also important to INL's research excellence, including invention disclosures, software disclosures, patent applications, copyrights, and licenses.

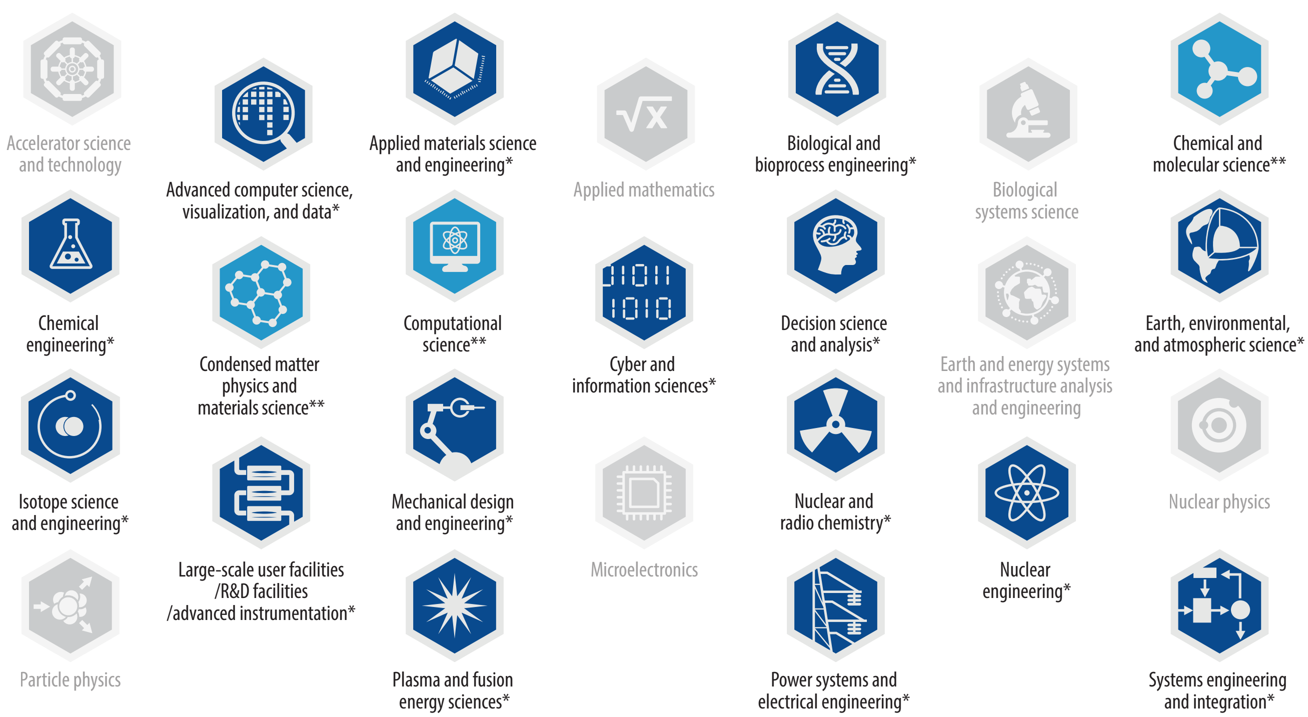
Core Capabilities

INL creates a discovery and solution driven research, development, and demonstration (RD&D) environment through unique experimental systems, infrastructure, and fundamental engineering and science capabilities. Of the 25 core capabilities foundational to DOE's mission and shared across the 17 national laboratories, DOE acknowledges that INL has 15 core capabilities and three emerging core capabilities. These core capabilities represent a comprehensive science and engineering skill set that extends across a continuum, connecting basic and applied research to develop, test, demonstrate, and validate technologies at scale.

These core capabilities are sustained and enhanced through INL's LDRD projects. To demonstrate that the emerging core capabilities are intrinsic at INL, the LDRD program included the three emerging core capabilities as strategic scientific initiatives. Of the 156 active projects in FY-25, 76 demonstrated one or more emerging core capabilities, including 30 of the 63 projects highlighted in this report. Throughout this report, icons will indicate the core capabilities supported by LDRD projects.

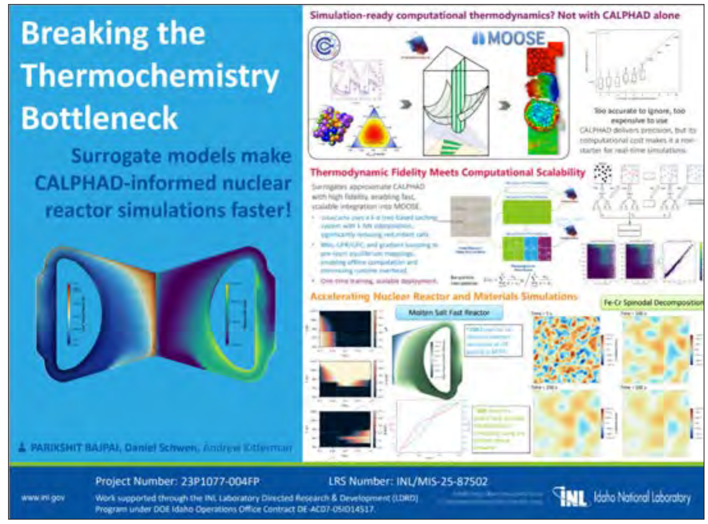
Project Selection & Oversight

INL ensures that the LDRD program goals and objectives are aligned with DOE Order 413.2C, Chg. 1, and that the LDRD portfolio is managed with integrity, transparency, and accountability. Project proposals undergo multiple layers of rigorous review by subject matter experts and senior leadership. The deputy laboratory director for Science and Technology, in collaboration with the associate laboratory directors, evaluates recommended projects and makes final funding determinations for the LDRD portfolio. Additionally, concurrence from the DOE Idaho Operations Office is required for each new or continuing project prior to funding in the subsequent fiscal year.

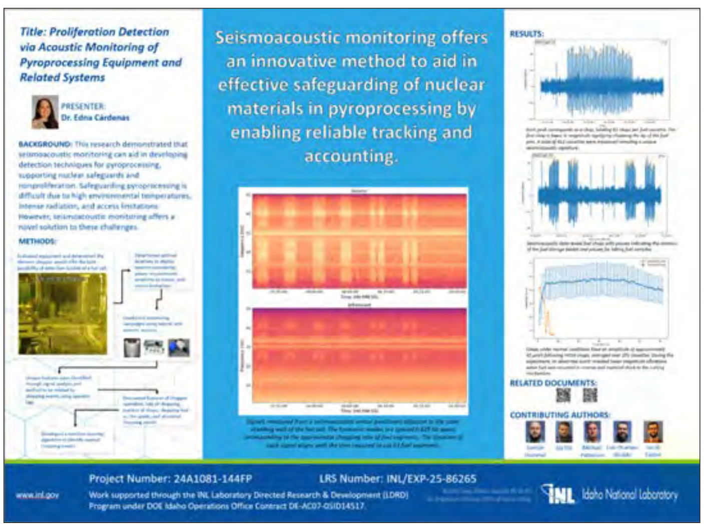


Core Capabilities *INL (dark blue) ** Emerging (light blue)

Nicolas Woolstenhulme won first place for "Unlocking the Power of Microreactors with Biomimicry and Additively Manufactured Nuclear Fuel."



Parikshit Bajpai won second place for "Accelerated Nuclear Materials Thermochemistry through Active Learning Surrogate Models."



Edna Cárdenas won third place for "Proliferation Detection via Acoustic Monitoring of Pyroprocessing Equipment and Related Systems."

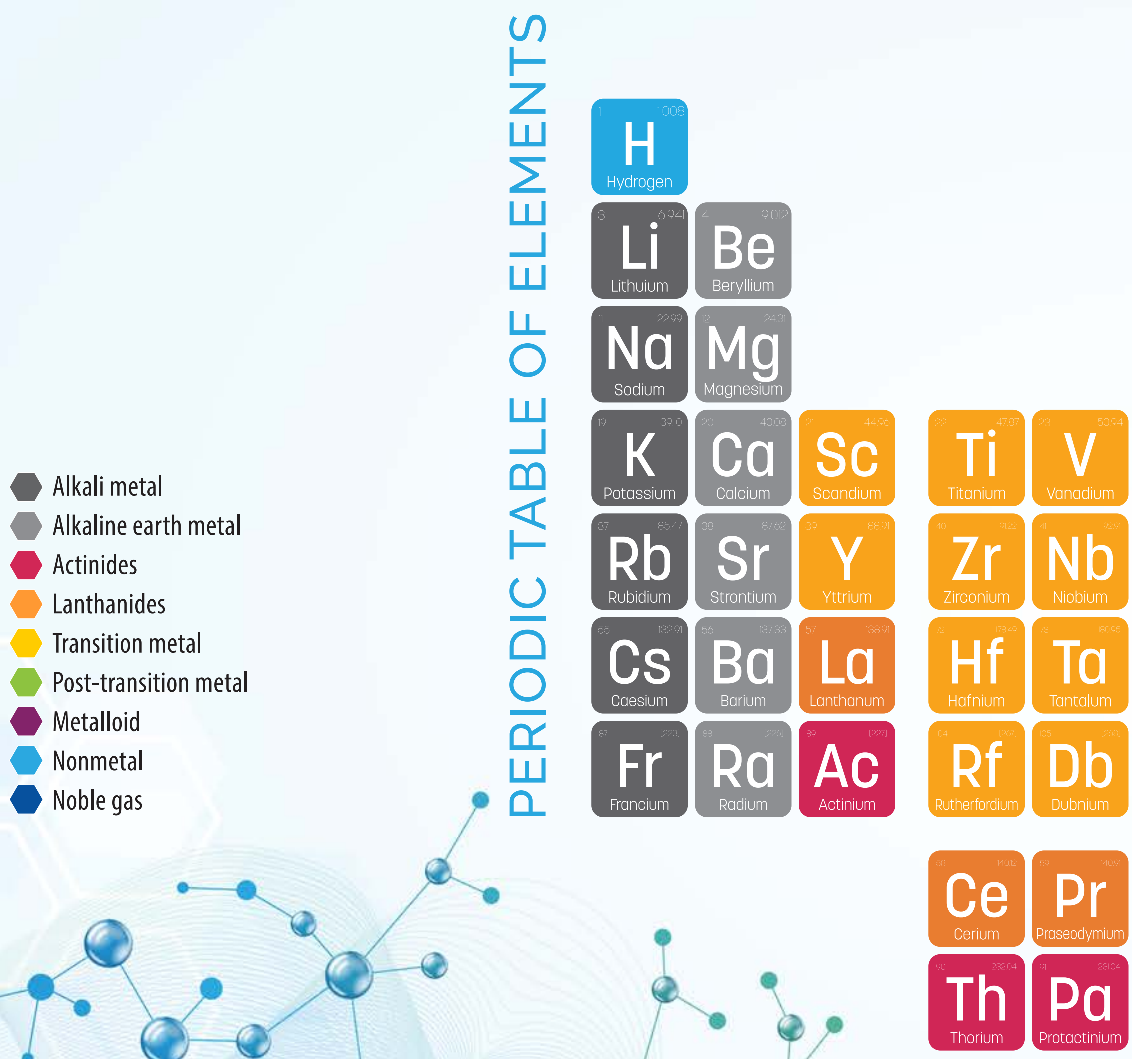
Showcasing Success

On September 8, 2025, INL hosted a poster session showcasing the LDRD projects that ended in FY-25. Attendees included INL researchers, industry and academic partners, external collaborators, and members of the public.

The poster session featured all 63 projects highlighted in this report. In a "best poster" competition, posters were evaluated on their creativity addressing cutting-edge science, technology, or engineering, the significance and impact of the project outcomes, the presentation clarity, and the potential for attracting future RD&D funding opportunities. Nicolas Woolstenhulme's project on "Unlocking the Power of Microreactors with Biomimicry and Additively Manufactured Nuclear Fuel," summarized on page 90, won first place for best poster. Parikshit Bajpai won second place for "Accelerated Nuclear Materials Thermochemistry through Active Learning Surrogate Models." See the project summary on page 128. Edna Cárdenas won third place for "Proliferation Detection via Acoustic Monitoring of Pyroprocessing Equipment and Related Systems," which is summarized on page 56.

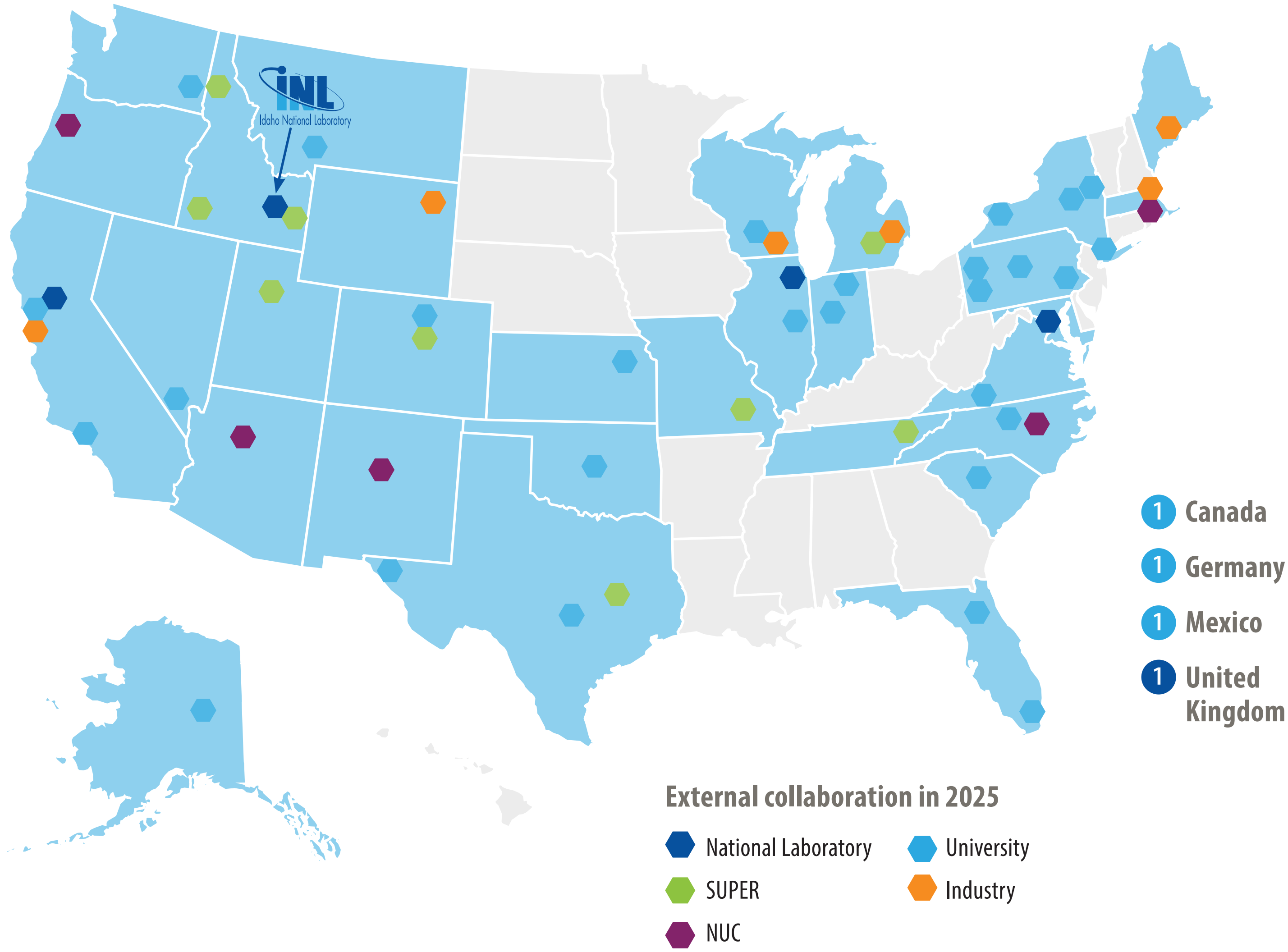
ACRONYMS & ABBREVIATIONS

DOE Department of Energy
INL Idaho National Laboratory
LDRD Laboratory Directed Research and Development
MOOSE Multiphysics Object-Oriented Simulation Environment
RD&D Research, development, and demonstration
US United States



												2 4.0026 He Helium
							5 10.81 B Boron	6 12.01 C Carbon	7 14.01 N Nitrogen	8 16.00 O Oxygen	9 19.00 F Fluorine	10 20.18 Ne Neon
							13 26.98 Al Aluminium	14 28.06 Si Silicon	15 30.97 P Phosphorus	16 32.06 S Sulfur	17 35.45 Cl Chlorine	18 39.95 Ar Argon
24 52.00 Cr Chromium	25 54.94 Mn Manganese	26 55.84 Fe Iron	27 58.93 Co Cobalt	28 58.96 Ni Nickel	29 63.55 Cu Copper	30 65.39 Zn Zinc	31 69.72 Ga Gallium	32 72.63 Ge Germanium	33 74.92 As Arsenic	34 78.97 Se Selenium	35 79.90 Br Bromine	36 83.80 Kr Krypton
42 95.94 Mo Molybdenum	43 [97.91] Tc Technetium	44 101.07 Ru Ruthenium	45 102.91 Rh Rhodium	46 106.42 Pd Palladium	47 107.87 Ag Silver	48 112.41 Cd Cadmium	49 114.82 In Indium	50 118.71 Sn Tin	51 121.76 Sb Antimony	52 127.60 Te Tellurium	53 126.90 I Iodine	54 131.29 Xe Xenon
74 183.84 W Tungsten	75 186.21 Re Rhenium	76 190.23 Os Osmium	77 192.22 Ir Iridium	78 195.08 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury	81 204.38 Tl Thallium	82 207.2 Pb Lead	83 208.98 Bi Bismuth	84 [209] Po Polonium	85 [210] At Astatine	86 [222] Rn Radon
106 [269] Sg Seaborgium	107 [270] Bh Bohrium	108 [269] Hs Hassium	109 [278] Mt Meitnerium	110 [281] Ds Darmstadtium	111 [281] Rg Roentgenium	112 [285] Cn Copernicium	113 [286] Nh Nihonium	114 [289] Fl Flerovium	115 [290] Mc Moscovium	116 [293] Lv Livermorium	117 [294] Ts Tennessine	118 [294] Og Oganesson

60 144.24 Nd Neodymium	61 [145] Pm Promethium	62 150.36 Sm Samarium	63 151.96 Eu Europium	64 157.25 Gd Gadolinium	65 158.93 Tb Terbium	66 162.50 Dy Dysprosium	67 164.93 Ho Holmium	68 167.26 Er Erbium	69 168.93 Tm Thulium	70 173.05 Yb Ytterbium	71 174.97 Lu Lutetium
92 238.03 U Uranium	93 [237] Np Neptunium	94 [244] Pu Plutonium	95 [243] Am Americium	96 [247] Cm Curium	97 [247] Bk Berkelium	98 [251] Cf Californium	99 [252] Es Einsteinium	100 [257] Fm Fermium	101 [258] Md Mendelevium	102 [259] No Nobelium	103 [266] Lr Lawrencium



COLLABORATION

INL's LDRD program encourages collaboration across organizational, institutional, and geographical boundaries to advance the frontiers of science, technology, and engineering. Of the more than 400 researchers working on LDRD projects in FY-25, nearly 100 of them were outside INL, representing 30 states as well as Canada, Germany, Mexico, and the United Kingdom. These collaborators came from four national laboratories, six companies and 45 universities, including 10 of the 12 Strategic Understanding for Premier Education and Research (SUPER) universities and four of the five National University Consortium (NUC) universities.

FY-25 PROGRAM STATISTICS

JOSEPH ONCKEN

NUCLEAR REACTOR SUSTAINMENT AND EXPANDED DEPLOYMENT

CORE CAPABILITIES

Advanced Computing Science, Visualization, and Data

Applied Materials Science & Engineering

Applied Mathematics

Computational Science

Condensed Matter Physics and Materials Science

Mechanical Design and Engineering

Network Security and Optimization

Nuclear Engineering

Plasma and Fusion Energy Sciences

Systems Engineering and Integration

As the nation's premier nuclear energy RD&D laboratory, we advance US energy dominance by ensuring the safe, reliable, and efficient operation of existing reactors while pioneering the next generation of nuclear technologies. We are expanding and modernizing nuclear infrastructure, experimental facilities, and modeling and simulation capabilities to accelerate discovery and demonstration. Our innovations will enhance the performance of current and future nuclear systems, including fuels, materials, and reactor designs. We are also advancing fusion energy through innovative RD&D in fusion-blanket technologies and integrated power-system components.

Resilient Remote Operation of Microreactors and Fission Batteries

PROJECT NUMBER:
23A1070-033FP

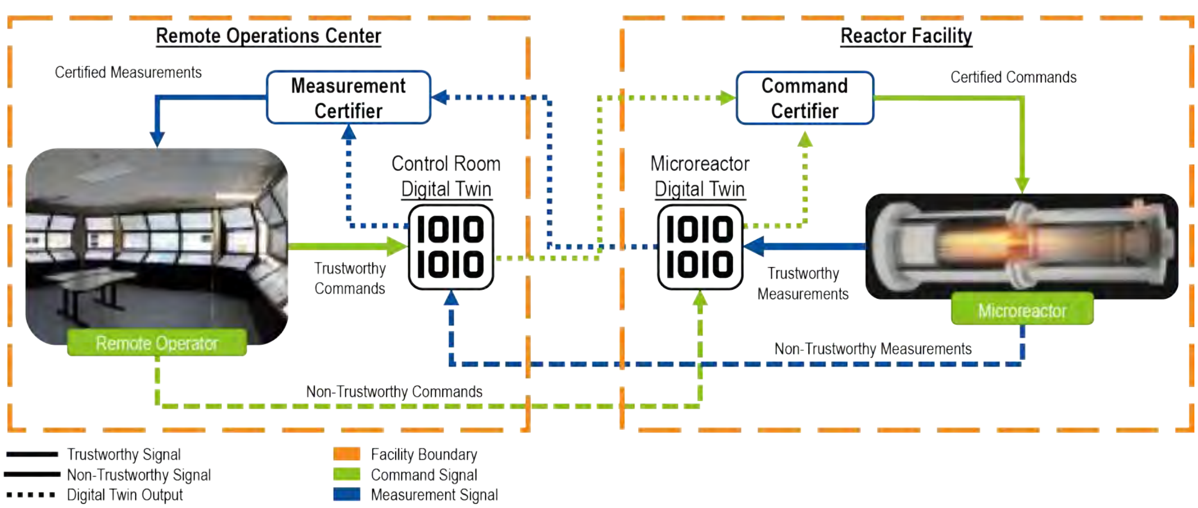
TOTAL APPROVED AMOUNT:
$1,600,000 over 3 years

PRINCIPAL INVESTIGATOR:
Joseph Oncken

CO-INVESTIGATORS:
Haydn Bryan, INL
Heather Ackenhusen, INL
Jack Cavaluzzi, INL
Jeren Browning, INL
Kaeley Stevens, INL
Megan Culler, INL
Ron Boring, INL
Stephen Bukowski, INL
Thomas Ulrich, INL
Troy Unruh, INL
Dylan Jurski, University of Florida

Remote operations enable widespread deployment of microreactors and fission batteries.

As the nuclear industry moves toward a new generation of advanced reactors, including microreactors and fission batteries, a major unresolved technical challenge to the full deployment of these systems is a reliable, resilient, and secure remote operation and monitoring capability. This project addressed that challenge by performing an investigation into the integration of remote operations with nuclear reactors and by developing a framework for the resilient remote operation and monitoring of microreactors. This remote operation and monitoring system addresses the operator, signal-monitoring, and verification needs unique to remote operation by introducing a digital-twin-based resilience system that ensures trustworthy data exchanges between the microreactor and remote operations facility and enhances operator awareness of reactor status. In addition, a communications architecture was developed that addresses the security and reliability needs of remote operations while adhering to the standards and best practices of remote communication systems proven in other industries such as oil and gas, the electric grid, and distributed energy resources. This project provided a platform to study the impact of remote operations pertaining to advanced reactors and created a scalable framework for reactor remote operations that can be applied to upcoming reactors such as the DOE Microreactor Applications Research Validation and Evaluation project. In addition, this project directly created new funding streams for INL including a new work package studying the security of remote operations supported by the DOE Advanced Reactor Safeguards and Security program.



Digital twin certification system for the resilient remote operation of advanced reactors.

TALENT PIPELINE:

- Joseph Oncken, Postdoc at INL, converted to staff
- Kaeley Stevens, student at University of Oregon
- Dylan Jurski, student at University of Florida

PAPERS AND PRESENTATIONS:

- Stevens, K., Oncken, J., Boring, R., Ulrich, T., Culler, M., Bryan, H., Browning, J., & Gutowska, I. "Opportunities, Challenges, and Research Needs for Remote Microreactor Operations." Nuclear Technology, vol. 210, pp. 2257–2273, 2024.
- Bryan, H., K. Jesse, K., Miller, C., and J. M. Browning, J., "Remote nuclear microreactors: a preliminary economic evaluation of digital twins and centralized offsite control." Frontiers in Nuclear Engineering, vol. 2, 2023.
- Oncken, J, Ulrich, T, J. Cavaluzzi, "Implementation and Demonstration of the Digital Twin Certification System Remote Operations Framework." 14th Nuclear Plant Instrumentation, Control & Human-Machine Interface Technologies, June 9-11, 2025, Chicago, IL.
- Culler, M., Oncken, J., Stevens, K., Ulrich, T., "Architecture Design for Remote Operation of Microreactors." Resilience Week 2024, December 3-5, 2024, Austin, TX.
- Culler, M., Oncken, J., Stevens, K., Ulrich, T., "Risk Analysis for Remote Operation of Microreactors." American Nuclear Society (ANS) Pacific Basin Nuclear Conference 2024, October 7–10, 2024, Idaho Falls, ID.
- Bryan, H., Larsen, L., Culler, M., Oncken, J., "Remote Nuclear Power Plant Operation: Navigating the Opportunities and Challenges in Public Perception." ANS Pacific Basin Nuclear Conference 2024, October 7–10, 2024, Idaho Falls, ID
- Jurski, D. L., Ulrich, T. A., "The Challenge of Data Integration—Digital Twin Certification to Support Remote Operations." Human Factors and Ergonomics Society Annual Meeting, Sept 2024, Phoenix, AZ.
- Oncken, J., Ulrich, T., Stevens, K., Sellers, Z., Browning, J., "Development and Demonstration Testbed for the Remote Operations and Monitoring of Microreactors." 31st International Conference on Nuclear Engineering, August 4-8, 2024, Prague, CZ.
- Stevens, K., Oncken, J, Gutowska, I., "Modeling for a Digital Twin-Based Remote Operation System Framework." 2024 ANS Annual Conference, June 16-19, 2024, Las Vegas, NV.
- Stevens, K., Oncken, J., Culler, M., Bukowski, S., Ulrich, T., Gutowska, I., Boring, R., "Digital Twin Framework for the Resilient Remote Monitoring and Operation of Nuclear Microreactors." AHFE 2023 International Conference. AHFE Open Access, vol. 117. AHFE International, USA.
- Ulrich, T., Oncken, J., Boring, R., Stevens, K., Culler, M., Bukowski, S., Unruh, T., Browning, J., "Digital Twin Verification for Advanced Reactor Remote Operations." AHFE 2023 International Conference. AHFE Open Access, vol. 82. AHFE International, USA.
- Boring, R., "Human Factors for Advanced Reactors." AHFE 2023 International Conference. AHFE Open Access, vol. 94. AHFE International, USA.
- Stevens, K., Oncken, J., Boring, R., Ulrich, T., Bryan, H, Culler, M., Gutowska, I., "Opportunities and Challenges for Remote Microreactor Operations." 13th Nuclear Plant Instrumentation, Control & Human-Machine Interface Technologies, July 15-20, 2023, Knoxville, TN.

Integral Reactor Shield Structures for Fission Batteries

PROJECT NUMBER:
23A1070-041FP

TOTAL APPROVED AMOUNT:
$2,468,827 over 3 years

PRINCIPAL INVESTIGATOR:
Samuel Bays

CO-INVESTIGATORS:
Abderrafi Ougouag, INL
Adam Zabriskie, INL
Adrian Wagner, INL
Joshua Zelina, INL
Robert Spears, INL
Ryan Stewart, INL

COLLABORATORS:
Element Materials Technology
Idaho State University
RPM Innovations
Stanford Advanced Materials

Integrating radiation shields and reactor vessels into a single stronger and lighter composite material system revolutionizes nuclear reactor design.

The purpose of this study was to discover a composite material system that simultaneously functions as a reactor pressure vessel and a radiation shield. The motivation for achieving such a material system is to significantly reduce the weight contributed by these components to a mobile nuclear microreactor. This novel lightweight material system is accomplished by forming a nuclear grade sandwich composite. Nuclear grade sandwich composite consists of additively manufactured 316 grade stainless steel cells. The cells can be closed honeycombs or open vertical channels depending on fabrication method. Shear strength between layers is ensured through connecting stainless steel 316 ribs (i.e., honeycombs or channels) extending in the radial direction. These ribs connect stainless steel 316 circumferential skins, thus forming layers. The spaces between the layers constitute cells. These cells are backfilled by radiation attenuating ceramics, boron carbide and tungsten tetraboride. Such a material system reduces the radius of the shield annulus while simultaneously reducing the volume of steel used to form a pressure boundary. The nuclear grade sandwich composite multilayered construction ensures that transverse (i.e., radial) stresses are transmitted from inner to outer layers which ensure all layers participate in pressure retention. The boron carbide and tungsten tetraboride layers offer very little tensile strength, but significant shear strength. The shear strength ensures that the connecting ribs do not buckle under load. The connecting ribs then carry most transverse stresses between the skins. Optimized boron carbide and tungsten tetraboride configurations ensure simultaneous reduction of neutrons and gamma rays during both reactor operation and transportation. Overall, we found that nuclear grade sandwich composite could replace approximately 30% of the transportable weight of a microreactor.

The discoveries made through fundamental research gave us confidence that a scaled prototype of a nuclear grade sandwich composite reactor pressure vessel could be constructed and hydrostatically tested. The stainless steel 316 vertical triangular channels are manufactured via wire arc additive manufacturing. These channels are filled with boron carbide powder and tap-densified using a vertical shake table. The prototype was pressurized to 5,000 psi prior to failure. Failure was premature, but we still have confidence that refined manufacturing controls will improve pressure retention.

TALENT PIPELINE:

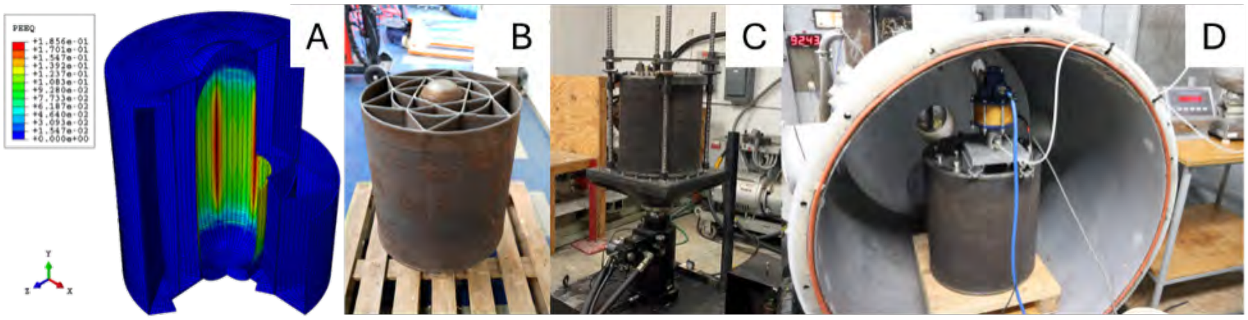
- Kyler Egan, student at Idaho State University
- Samuel Garcia, student at University of Wisconsin

PAPERS AND PRESENTATIONS:

- S. Bays, A. Ougouag, H. Hiruta, R. Stewart, "Challenge and Opportunity Specific to Microreactors: Compact and Lightweight Shielding During Operation and Transportation." Nuclear Science and Engineering, (2025).
- R. Stewart, S. Bays, J. Zelina, R. Spears, A. Zabriskie, E. Kurt, A. Ougouag, "Mass Optimization of a Multilayered Shield for Transportable Microreactors." Nuclear Science and Engineering, (2024).
- R. Stewart, S. Bays, A. Zabriskie, J. Zelina, R. Spears, "Streaming in a Nuclear Grade Sandwich Composite for Microreactor Shielding." Transactions of the ANS, Vol. 131, (1), November 18, 2024.
- S. Bays, H. Hiruta, W. Scates, A. Ougouag, "Effectiveness of Various Shielding Materials for Mobile Microreactors." Pacific Basin Nuclear Conference, Idaho Falls, Idaho, October 7-10, 2024.
- Stewart, S. Bays, A. Zabriskie, J. Zelina, A. Ougouag, R. O'Brien, "Preliminary Analysis of a Nuclear Grade Sandwich Composite for Transportable Microreactor Shielding." International Conference on Physics of Reactors, San Francisco, California, April 21-24, 2024.

EXTERNAL INTELLECTUAL PROPERTY:

- S. E. Bays, A. M. Ougouag, T.-L. Sham, J. N. Zelina, R. H. Stewart, A. X. Zabriskie, R. C. O'Brien, R. Spears, A. R. Wagner, K. Egan "Integrated Reactor Shield Structures." Patent BA-1453. (2024)



(A) Nuclear Grade Sandwich Composite Prototype: Plastic strain analysis using the Abaqus code, (B) Additive manufacturing by three-dimensional wire arc additive manufacturing, (C) boron carbide powder and tap densification at Idaho State University, (D) ready for hydrostatic pressure testing at Element Materials Technology.

Accelerating Assessment of High-Temperature Helium Embrittlement in Nickel-bearing Structural Materials

PROJECT NUMBER:
23A1070-069FP

TOTAL APPROVED AMOUNT:
$1,468,800 over 3 years

PRINCIPAL INVESTIGATOR:
Yachun Wang

CO-INVESTIGATORS:
Boopathy Kombaiah, INL
Masashi Shimada, INL
Chase Taylor, INL

COLLABORATORS:
University of Wisconsin
University of Michigan

Newly discovered helium diffusion mechanism in nickel-chromium alloys challenges prior understanding.

Nickel-chromium alloys are promising structural materials for nuclear reactor applications but are susceptible to high-temperature helium embrittlement due to helium generation from transmutation reactions and subsequent helium bubble formation. The kinetics of high-temperature helium embrittlement are governed by helium diffusion, which is affected by the presence of chromium and other solute atoms. Therefore, uncovering the mechanisms of helium diffusion in the presence of solute atoms is fundamental to understanding and mitigating high-temperature helium embrittlement.

Conventionally, the impact of solute atoms on helium diffusion is often investigated by coupling atomistic calculations and theoretical models. The binding energies between helium and solute atoms obtained from atomistic calculations, e.g., density functional theory, are fed to analytical models to predict helium diffusivity in alloys. The models are often derived in the dilute concentration regime and are incapable of dealing with the presence and interconnection of multiple trapping sites in alloys with high solute concentrations, resulting in a standard belief that increasing chromium concentration monotonically slows down helium diffusion in nickel-chromium alloys.

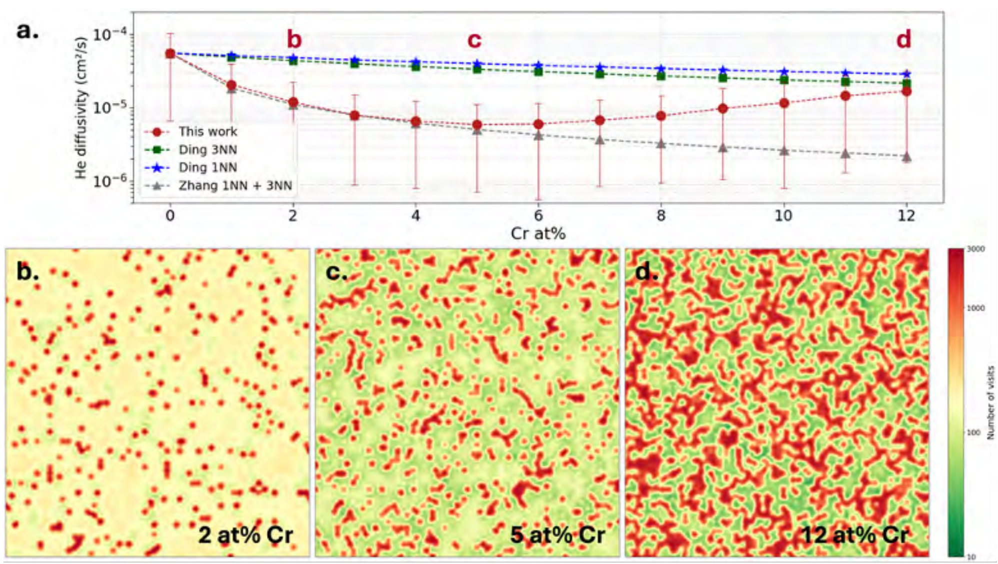
This study investigated helium diffusion in pure nickel and nickel-chromium alloys by integrating high-fidelity density functional theory with atomic kinetic Monte Carlo simulations, to overcome the challenge of dealing with high solute concentrations. The findings reveal a non-monotonic relationship between helium diffusivity and chromium concentration, contradicting the monotonic trends predicted in the literature. At low chromium concentrations (<5 at%), helium diffusion is dominated by short-range trapping, characterized by multiple trapping sites and a distinct mechanism within the first nearest neighbor (1NN) of chromium, differing from the behavior in pure nickel. In contrast, at high chromium concentrations (>5%), these local traps become interconnected, forming long-range fast diffusion channels that enhance helium mobility. The size of the channels increases with chromium concentration. This interplay between localized trapping and extended channeling results in helium diffusivity that first decreases and then increases with increasing chromium content. These atomic-scale insights are critical for designing radiation-tolerant nickel-based alloys. Furthermore, the combined density functional theory with atomic kinetic Monte Carlo methodology and the concept of random walker diffusion through interconnected energy basins provide a broadly applicable framework for studying transport phenomena in disordered systems.

TALENT PIPELINE:

- Volodymyr Buturlim, distinguished postdoc at INL
- Tzu-Yi Chang, postdoc at INL
- Yalei Tang, postdoc at INL
- Ximeng Wang, postdoc at University of Wisconsin
- Ziang Yu, postdoc at University of Wisconsin
- Justin, Hamil, student at University of Michigan
- Ian Steigerwald, student at the University of Michigan

PAPERS AND PRESENTATIONS:

- Wang, X., Wang, Y., and Zhang, Y. 2025. "Density Functional Theory Study of Helium Diffusion in Ni-M Alloys (M= Cr, Mo)." Presented at The Minerals, Metals & Materials Society (TMS) 2025 Annual Meeting & Exhibition (Las Vegas, NV, USA, March 23-27).
- Wang, X., Wang, Y., and Zhang, Y. 2024. "Density Functional Theory Study of Helium diffusion in Ni-M Alloys (M= Cr, Mo)." Presented at TMS Fall Meeting 2024 at Materials Science & Technology (MS&T) (Pittsburgh, Pennsylvania, USA, October 6-9).



(a) Helium diffusivity was calculated from this work and calculated by the widely used theoretical model in nickel-chromium as a function of chromium (Cr) concentration, as well as the helium visit time at different sites in nickel-chromium under (b) 2 atomic percent (at%) (isolated traps), (c) 5 at% (increased isolated traps), and (d) 12 at% (fast diffusion channels formed by the interconnected traps) chromium concentrations.

Development of Lightweight Structural Materials with Improved Properties for Fission Batteries

PROJECT NUMBER:
23A1070-132FP

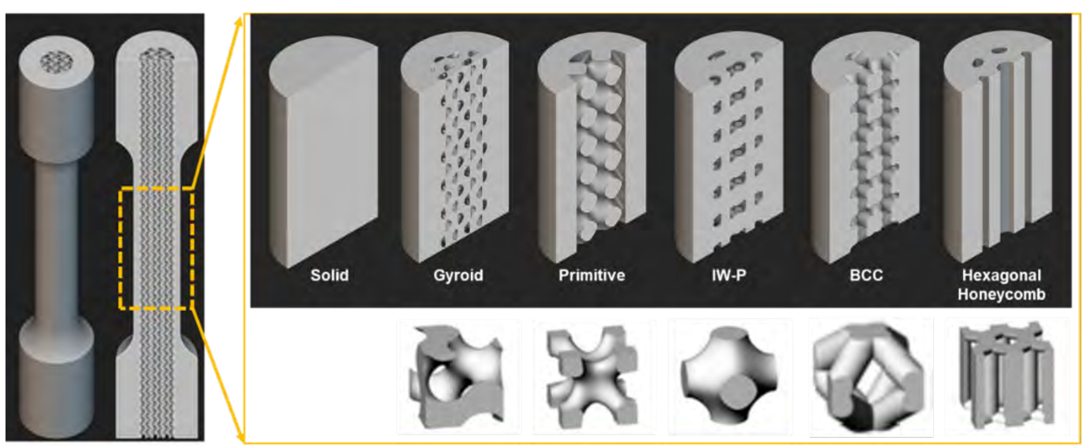
TOTAL APPROVED AMOUNT:
$1,618,200 over 3 years

PRINCIPAL INVESTIGATOR:
Rongjie Song

CO-INVESTIGATORS:
Dewen Yushu, INL
Donna Guillen, INL
Jia-Hong Ke, INL
Michael Heighes, INL
Michael McMurtrey, INL
Michael Moorehead, INL
Timothy Yoder, INL
Kevin Field, University of Michigan

Novel, lightweight, lattice structured, and nanotube-reinforced stainless steel provides superior performance and radiation tolerance for fission batteries.

Lightweight, high-performance materials are essential for transportable nuclear systems, such as fission batteries and plug-and-play microreactors. This project focuses on developing stainless steel 316L with lattice structures to achieve superior strength-to-weight ratios and enhanced radiation tolerance. Advanced modeling and simulation guided the design of lattice geometries, which were fabricated using laser powder bed fusion. Tensile testing confirmed the accuracy of the predicted mechanical behavior. Tensile and fatigue tests demonstrated that hexagonal honeycomb and gyroid lattices provide improved mechanical performance while reducing material weight. Radiation tolerance was further enhanced by incorporating carbon nanotubes into the stainless steel 316L matrix via laser powder bed fusion. The project establishes a workflow linking lattice design, multiphysics modeling, and additive manufacturing to produce lightweight, mechanically robust, and radiation-tolerant materials. These findings offer a pathway to next-generation structural materials for advanced nuclear systems, extending component lifetimes, reducing operational costs, and enabling more efficient deployment of portable nuclear energy technologies.



Tensile bar models generated in nTopology with different lattice types, enabling model-based prediction of tensile performance. Such modeling provides insights into the influence of lattice parameters and geometries, allowing the identification of optimized design prior to experimental fabrication. The benefit is model-based lattice design and properties prediction reduces experimental cost and time while enabling rapid optimization of mechanical performance.

TALENT PIPELINE:

- Jingfan Yang, postdoc at INL
- Junaid Dar, student at Oregon State University
- Lanh Trinh, student at University of Nebraska-Lincoln
- Matthew Lynch, student at University of Michigan
- Michael Moorehead, postdoc at INL, converted to staff
- Yisong Zhang, student at Oregon State University

PAPERS AND PRESENTATIONS:

- R. Song, M. Moorehead, D. Yushu and J.-H. Ke. "Lattice Design and Advanced Modeling to Guide the Design of High-Performance Lightweight Structural Materials." Energies, vol. 17, issue 6, 2024, pages 1468–1479.
- R. Song, M.J. Moorehead, D. Yushu and J.-H. Ke. "Computer-aided Lattice Design and Advanced Modeling for the Development of Lightweight Structural Materials." Transactions of 27th International Conference on Structural Materials in Reactor Technologies (SMiRT27), Yokohama, Japan, March 3-8, 2024.
- R. Song, M. Moorehead, X. Zhang, D. Yushu and J.-H. Ke. "Effect of Heat Treatment on Microstructure and Mechanical Property of 316L Stainless Steel Produced by Laser Powder Bed Fusion." Transactions of ANS Annual Conference, Las Vegas, NV, vol. 130, No. 1, June 2024, page 708.
- R. Song, M. Moorehead, D. Yushu, J. Yang and J.-H. Ke. "Lattice Structured Lightweight Structural Materials." Transactions of ANS Annual Conference, Chicago, IL, vol. 132, No. 1, June 2025, page 664.
- J. Yang, X. Zhang and R. Song. "Thermal Stability and Strengthening Mechanism of BNNT Reinforced 316L Stainless Steel Composites." Transactions of ANS Annual Conference, Chicago, IL, vol. 132, No. 1, June 2025, page 662.

Assessment of Long-range Ordering on the Corrosion Performance of Nickel-based Commercial Alloys in Molten Salts

PROJECT NUMBER:
23A1070-147FP

TOTAL APPROVED AMOUNT:
$1,675,000 over 3 years

PRINCIPAL INVESTIGATOR:
Trishelle Copeland-Johnson

CO-INVESTIGATORS:
Fei Teng, INL
Jia-Hong Ke, INL
Michael Woods, INL
Julie Tucker, Oregon State University
Kevin Field, University of Michigan

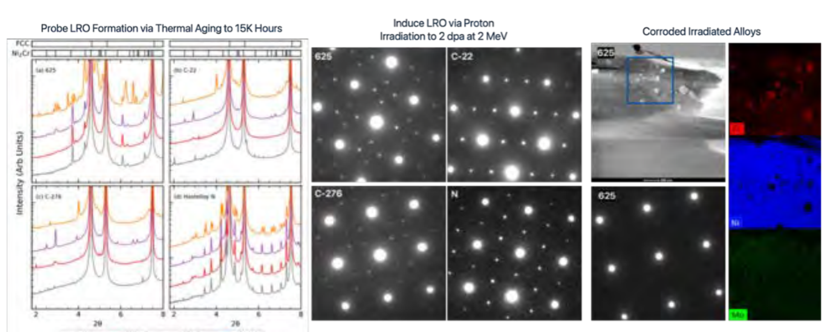
COLLABORATORS:
Stony Brook University

Nickel-chromium-molybdenum alloys enhance resistance to chloride molten salt corrosion.

Structural materials in molten salt reactors face corrosion, irradiation, and long-term thermal exposure, requiring alloys with stable performance over reactor lifetimes. Nickel-chromium-molybdenum (Ni-Cr-Mo) alloys show excellent corrosion and high-temperature strength, but can form a $Ni_2(Cr,Mo)$ long-range ordered phase under 400–700°C thermal or irradiation exposure, leading to lattice contraction and increased hardness that may reduce corrosion resistance.

This study investigated the likelihood of long-range order formation in structural candidates Hastelloy N, C-276, C-22, Alloy 625 versus model Ni-Cr-Mo alloys, identifying critical temperatures for ordering under operational conditions. A cluster-based computational model using density functional theory and Monte Carlo simulations was developed to predict long-range order stability and simulate chromium diffusion during corrosion. Experimental validation involved isothermal aging and 2 MeV proton irradiation up to 2 displacements per atom followed by molten salt corrosion testing at 550°C in sodium chloride–magnesium chloride for 500 hours. Microhardness testing, synchrotron x-ray diffraction, transmission electron microscopy, and selected area electron diffraction confirmed ordered phases. Scanning electron microscopy, energy-dispersive x-ray spectroscopy, and electron backscatter diffraction characterized post-corrosion microstructures. Results showed:

1. The predictive model successfully identified long-range order onset and chromium diffusion trends
2. Irradiation accelerated ordering, producing larger precipitates at lower temperatures and shorter times compared to thermal aging
3. Ordered precipitates persisted after corrosion, but corrosion extent did not significantly differ between ordered and as-received alloys, refuting the initial hypothesis
4. Overall, the study established that the $Ni_2(Cr,Mo)$ long-range ordered phase forms readily under irradiation but remains corrosion resistant. Future work will focus on property-to-performance correlations to clarify how long-range order influences molten salt corrosion and to inform alloy qualification for molten salt reactor applications.



(a) Synchrotron x-ray diffraction for each commercial alloy investigated in this work, plotted for each aging temperature after 15,000 h of aging, illustrating the presence/absence of long-range order at each temperature. (b) selected area electron diffraction micrographs on [001] zone axis of proton irradiated alloys, exhibiting superlattice reflections indicative of long-range order. (c) Brightfield transmission electron microscopy and associated energy-dispersive x-ray spectroscopy maps for Alloy 625 after a 500 h static corrosion test in sodium chloride–magnesium chloride.

TALENT PIPELINE:

- Xavier Quintana, student at Oregon State University
- Mackenzie Warwick, student at University of Michigan
- Hamdy Arkoub, student at Pennsylvania State University

PAPERS AND PRESENTATIONS:

- Teng, F., Copeland-Johnson, T. M., Tucker, J. D., Cao, G. "Accelerated corrosion of Ni-based alloys in molten chloride salts, due to Ni_2Cr phase formation." Materialia 31 (2023).
- F. Teng, T.M. Copeland-Johnson, G. Cao, J. D. Tucker, "Ni2Cr Long-Range Ordered Transgranular Precipitation-accelerated Corrosion of Ni-Cr Alloys in Chloride Molten Salt." The Minerals, Metals, and Materials Society (TMS), Mar. 3rd to 7th, 2024.
- F. Teng, "Degradational effects of atomic LRO in single-crystal deformation mode and corrosion resistance of Ni-based alloys for nuclear applications." TMS Fall 2024 Annual Meeting, Invited Speaker, Oct. 6th to 9th, 2024.
- X. Quintana, T. Copeland-Johnson, "Irradiation Effects on Ni-Cr-Mo Alloys with LRO." The Nuclear Materials Conference (NuMat), Invited Speaker, Oct. 14th to 17th, 2024.
- J. D. Tucker, "Enhanced Corrosion in Ni-Cr-Mo alloys with LRO." NuMat, Symposium Organizer/Invited Speaker, Oct. 14th to 17th, 2024.
- Quintana, X., Warwick, M., Teng, F., Tucker, J., Copeland-Johnson, T. European Corrosion Congress 2025 Presentation. "Assessment of Ni_2(Cr,Mo) Long-Range Ordering on the Corrosion Performance of Ni-Based Alloys in Molten Salt." Stavanger, Norway. Sept. 2025.
- Copeland-Johnson, T., Hawkins, L., Newell, B., Rittenhouse, J., Woods, M., Murray, D., Gakhar, R. European Corrosion Congress 2025 Presentation. "Evaluation of corrosion performance of Ni-Cr-Mo Hastelloy systems in NaCl-UCl_3." Stavanger, Norway. Sept. 2025.
- Quintana, X., Warwick, M., Teng, F., Tucker, J., Copeland-Johnson, T. "Anisotropic Growth of Ni_2(Cr,Mo) Ordered Phase in Proton Irradiated Ni-based Alloys." Scripta Materialia (2025).
- Quintana, X., Warwick, M., Teng, F., Tucker, J., Copeland-Johnson, T. "Assessment of the Impact of Mo on Long-Range Ordering on Thermally-Aged and Proton Irradiated Ni-Cr-Mo Alloys." Journal of Nuclear Materials (2025).
- Quintana, X., Warwick, M., Teng, F., Tucker, J., Copeland-Johnson, T. "Long-Range Ordering and its Synergistic Effects on the Corrosion Mechanism of Proton Irradiated Ni-Cr-Mo alloys." Journal of Nuclear Materials (2025).
- Teng, F., Zhou, W., Zhu, Y., Wang, Y., Liu, X., Murray, D., Yang, Y., Short, M., He, L. "Micromechanical characterization of irradiated/corroded Ni2Cr model alloys with Push-to-Pull (PTP) apparatus." Materials & Design (2025).
- Hamdy, A., Ke, J., Jin, M. "Understanding the Role of Chemical Ordering in Molten Salt Corrosion of Ni-Cr Alloys." Journal of Materials Science (2025).

Rapid Creep Strength Testing Through Multi-Stress Specimens

PROJECT NUMBER:
23A1070-155FP

TOTAL APPROVED AMOUNT:
$878,000 over 3 years

PRINCIPAL INVESTIGATOR:
Michael McMurtrey
Co-investigators:
Patrick Behne, INL
Robert Hansen, INL
Ninad Mohale, INL
Stephanie Pitts, INL

Novel pairing of digital image correlation, new specimen design, and computer simulation enables high-throughput creep testing.

The project focused on addressing the extended duration typically associated with creep testing in materials, which has traditionally been challenging to accelerate without compromising the integrity of the mechanisms involved. Utilizing a multi-stress specimen design with varying gauge thicknesses within a single specimen, significant reductions in the time required for testing and assessing creep properties were achieved. This innovative methodology was integrated with comprehensive microstructural analysis and advanced mathematical modeling to ensure accurate and reliable results. The fundamental mechanisms were preserved, providing precise data that could be extrapolated to real-world conditions.

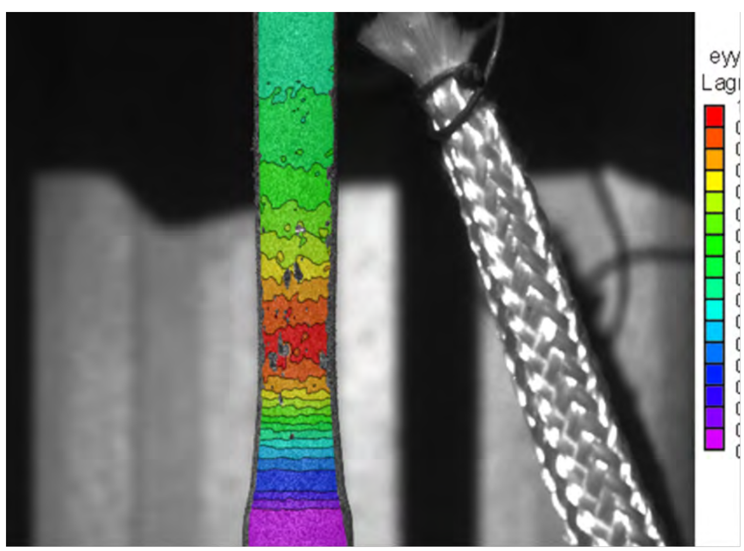
The primary objective was centered on developing a faster, yet accurate, method for creep testing, which was successfully realized. The results demonstrated substantial improvements over traditional methods, significantly reducing testing time while maintaining data integrity.

TALENT PIPELINE:

- Ninad Mohale, postdoc at INL, converted to staff

PAPERS AND PRESENTATIONS

- Behne, P., Mohale, N., Hansen, R., Pitts, S., McMurtrey, M., “Multiobjective Constrained Symbolic Regression for Predictive Modeling of Material Creep Behavior.” [POSTER] Machining Learning and Artificial Intelligence Exposition, Idaho Falls, ID, June 25, 2024
- Hansen, R., Mohale, N., McMurtrey, M., “Rapid Creep Strength Tests Using Multi-Stress Specimens and Digital Image Correlation.” Society for Experimental Mechanics, Milwaukee, WI, June 2-5, 2025.



Creep sample speckled for digital image correlation with a strain overlay. The color scale indicates strain levels, with red representing high strain and purple representing low strain.

High Spatial Resolution Mapping of Retained Fission Gas

PROJECT NUMBER:
24A1081-193FP

TOTAL APPROVED AMOUNT:
$1,050,000 over 2 years

PRINCIPAL INVESTIGATOR:
Alonzo Martinez

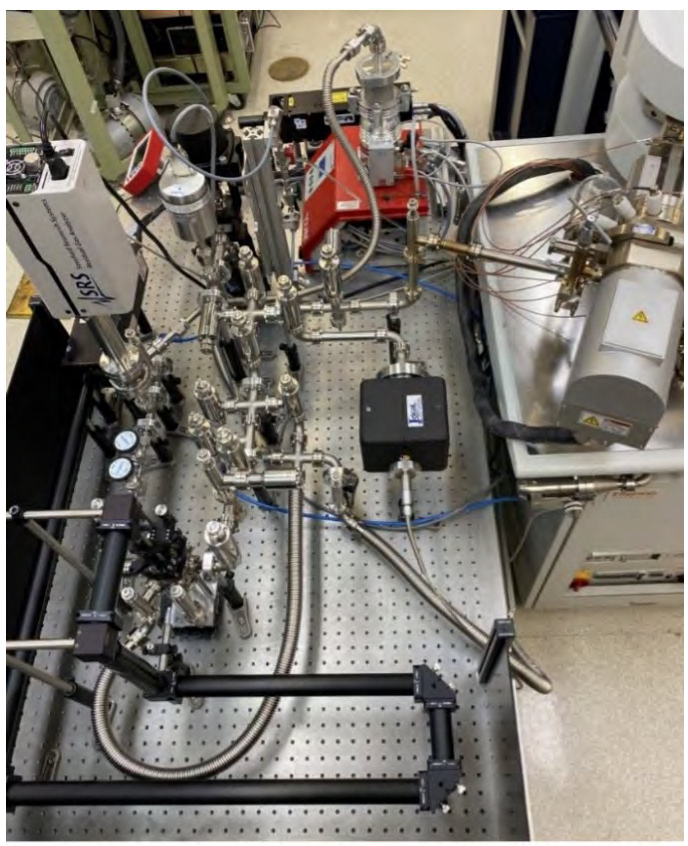
CO-INVESTIGATORS:
Gregory Eiden, INL
Heather Chichester, INL
John Olson, INL

Novel mass spectrometry capability informs nuclear fuel performance models.

Krypton and xenon gas are fission products, the isotopic analysis of which gives a quantitative determination of irradiated nuclear fuel burnup, provides other diagnostics such as age for unknown samples, and informs nuclear fuel performance models. A proof-of-concept was demonstrated for a measurement capability to map the isotopic composition of retained krypton and xenon gases at high spatial resolution (tens of micrometers). The capability was demonstrated using pulsed laser release of xenon implanted metal foils. Isotopic ratios of the released gas were measured with a static noble gas mass spectrometer. The foils were prepared with a mass separator modified under this project to enable implantation of multiple isotopes at a well-controlled isotope ratio. Focused ion beam sub-sampling was scheduled to prepare samples with which to demonstrate the method using irradiated fuel. However, sample production delays resulted in samples not being prepared with enough time to include in this report.

PRESENTATION:

- Martinez, A., Brookhart, J.L., Meiers, J.L., Olson, J.E., Eiden, G.C., Chichester, H.J.M. "High Spatial Resolution Mapping of Retained Fission Gas." [Poster session] GLOBAL2024, Tokyo, Japan, October 6–10, 2024.



The gas manifold that was assembled at the inlet to the static noble gas mass spectrometer. To the left on the optical table is the gas manifold that allows laser sampling and preparation of the extracted gas sample for mass spectrometer analysis. The manifold includes a sample chamber with a viewport for laser access, chemical getters and cold fingers for purification and cryogenic transfer of gases, and a gas pipette containing isotopically natural krypton and xenon with which to characterize instrument response. To the right is the inlet section of the static noble gas mass spectrometer.

Investigation Using the Multiphysics Object-Oriented Simulation Environment

PROJECT NUMBER:
24P1084-027FP

TOTAL APPROVED AMOUNT:
$132,000 over 1 year

PRINCIPAL INVESTIGATOR:
Pierre-Clément Simon

CO-INVESTIGATORS:
Mauricio Tano Retamales, INL
Carlo Fiorina, Texas A&M University
Susana Reyes, Xcimer Energy

Pierre-Clément Simon, Lab Director Award, Inclusive Diversity

Advancement of Experiment Interpretation with the Auto Corrected Reactimeter Algorithm

Project number:
24P1086-002FP

TOTAL APPROVED AMOUNT:
$250,000 over 2 years

PRINCIPAL INVESTIGATOR:
Paul Ferney

CO-INVESTIGATORS:
DeHart Mark, INL

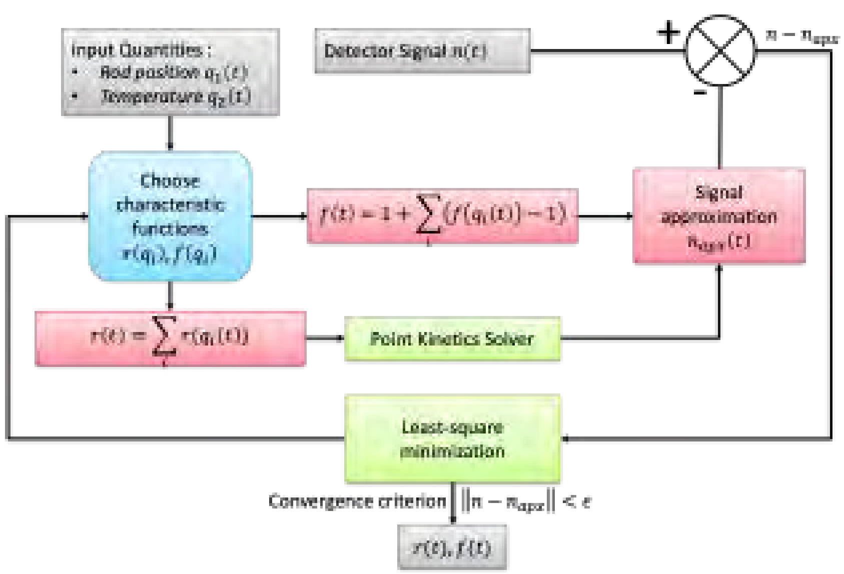
IMPACT STATEMENT:

Novel signal processing algorithm eliminates the need for simulations.

Analyzing neutron flux measurements often presents challenges in distinguishing global flux variations from local ones, complicating the understanding of reactor dynamics. Traditionally, simulations have been employed to compute corrections for these local flux variations. However, these simulations are often validated against the same experiments they aim to correct, leading to a significant flaw in the validation methodology. This project introduced the Signal Processing Algorithm for Reactivity and Transient Analysis (SPARTA), an innovative flux adjustment methodology designed to independently correct neutron flux measurements without relying on simulations. SPARTA processes experimental data, such as rod position and temperature, to iteratively generate quantities related to both global and local flux variations. Based on these quantities, SPARTA's algorithm generates a signal using point kinetic equations; the signal is then aligned with the experimental signal to minimize the difference between the two. SPARTA was rigorously tested and validated using a heat balance experiment conducted at the Transient Reactor Test Facility. The results obtained from SPARTA were consistent with both traditional interpretation methods and simulation data, demonstrating its reliability as an experimental analysis tool. Future methodologies like SPARTA can significantly enhance the interpretation of complex experiments involving temperature variations, thereby improving the accuracy of reactor models and advancing our understanding of reactor dynamics.

PAPER AND PRESENTATION:

- Paul A. Ferney, Ben A. Baker, Mark D. DeHart, "SPARTA: A flux adjustment methodology to interpret complex experiments." Annals of Nuclear Energy, Volume 223, 2025, 111623.
- Paul A. Ferney, Mark D. DeHart, "Benchmarking of Different Inverse Point Kinetics Implementations for an Autocorrected Reactimeter Algorithm." 2024 ANS Annual Conference.



Workflow of the SPARTA Algorithm. SPARTA is a flux adjustment method that utilizes point kinetics to iteratively fit detector signals with experimental data (e.g., rod position, temperature), thereby eliminating the need for transient simulations.

Development of Diffraction Contrast Tomography Technique to Study Crystallographic Grain Structures of Nuclear Materials

PROJECT NUMBER:
24P1087-013FP

TOTAL APPROVED AMOUNT:
$150,000 over 1 year

PRINCIPAL INVESTIGATOR:
Swapnil Morankar

CO-INVESTIGATORS:
Boopathy Kombaiah, INL
William Chuirazzi, INL

COLLABORATORS:
Xnovo Technology ApS
ZEISS Microscopy

X-ray diffraction contrast tomography unlocks insights into grain boundary characteristics and microstructural evolution in nuclear materials.

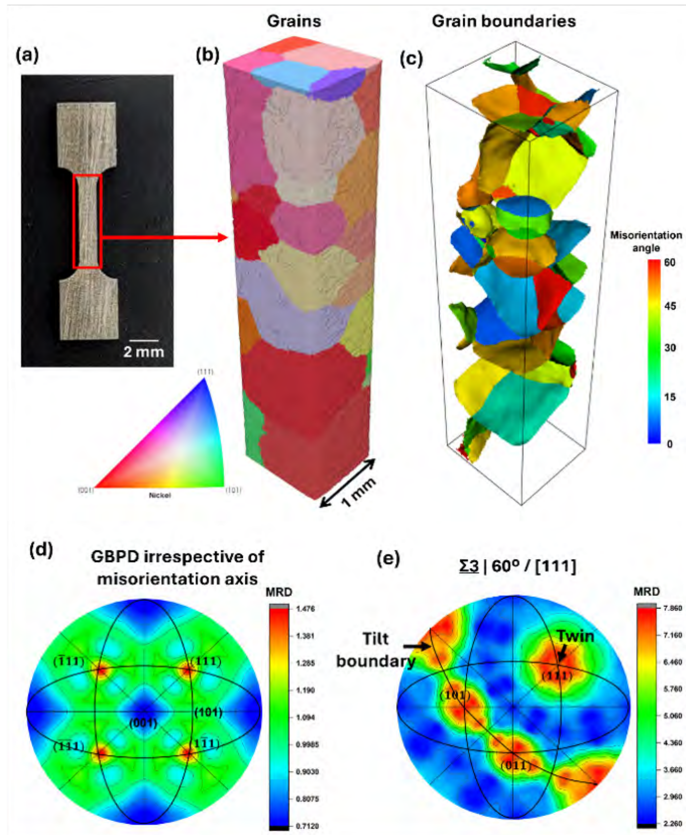
Structural materials used in nuclear reactors are subjected to extreme environments, including ultra-high temperatures and intense radiation, which drive grain growth and degrade material performance. Understanding the mechanisms and kinetics of grain growth is therefore essential for predicting material behavior and improving reactor component reliability. Grain characterization has traditionally relied on electron backscatter diffraction, a two-dimensional technique limited to surface analysis. While three-dimensional electron backscatter diffraction is possible, it is destructive and labor-intensive, making it unsuitable for in situ studies or tracking microstructural evolution over time. To overcome these limitations, this project successfully developed a complete workflow for data acquisition and analysis using the x-ray diffraction contrast tomography technique. Diffraction contrast tomography enables nondestructive, three-dimensional characterization of grains and grain boundaries. The technique was demonstrated using a nickel-8 chromium alloy sample, where grains and grain boundaries were reconstructed in three-dimensions and validated against electron backscatter diffraction measurements. Grain and grain boundary characteristics as a function of annealing were also studied. A post-processing pipeline was also developed to perform quantitative analysis of grain size, misorientation angles, and grain boundary characters. In the nickel-8 chromium alloy, grain boundaries exhibited prominent misorientation angle peaks around 51 and 60 degrees. Further analysis revealed that many of these boundaries had twin and tilt characters. In addition, most grain boundary planes were oriented along {111}, which are the closest-packed and lowest-energy planes in face-centered cubic structures. These findings align with theoretical expectations for equilibrium microstructures. The successful implementation of the diffraction contrast tomography technique provides a powerful new capability for three-dimensional grain structure analysis in nuclear materials. It opens new avenues for investigating both fundamental mechanisms and applied challenges in materials science, including those relevant to nuclear energy systems.

TALENT PIPELINE:

- Swapnil Morankar, postdoc at INL, converted to staff

PRESENTATIONS:

- S. Morankar, B. Kombaiah, W.C. Chuirazzi, "Thermomechanical Effects on Grain Structure Evolution in Ni-8Cr Alloy Using X-ray Diffraction Contrast Tomography." The Minerals, Metals, and Materials Society's Annual Meeting, Las Vegas, NV, March 2025.



(a) Tensile sample of nickel-8 chromium alloy. (b) Reconstructed three-dimensional grain structure of the gauge section. Grains are color-coded based on inverse pole figure. (c) Isolated grain boundaries color-coded based on their misorientation angles. (d) Grain boundary plane distribution irrespective of misorientation axis in terms of multiples of random distribution. (d) Grain boundary character distribution for Σ3 type boundaries in terms of multiples of random distribution.

Reconfigurable Intelligent Surface for Improved Coverage and Enhanced Security for Nuclear Power Plants

PROJECT NUMBER:
24P1087-024FP

TOTAL APPROVED AMOUNT:
$157,400 over 1 year

PRINCIPAL INVESTIGATOR:
Imtiaz Nasim

CO-INVESTIGATORS:
Vivek Agarwal, INL
Shannon Eggers, INL
Ahmed Mohamed, Florida International University

Reconfigurable intelligent surface technology enhances wireless communication coverage and security in nuclear facilities.

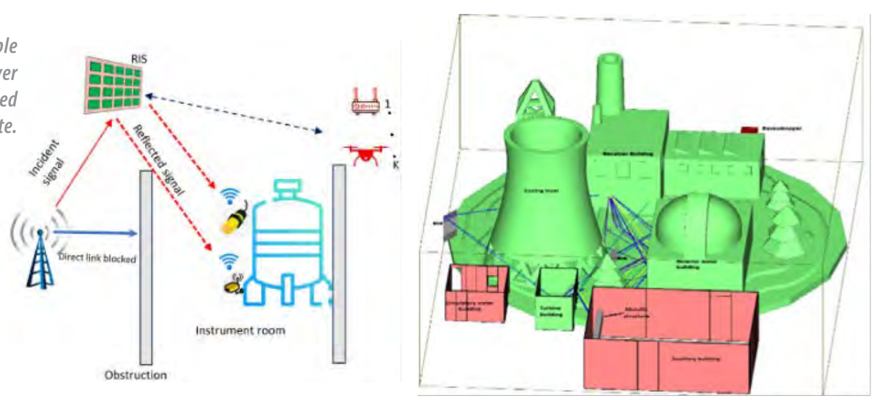
This project focused on addressing the challenges of wireless communication in nuclear power plants, specifically issues related to coverage and data transmission security. Given the high data security requirements of nuclear power plants due to the transmission of sensitive information, ensuring robust and secure wireless communication is critical. The wireless coverage is hindered by high signal attenuation due to the reflective environment, dense metallic structures, electromagnetic interference, and concrete walls of nuclear reactors. For security, the signal received by legitimate receivers must be protected against eavesdropping or other interception, as open-air communication is vulnerable to such attacks. To address these issues, this research demonstrated via simulation that the use of reconfigurable intelligent surfaces can control the reflection of incident radio waves. The research compared the effects of no reconfigurable intelligent surfaces (i.e., baseline model) and multiple reconfigurable intelligent surfaces on wireless coverage and security, designing their locations and parameters to achieve improved results. Our methodology involves generating a simulation dataset that mimics wireless propagation and characteristics in a typical nuclear plant environment. A novel data-driven solution, a multi-armed bandit-based algorithm is developed, to determine the optimal reconfigurable intelligent surface locations and reflection parameters to maximize the wireless coverage and security. This algorithm is effective in both dynamic and static environments because it is updated based on changes in the eavesdropper's position, making it suitable for various scenarios. This project's success is significant because it can provide critical evidence to regulatory agencies about potential improvements achievable with emerging wireless applications like reconfigurable intelligent surfaces in nuclear plants.

TALENT PIPELINE:

- Deniz Aytemiz, student at Virginia Tech University

PRESENTATION:

- I. Nasim, V. Agarwal, A. S. Ibrahim and S. Eggers, "Revisiting Reconfigurable Intelligent Surface for Improved Coverage in Nuclear Plants." Nuclear Plant Instrumentation, Control & Human-Machine Interface Technologies, 2025.



(a) A nuclear facility with reconfigurable intelligent surfaces, transmitter and receiver nodes, and multiple attacker, and (b) Simulated nuclear power plant using Wireless Insite.

Scramjet Hydrogen Injection Fission-Fusion Thermal Propulsion Reactor

PROJECT NUMBER:
24P1088-011FP

TOTAL APPROVED AMOUNT:
$86,000 over 1 year

PRINCIPAL INVESTIGATOR:
Boone Beausoleil

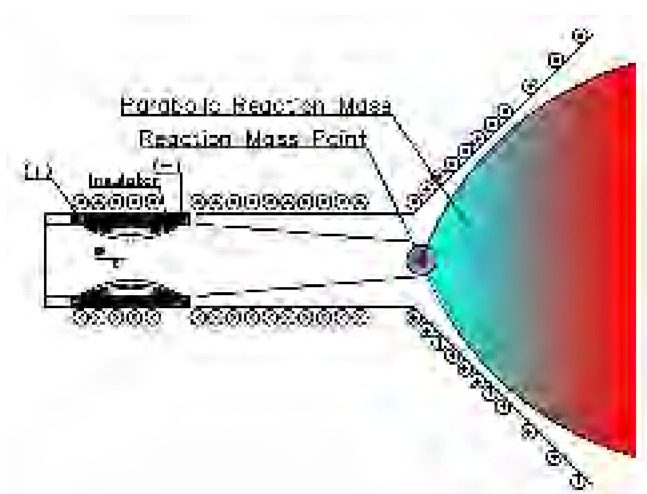
CO-INVESTIGATORS:
Casey Icenhour, INL

Hybrid fission-fusion reactor provides significant propulsion gains for interplanetary travel.

This project validated the hypothesis that a fission based nuclear thermal propulsion system could be used in conjunction with a compression system similar to a scramjet to produce sustained fusion for a direct energy propulsion drive. This project performed a series of analyses to develop this concept, which is referred to as the Fission Assisted Ramjet Ignition System reactor. First, a survey of existing and demonstrated fission based nuclear thermal propulsion systems was performed to characterize the potential thresholds needed to create a steady stream of high temperature hydrogen within the exhaust stream that could be ionized to plasma. The exhaust stream was approximated as an adiabatic compressible fluid flow through a magnetic coil that compresses the plasma into a pinch (Z-pinch). The results of this first analysis were used to show a relative comparison to the Lawson criteria of the plasma and as constraints to plasma modeling. The second analysis performed was done in the MOOSE-based plasma fluid code, Zapdos. Here, one-dimensional analyses were performed using magnetohydrodynamics equations—a plasma model representing constitutive gases as fluids—to simulate plasma flow and conditions within the pinch. Both analyses suggest that plasma densities comparable to those needed for a sufficient level of fusion energy are possible with such a configuration. However, it was noted that higher-dimensional analysis needs to be performed in future efforts to capture all possible plasma flow conditions and more accurately calculate plasma density.

TALENT PIPELINE:

- Corey DeChant, Russell L. Heath distinguished postdoc at INL
- Noah Simon, student at North Carolina State University



A representation of the Fission Assisted Ramjet Ignition System reactor concept. This would be attached to a nuclear thermal propulsion fission reactor and utilize electricity produced by the reactor to maintain continuous magnetic confinement and magnetically assisted nozzle.

Stochastic Space Fission and Microreactor Design Analysis to Support Design Optimization Using Artificial Intelligence Methods

PROJECT NUMBER:
24P1091-002FP

TOTAL APPROVED AMOUNT:
$700,000 over 2 years

PRINCIPAL INVESTIGATOR:
Jackson Harter

CO-INVESTIGATORS:
Venkateswara Dasari
Mark DeHart
Nicolas Martin

COLLABORATORS:
Antares
Argonne National Laboratory
BWX Technologies
Dark Fission
Los Alamos National Laboratory
National Aeronautics and Space Administration
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
RAND School of Public Policy
Tennessee Tech University
Texas A&M University, Galveston
University of New Mexico
University of Texas at San Antonio
X-energy

Modeling and simulation advance nuclear power in space.

This project focused on the design, analysis, and optimization of advanced microreactor systems to support fission surface power and nuclear electric propulsion applications. Work encompassed the characterization of three distinct microreactor concepts, including two heat-pipe-cooled configurations and one sodium-potassium-cooled design. A significant component of the effort involved developing expertise in the MOOSE-based code DireWolf, particularly its coupling with the Stochastic Tools Module to perform uncertainty quantification and sensitivity analyses. This training equipped participating interns with the computational and analytical skills necessary for high-fidelity reactor modeling.

Building upon this foundation, the team conducted extensive optimization studies on the heat-pipe microreactor design. Using gradient descent and Bayesian optimization methods, researchers established a methodology to optimize key reactor parameters—such as fuel temperature and reactivity—based on physical geometry and material characteristics. These results provide a framework for systematic design improvement and inform future efforts to enhance the performance and safety of compact reactor systems for both space and terrestrial applications.

The project led the organization of two Space Technology for Advanced Reactor Fueling Innovation in Research and Exploration (STAR☆FIRE) summer workshops in 2024 and 2025. These events convened students, researchers, and professionals from industry, academia, and national laboratories to advance space nuclear technology through education and collaboration. The 2024 workshop, hosted at Idaho National Laboratory, engaged 28 students from 12 universities, while the 2025 session at the Atomic Museum in Las Vegas welcomed 40 students from 20 universities. Together, these workshops strengthened the community of emerging researchers and fostered innovation in space nuclear systems.

Overall, the project advanced computational methodologies, fostered technical workforce development, and strengthened collaborative networks supporting the next generation of microreactor design and space nuclear power research. INL staff assisted in the planning, development, and mentoring of interns during FY-24 and FY-25, and also added input to the planning and execution of STAR☆FIRE. These staff members were Hikaru Hiruta, Matthew Johnson, Sonali Sinha Roy, and Dean Price (joint appointment).

TALENT PIPELINE:

- Brandon Bloss, student at Missouri University of Science and Technology
- Jonathan Geymer, student at North Carolina State University
- Felicity Griffin, student at Pennsylvania State University
- Wafaa Osman, student at North Carolina State University
- Leo Tunkle, student at University of Michigan

Astronaut Colonel Mike Fossum takes a selfie with the attendees of Space Technology for Advanced Reactor Fueling Innovation in Research and Exploration 2025 at the Atomic Museum in Las Vegas, Nevada.

Optimization Oriented Surrogate Models for Control in Digital Twinning

PROJECT NUMBER:
25P1094-006FP

TOTAL APPROVED AMOUNT:
$175,000 over 1 year

PRINCIPAL INVESTIGATOR:
Dean Price

CO-INVESTIGATORS:
Linyu Lin, INL
Mark DeHart, INL

Optimization oriented surrogate models enhance advanced reactor safety and operational flexibility.

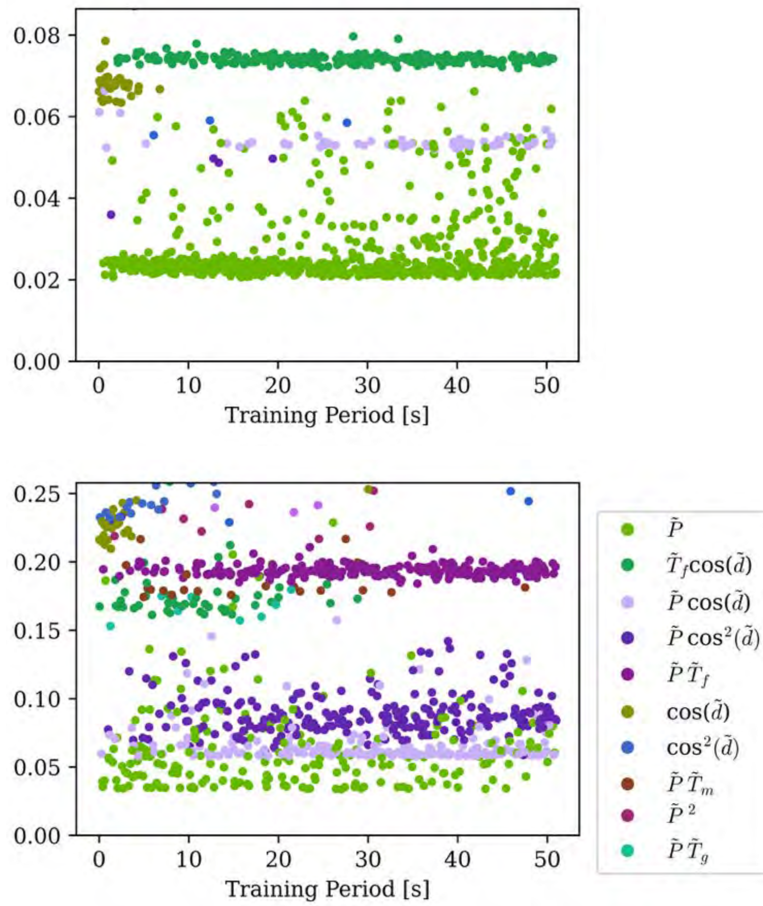
The project aimed to develop physics-informed (PIN) sparse identification of nonlinear dynamics (SINDy) models to enhance the accuracy and efficiency of dynamic modeling for nuclear microreactors. These models are formulated such that their gradients are computable and should therefore be considered an optimization-oriented surrogate model. Recognizing the complexities and constraints associated with real-time control applications, the research focused on integrating physics-based models with data-driven techniques to achieve a robust representation of reactor dynamics. By leveraging the existing SINDy methodology, the project sought to identify key relationships and behaviors within the reactor system using observational data while also incorporating established physical principles to mitigate the challenges of poor conditioning often encountered in data-driven approaches.

Throughout the project, notable advancements were made in developing and demonstrating the PIN-SINDy framework, which successfully enhanced the predictive capabilities of surrogate models for microreactor dynamics. The methodology was rigorously tested using data generated from high-fidelity simulations, showcasing its effectiveness in accurately capturing the complex interactions within the reactor during various operational scenarios.

The accomplishments included the successful application of PIN-SINDy to datasets of varying complexity, demonstrating its versatility and potential for real-time control applications. This work significantly contributed to the field of nuclear reactor dynamics by providing a novel methodology that combines physics-informed insights with machine learning techniques to yield high-accuracy models that can support digital twin controllers.

TALENT PIPELINE:

- Dean Price, Russell L. Heath distinguished postdoc at INL



Notable result from project, performance of PIN-SINDy model varies depending on dynamic term included in surrogate model. Mean relative absolute error in predicted power is shown on y-axis and time require.

INTEGRATED FUEL CYCLE SOLUTIONS

CORE CAPABILITIES

Advanced Computer Science

Applied Materials Science & Engineering

Applied Mathematics

Chemical Engineering

Chemical and Molecular Science

Computational Science

Earth and Energy Systems and Infrastructure Analysis and Engineering

Earth, Environmental, and Atmospheric Science

Nuclear Engineering

Nuclear Physics

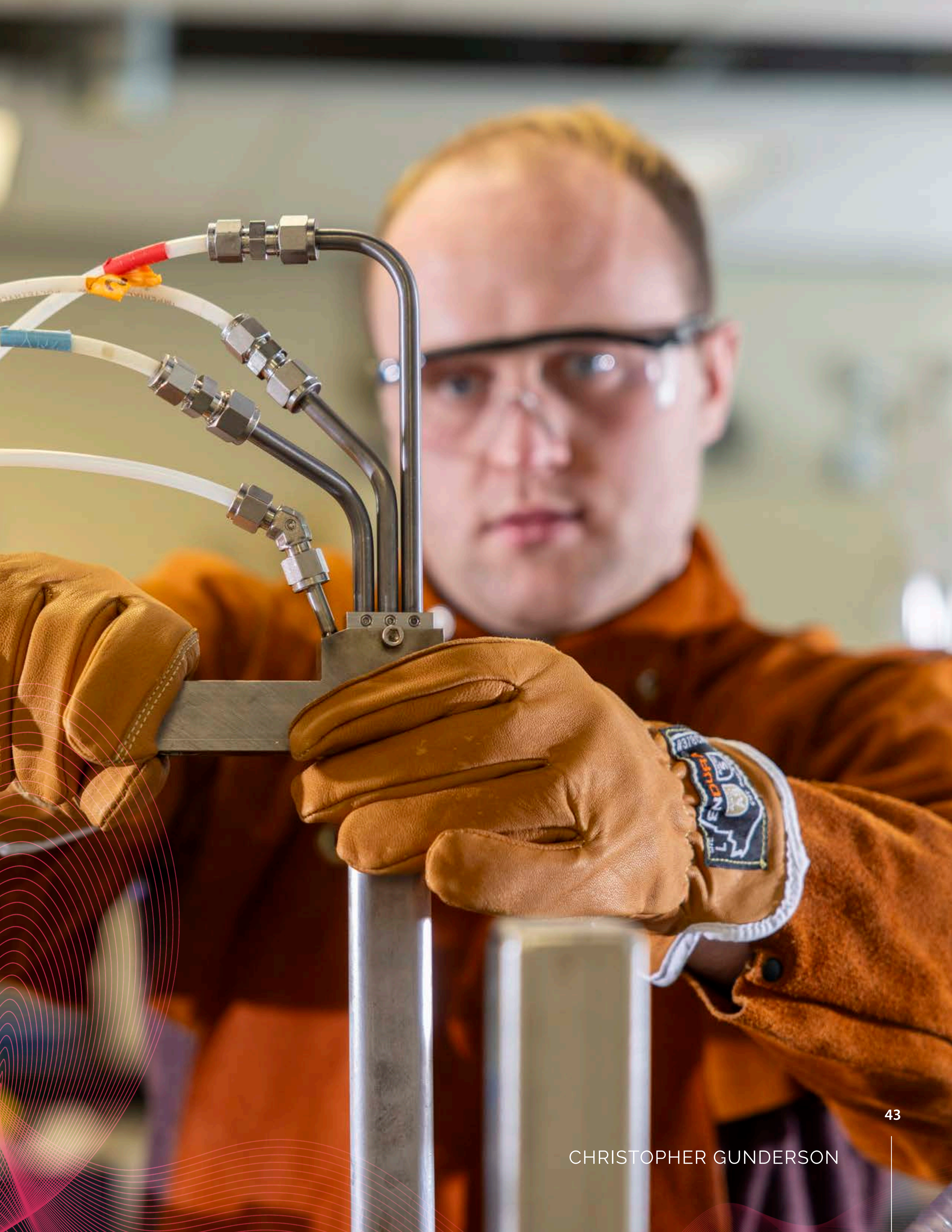
Nuclear and Radio Chemistry

Nuclear and Radiochemistry

Systems Engineering and Integration

Visualization, and Data

We develop integrated fuel cycle solutions that sustain the existing commercial reactor fleet and enable US energy dominance. Our work spans the development of innovative fuel cycle technologies and capabilities that support advanced reactor systems as well as the safe management and disposition of current and future radiological waste materials. Our focused RD&D in recycling and waste minimization improves the economics and security of nuclear energy systems.



CHRISTOPHER GUNDERSON

Understanding the Behavior of Oxides in Molten Chloride Salts and Their Effects on Speciation of Molten Salts for Molten Salt Reactors

PROJECT NUMBER:
23A1070-007FP

TOTAL APPROVED AMOUNT:
$1,590,000 over 3 years

PRINCIPAL INVESTIGATOR:
Guoping Cao

CO-INVESTIGATORS:
Ruchi Gakhar, INL
Jianguo Yu, INL
Trishelle Copeland-Johnson, INL

New electrochemistry technique measures dissolved oxide impurities in molten salt reactors in real time.

Impurities like oxides and moisture in molten salts for molten salt reactors can change the redox chemistry and may also lead to the precipitation of fissile materials, thus violating the reactivity control fundamental safety function. It is important to understand the precipitation of fissile materials such as uranium chloride, redox chemistry change due to impurities, and the speciation of the oxides and chloride salts and their interactions.

In this project, a combination of bi-modal spectroscopy and electrochemistry (or spectroelectrochemistry) was employed to investigate the fundamental chemical behavior of oxides in chloride salts and how the oxides affect the speciation of chloride salts. Meanwhile, first-principles molecular dynamics modeling was used to understand the solubility of uranium oxides in molten chloride salts. Based on systematic experimentation and first-principles molecular dynamics modeling, the following major important findings and accomplishments were made on behavior of oxides in molten chloride salts and their effects on speciation of molten salts for molten salt reactors:

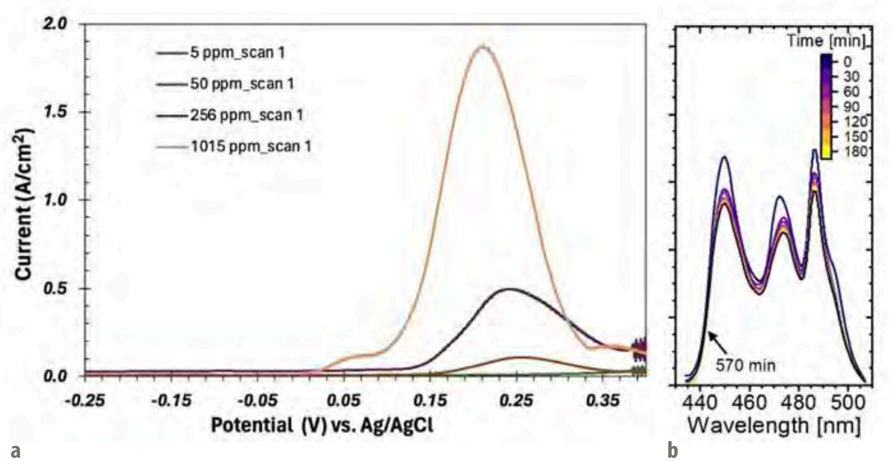
1. Unique experimental spectroelectrochemistry capability has been developed for fundamental studies on molten salt chemistries and speciations of impurities in molten salts.
2. Spectroscopy studies were conducted to characterize the effects of oxides on the salt chemistries, speciation of the rection products between lithium oxide (Li_2O) and neodymium(III) chloride ($NdCl_3$) in lithium chloride (LiCl)-potassium chloride (KCl)-3.4wt%$NdCl_3$ salt, and kinetics of the reaction between the oxide and $NdCl_3$. The $Li_2O/NdCl_3$ ratio determined the rection products neodymium oxychloride or neodymium oxide and the reaction kinetics.
3. The square wave voltammetry is sensitive and reliable to measure very small amounts (as low as 5 ppm) of dissolved oxides in molten chloride salts. It can also be used for measurement of the solubility of rare earth oxides in molten salts. Both iridium and gold can be good working electrodes for oxide measurement.
4. The solubility of oxides (uranium oxide and neodymium oxide) in molten salts was evaluated by combining ab initio molecular dynamics and thermodynamics analysis, enabling the estimate of oxide solubility in fuel salt with high concentration of uranium chloride for molten salt reactors.

TALENT PIPELINE:

- Kavindan Balakrishnan, student at University of Idaho
- Garrett LeCroy, postdoc at INL
- David Ramgren, student at Colby College
- Kelly Varnell, student at Penn State University
- Qiufeng Yang, postdoc at INL, converted to staff

PRESENTATIONS:

- Guoping Cao, Ruchi Gakhar, "Corrosion of 316H in different crucible materials in 800°C NaCl-MgCl2 salt," Molten Salt Symposium, 2023 American Chemical Society (ACS) Fall Meeting.
- Qiufeng Yang, Ruchi Gakhar, Guoping Cao, "Electrochemical and Spectroscopy Study of Oxide Speciation in Molten Chloride Salts," Molten Salt Symposium, 2023 ACS Fall Meeting.
- Guoping Cao, Qiufeng Yang, Garrett S. LeCroy, Kelly Varnell, Ruchi Gakhar, Electrochemical methods for oxide impurity measurement in chloride salts for MSRs, Molten Salt Thermal Properties Working Group Workshop on Effect of Oxygen, Hydrogen, and Moisture on Molten Salt Behavior June 3-4, 2025.
- Garrett LeCroy, Qiufeng Yang, Guoping Cao, Ruchi Gakhar, *In situ* Monitoring of Lanthanide Reactions with Oxide Species via Combined Absorption Spectroscopy and Electrochemical Methods, 13th International Conference on Methods and Applications of Radioanalytical Chemistry (MARC XIII), March 23–28, 2025, Kailua-Kona, HI, USA.



(a) Square wave voltammetry of LiCl-KCl with different concentration of Li_2O at 600°C (b) In situ electronic absorption spectroscopy monitoring of reaction of praseodymium ions with 1153ppm Li_2O in LiCl-KCl-NaCl-3.4wt% praseodymium chloride salt at 500°C.

Online Process Monitoring and Uncertainty Quantification of Nuclear Material in Molten Salt Reactor Fuel Salt Using Spectroscopy Techniques

PROJECT NUMBER:
23A1070-034FP

TOTAL APPROVED AMOUNT:
$1,170,000 over 3 years

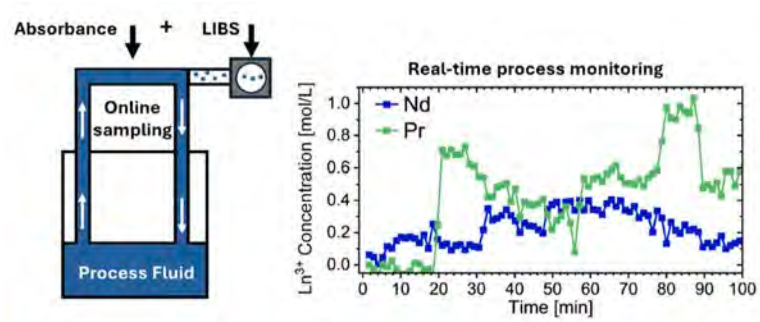
PRINCIPAL INVESTIGATOR:
Ammon Williams

CO-INVESTIGATORS:
Matt Jones, INL
Nick Erfurth, INL
Piyush Sabharwall, INL
Ruchi Gakhar, INL
Igor Jovanovic, University of Michigan

COLLABORATORS:
University of Michigan

A novel online sampling mechanism monitors complex salt streams in molten salt reactors.

This project successfully developed and demonstrated a novel online molten salt sampling mechanism that enables real-time spectroscopic characterization of molten salts, thus allowing continuous monitoring of complex salt streams in molten salt reactors and pyroprocessing applications. By providing a continuous, real-time sampling method, this innovative approach bridges a critical gap in existing technologies, enhancing operational efficiency, nuclear safeguards, and nuclear material accountancy. This project resulted in the patent of our molten salt reactor high-temperature aerosol spectroscopy system, marking a significant contribution in the field. Utilizing state-of-the-art spectroscopy techniques, including laser-induced breakdown spectroscopy and ultraviolet-visible absorption spectroscopy, the team achieved precise measurements on high-temperature chloride salts containing rare earth fission product surrogates. The system showed real-time concentration monitoring with errors in prediction of less than 0.2 weight percent. These techniques, combined with advanced chemometric modeling, have substantially improved the accuracy and reliability of monitoring systems, significantly reducing uncertainty in material quantification. Enhancements in resonant and double-pulse laser-induced breakdown spectroscopy techniques were also achieved, resulting in higher sensitivity measurements. These advancements provide promising results for online monitoring in molten salt reactor and pyroprocessing applications. The impact of this work extends beyond nuclear safeguards, with applications in monitoring corrosion products, tritium buildup, and other critical aspects of molten salt reactor safety. This project has made substantial contributions to the field of nuclear engineering, providing innovative solutions for real-time monitoring and uncertainty quantification in molten salt systems, thereby paving the way for safer and more efficient nuclear energy applications.



Absorbance and laser-induced breakdown spectroscopy were performed on the online sampling stream. The combination of these two techniques allowed real-time process monitoring wherein trivalent lanthanide fission product surrogates (Ln^{3+}) were monitored as the process fluid underwent spikes of either neodymium (Nd) or praseodymium (Pr).

TALENT PIPELINE:

- Ashton Dziengue, student at Savannah State University
- Chris Gundersen, student at Idaho State University, hired as staff
- Cooper Rokop, student at Michigan State University
- Garrett LeCroy, postdoc at INL
- George Sun, student at University of Michigan
- Juan Avila Gutierrez, student at Florida International University
- Londrea Garrett, student at University of Michigan
- Micah Raab, postdoc at INL
- Qiufeng Yang, postdoc at INL, converted to staff
- Rachelle Austin, postdoc at INL

PAPERS AND PRESENTATIONS:

- G. LeCroy, Q. Yang, M. Raab, R. Gakhar, A.N. Williams, "Online monitoring of Lanthanide species with combined spectroscopy in flowing aqueous aerosol systems." RSC Advances, 2025, 15, 35036-35046.
- G. Sun, L. Garrett, A.N. Williams, I. Jovanovic, "Preliminary Measurements of Solid FliNaK Samples with Double-Pulse Laser-Induced Breakdown Spectroscopy." ANS Winter Meeting, Nov. 9-12, 2025.
- A.N. Williams, G. LeCroy, J. Meiers, R. Austin, R. Gakhar, "Molten Salt Reactor Process Monitoring using Laser and Optical Spectroscopy Techniques." ANS Winter Meeting, Nov. 9-12, 2025.
- I. Jovanovic, L. Garrett, G. Sun, M. Burger, A.N. Williams, "Molten Salt Composition Measurements with Double-Pulse and Resonant Laser-Produced Plasmas." Material Science & Technology 2025, Columbus OH, Sept. 28-Oct. 1, 2025.
- G. LeCroy, R. Gakhar, R. Roper, A.R. Ballesteros, J. Meiers, A.N. Williams, "In Situ Spectroscopic Monitoring of MSR Molten Salt and Off-Gas Systems." Institute of Nuclear Materials Management (INMM) Annual meeting, Washington DC, Aug. 25-28, 2025.
- R. Roper, R. Gakhar, A.R. Ballesteros, A.N. Williams, "A high-temperature optical cell for chemical analysis of vapor using combined spectroscopy approaches." RSC Advances, 2025, 15, 12563-12576.
- G. Sun, L. Garrett, A.N. Williams, I. Jovanovic, "Toward the Development of Molten Salt Reactor Diagnostics based on Resonantly Enhanced Laser Spectroscopy." ANS Annual Meeting, Chicago IL, June 15-18, 2025.
- 8. G. Sun, L. Zhao, L. Garrett, A.N. Williams, I. Jovanovic, "Development of Automated Data Collection for Laser-Induced Fluorescence Measurements of Fission Fragments." ANS - Student Conference, Albuquerque NM, April 3-5, 2025.
- L. Garrett, M. Burger, A.N. Williams, I. Jovanovic, "Detection of Neodymium and Surrogate Materials via Laser-Induced Fluorescence." ANS Winter Meeting, Orlando FL, Nov. 17-21, 2024.
- A.N. Williams, R. Gakhar, Q. Yang, A. Butikofer, C. Rokop, M. Raab, "A Molten Salt Aerosol Spectroscopy Approach to Online Process Monitoring in Molten Salt Reactors." INMM Annual Meeting, Portland OR, July 19-25, 2024.
- M. Raab, A.N. Williams, R. Gakhar, Q. Yang, R. Roper, "*In Situ* Monitoring of Molten Salts and Off-Gases Using a Combined Spectroscopic Approach.", ACS Norm, Pullman WA, June 23-26, 2024.
- R. Gakhar et al., "Online Molten Salt and Off-Gas Monitoring Using Coupled Spectroscopy Techniques" The Minerals, Metals & Materials Society (TMS), 2024 Meeting, Orlando, FL, March 3-7, 2024.
- A.N. Williams, J. Avila, R. Gakhar, Q Yang. "Design and Optimization of an Aerosol Optical Cell for Spectroscopy Analysis for Molten Salt Reactor Safeguards." American Nuclear Society—Winter Meeting, Washington DC, Nov.12-15, 2023.
- A.N. Williams, R. Gakhar, Q. Yang, J. Avila, I. Jovanovic, M. Burger, L. Garrett. "Online Molten Salt Reactor Sampling Approach using Laser and Optical Spectroscopy Techniques in Molten Salt Aerosol." ANS Winter Meeting, Washington DC, Nov.12-15, 2023.
- A.N. Williams, R. Gakhar, J. Avila, Q. Yang, "Ultraviolet-Visible Spectroscopy (UV-VIS) Measurement of Rare Earth Chlorides in Aerosol." ACS Fall Meeting, San Francisco CA, Aug. 13-17, 2023.

EXTERNAL INTELLECTUAL PROPERTY:

- A.N. Williams, R. Gakhar, S. Sabharwall, 2339-1709US Provisional Patent. "Nuclear Material Management with Continuous Online High-Temperature Liquid Sampling and Analysis." Filed March 2023.

EXTERNAL AWARDS:

- Londrea Garrett received a Hoffman Postdoctoral Fellowship at Lawrence Berkeley National Laboratory

Enhancement of Gamma Ray Emission Modeling Through Advanced Analysis of Random and True Coincidence Summing Effects

PROJECT NUMBER:
23A1070-062FP

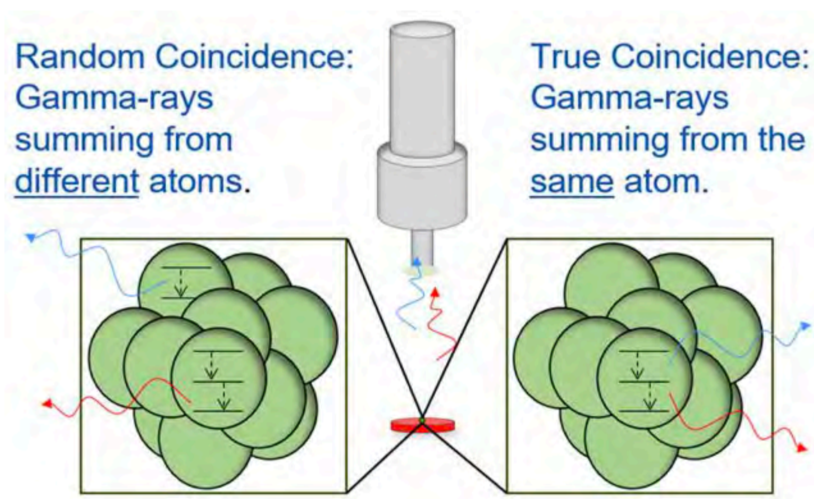
TOTAL APPROVED AMOUNT:
$1,308,000 over 3 years

PRINCIPAL INVESTIGATOR:
Thomas Holschuh

CO-INVESTIGATORS:
Jay Hix, INL
James Johnson, INL
Teancum Quist, INL
Scott Thompson, INL
Jaime Diaz, INL
Ethan Bauer, INL

New gamma ray spectroscopy capabilities improve nuclear forensics.

Advanced modeling and simulation efforts have improved at INL in recent years with a solid foundation of experimental results. Current computational methods represent significant modeling capabilities but are limited by the accuracy and availability of nuclear data. The creation of pre- and post-processing software tools to address these limitations is fundamental to the improvement of nuclear science modeling capacities. One aspect of predictive modeling tools deals with gamma rays emitted from radionuclides, including fissile or fissionable material, fission products, or activation products, produced in reactor experiments or other neutron environments. The resulting radionuclides decay in unique ways, providing complications upon measurement as a result of random and cascade or true coincidence summing. These effects are not easily quantified during modeling efforts of gamma ray source terms. Several of the challenges in this field have now been addressed. Random coincidence summing can now be accounted for in measured and simulated gamma ray spectra, which eases efforts when comparing the two methodologies for analyzing radiation detector outputs. Next, the germanium rotational measurements for angular correlation systems have been designed and assembled for use when measuring anisotropically emitted gamma rays. This is impactful for future nuclear forensics programs when determining origins of nuclear debris based on the trace isotopics of embedded fission products.



FDepiction of random and true coincidence summing similarities and differences.

TALENT PIPELINE:

- Jaime Diaz, student at Northern Arizona University
- Ethan Bauer, student at Idaho State University

EXTERNAL INTELLECTUAL PROPERTY:

- BEA Docket: BA-1599, Neutron Dosimeters and Related Methods, Thomas Holschuh
- CW-24-36: CRYPT—Calculator for Radioisotopic Yields, Products, and Targets
- CW-24-37: TRYC—Total Radioisotope Yield Calculator
- CW-24-38: GREASE—Gamma Ray Exportable Adjustable Spectrum Evolution

Transient Multiphysics Simulation of Spent Fuel Repositories for Pebble Bed Reactors

PROJECT NUMBER:
23A1070-117FP

TOTAL APPROVED AMOUNT:
$1,050,000 over 3 years

PRINCIPAL INVESTIGATOR:
Rodrigo de Oliveira

CO-INVESTIGATORS:
Gordon Petersen, INL
Alexander Lindsay, INL
Paolo Balestra, INL
Ahmed Almetwally, University of Texas at Austin
Mary Wheeler, University of Texas at Austin

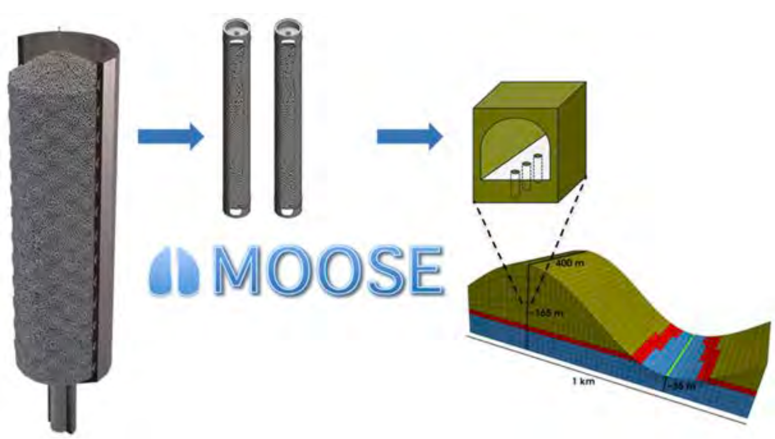
New models and methods advance pebble bed reactor fuel cycle understanding.

There is a significant gap in understanding of used nuclear fuel from pebble bed reactors. While the understanding of the fuel during operation is robust, the understanding of behavior of the fuel during long-term storage after irradiation is outdated. This project aimed to use state-of-the-art computational tools to fill gaps in understanding of this waste form after it is discarded from the reactor to during its storage in a final repository.

Big problems studied included the cool down, transmutation, and criticality of pebbles as they leave the reactor and are placed in a canister for storage. A new methodology and software capabilities have been developed to address analysis of canisters in MOOSE. In addition, the problem of porous flow in repository bedrock has been tackled, where new capabilities and methodologies have also been developed and implemented in MOOSE to simulate nuclide geo-transport.

Results of the studies indicate that, in principle, a pebble of relatively high burnup can be put into a canister straight from the discard outlet because it takes days for activity to reduce sufficient for gamma spectroscopy to be done and to decide whether a pebble will be recycled or discarded. Geological disposal models have shown accuracy relative to available benchmarks, making them a promising approach to future geological repository studies.

Plans to discard pebbles directly into canisters are feasible assuming that the canister's external surface is appropriately cooled. Also, geological repositories housing disposed pebbles seem resilient to nuclide dispersal to the environment, highlighting the simplicity of disposal after use.



Concept of the project, where pebbles are discarded from a pebble bed reactor, put inside a canister, and the canister is put in a geological repository where it will stay for an indeterminate amount of time safely.

TALENT PIPELINE:

- Ahmed Almetwally, student and postdoc at the University of Texas at Austin
- Brecken Allegood student at Idaho State University

PRESENTATIONS:

- Almetwally, A. G., and Wheeler, M. F. (March 2025). "Compositional Reservoir Simulation Using Enriched Galerkin and Phase Field Formulation." SPE Reservoir Simulation Conference. Galveston, TX, USA.
- Almetwally, A. G., Wheeler, M. F., and de Oliveira, R. (June 2025). "MOOSE-Based Application for Performance Assessment of Nuclear Waste Geologic Disposal." ANS Annual Conference 2025. Chicago, IL, USA.
- Almetwally, A. G., Wheeler, M. F., and Podgorney, R. K. (October 2024). "FORGE Geothermal Project Modeling using Phase Field Finite Element." 2024 Geothermal Rising Conference. Waikoloa, HI, USA.
- Almetwally, G. A., Wheeler, F. M., and Podgorney, R. K. (Fabruary 2025). "Simulation of EGS Fracturing Dynamics Using Phase field Finite Element." 50th Workshop on Geothermal Reservoir Engineering. Stanford, CA, USA.
- de Oliveira, R., Hanophy, J., Balestra, P., and Gaston, D. (2024). "Long Time Scale Multiphysics Simulation of Spent Nuclear Fuel Canister in MOOSE." PHYSOR24. San Francisco.

Development of Two-Phase Separation Techniques for Advanced Fuel Cycle Studies

PROJECT NUMBER:
23A1070-162FP

TOTAL APPROVED AMOUNT:
$1,150,000 over 3 years

PRINCIPAL INVESTIGATOR:
Corey Pilgrim

CO-INVESTIGATORS:
Colt Heathman, INL
Gregory Holmbeck, INL
Dean Peterman, INL

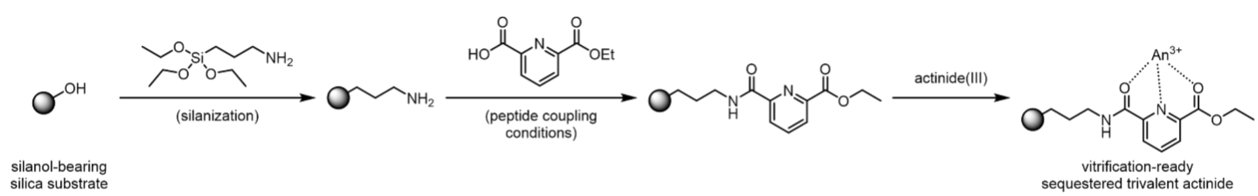
COLLABORATORS:
Pacific Northwest National Laboratory
University of Nevada, Las Vegas
University of Notre Dame

Silica-grafted chelators make used nuclear fuel processing easier and cheaper.

Standard hydrometallurgical systems for reprocessing used nuclear fuel typically result in large volumes of waste that must undergo further processing to allow for disposition. However, if the radiotoxicity of the large solution volumes can be reduced, handling and storage of the subsequent liquid becomes easier and cheaper. The vision of this project was to address this issue by designing a method to extract these radioactive metals—primarily the minor actinides—utilizing a heterogeneous separation technique where the liquid would be contacted with a solid phase that would retain these deleterious metals. Solid phase extractants are already used within reprocessing systems but are typically organic in nature (i.e., impregnated resins). We hypothesized that the use of silica-based extractants would provide a more streamlined approach because the used extractants could then be directly fed into a vitrification process.

Leveraging the vast literature of solution-based complexants synthesized for metal extraction, we targeted specific functional groups to attach to the silica substrate that we hoped would be selective for the minor actinides, which typically have a +3 charge. We started with commercially available materials but transitioned to compounds that were synthesized in-house because the efficiency of the commercially available materials was not adequate for our needs. Subsequent testing of the materials showed that picolinic acid and malonic acid-derived chelators might prove favorable in the two-phase extraction systems.

While there are challenges—i.e., material loading issues and stability in highly acidic media—to these silica-based systems, we also developed means to increase functionalization density on the silica substrate and have explored different linkages between the silica and the chelators that can better withstand hydrolysis.



The simple yet effective synthetic recipe to couple a chelator (in this case, a dipicolinic acid derivative) to the silica substrate.

TALENT PIPELINE:

- Kash Anderson, early career research scientist at INL
- Steven Rehbein, *Glenn T. Seaborg distinguished postdoc at INL*
- Logan Smith, student at University of Nevada, Las Vegas
- Zoe Smith, student at University of Notre Dame

PRESENTATIONS:

- Rehbein, S. M., K. R. Anderson, C. R. Heathman, C. D. Pilgrim, D. R. Peterman, 2025. "Vitrification-Ready Functionalized Silica Materials for Actinide(III)-Lanthanide(III) Separations." 48th Annual Actinide Separations Conference (Lemont, IL, May 20–22).
- Peterman, D. R., C. D. Pilgrim, K. R. Anderson, S. M. Rehbein, G. P. Holmbeck, C. R. Heathman, 2025. "Encapsulation of Metal Ions Using Functionalized Solid Phase Extractants." Thirteenth International Conference of Methods and Applications of Radioanalytical Chemistry (Kailua-Kona, HI, March 23–28).
- Heathman, C. R., C. D. Pilgrim, K. R. Anderson, N. Rasmussen, G. P. Holmbeck, 2023. "Evaluation of Functionalized Particles for Solid-Liquid Separations." 46th Annual Actinide Separations Conference (Idaho Falls, ID, May 16–18).

Photochemical Manipulation and Radiolytic Evaluation of Aqueous Americium Separations

PROJECT NUMBER:
23P1077-006FP

TOTAL APPROVED AMOUNT:
$519,000 over 2 years

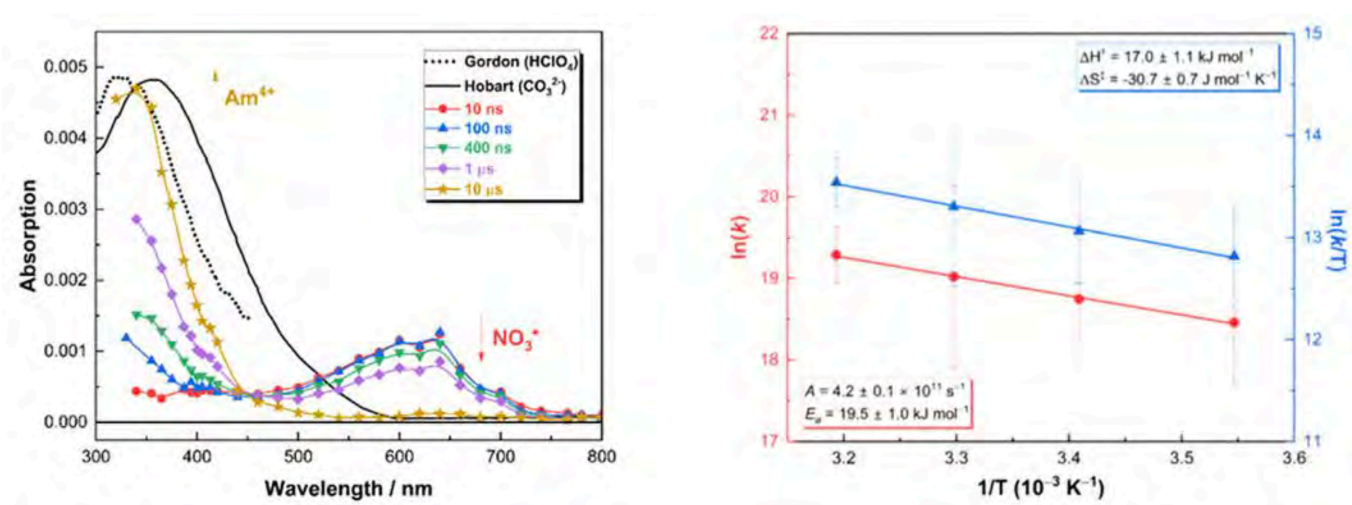
PRINCIPAL INVESTIGATOR:
Amy Kynman

CO-INVESTIGATORS:
Travis Grimes, INL
Gregory Holmbeck, INL

COLLABORATORS:
Brookhaven National Laboratory
Lawrence Berkeley National Laboratory
California State University, Long Beach
Lawrence Livermore National Laboratory

First-of-a-kind temperature-controlled irradiation experiments reveal fundamental chemistry that could lead to safer used nuclear fuel storage.

The separation and recovery of highly radioactive americium (Am) from used nuclear fuel using solvent extraction reprocessing technologies could mitigate the long-term impacts of nuclear waste on the environment by reducing the radiotoxic and thermal burden of Am on geological repositories. To improve existing technologies and establish innovative techniques to recover Am from used nuclear fuel, a deeper fundamental understanding of its inherent radiation-induced chemical behavior is required. Historically, this knowledge is limited. In this project, a series of radiation-induced chemical reactions of Am were studied, thereby improving our knowledge of complex mechanisms underpinning its molecular level behavior in solution. State-of-the-art electron pulse radiolysis facilities at Brookhaven National Laboratory were used to study the radiation-induced redox reaction of Am(III) with the oxidizing nitrate radical (NO_3•), allowing for the unusual Am(IV) oxidation state to be observed in concentrated nitric acid (HNO_3) for the first time. Furthermore, by designing and using a custom-built temperature cell, the first-ever temperature-dependent, radiation-induced kinetics study of an actinide element was performed. Finally, a systematic, time-resolved pulse radiolysis study of Am(III) complexed by organic minor actinide extractant was performed to explore the reactivity of Am(III) complexes with NO_3•. Here, enhanced reactivity (an order of magnitude faster) of NO_3• was seen upon Am(III) complexation, which has interesting implications for the functional lifetime of reprocessing solvents under radiation fields.



(a) Dose normalized transient absorption spectra from the electron pulse irradiation of 2.32 mM Am(III) in aerated 6.0 M HNO_3 at 21 ± 1°C for several time slices after the electron pulse. Scaled ambient temperature Am(IV) spectra reported by Gordon and Hobart are shown as a dotted and solid black lines, respectively. (b) Combined Arrhenius and Eyring plots utilizing second-order rate coefficient data from the reaction of Am(III) with NO_3• at 8, 22, 30, and 40 ± 1°C.

TALENT PIPELINE:

- Amy E. Kynman, *Glenn T. Seaborg distinguished postdoc* at INL, converted to staff

PAPERS AND PRESENTATIONS:

- Kynman, Amy E., Grimes, Travis S., Mezyk, Stephen P., Layne, Bobby, Cook, Andrew R., Rotermund, Brian M., and Horne, Gregory P. "Generation and study of Am(IV) by temperature-controlled electron pulse radiolysis," Dalton Transactions 2024, 53, 9262.
- Kynman, Amy E., Grimes, Travis S., Cook, Andrew R., Peterman, Dean R., and Horne, Gregory P. "Influence of americium complexation on the radiation-induced chemical reactivity of sulfophenyl bistriazinyl pyridine (SO_3-Ph-BTP) toward the nitrate radical," Radiation Physics and Chemistry 2026, 239, 113246.
- A. E. Kynman (Invited Talk), "Investigating radiation-induced actinide species in solution," TMS2025 Annual Meeting & Exhibition, Las Vegas, Nevada, USA, March 2025.
- A. E. Kynman, "Investigating radiation-induced actinide species in solution," Inorganic Reaction Mechanisms Gordon Research Seminar, Pomona, California, USA, March 2025.
- A. E. Kynman, "Generation and study of Am(IV) by temperature-dependent electron pulse radiolysis," Inorganic Reaction Mechanisms Gordon Research Conference, Pomona, California, USA, March 2025.
- A. E. Kynman, "Investigating radiation-induced actinide species in solution," Nuclear Energy Agency Global Forum Rising Stars Workshop, Karlsruhe, Germany, November 2024.
- A. E. Kynman, "Generation and study of Am(IV) by temperature-controlled electron pulse radiolysis," 4th International Conference on Ionizing Processes, Notre Dame, Indiana, USA, August 2024.
- A. E. Kynman, "Purification techniques for actinide radiation chemistry experiments," 4th International Conference on Ionizing Processes," Young Investigator Workshop, Notre Dame, Indiana, USA, August 2024.

EXTERNAL AWARDS:

- The Organisation for Economic Co-operation and Development Nuclear Energy Agency Global Forum Rising Star 2024.

Proliferation Detection via Acoustic Monitoring of Pyroprocessing Equipment and Related Systems

PROJECT NUMBER:
24A1081-144FP

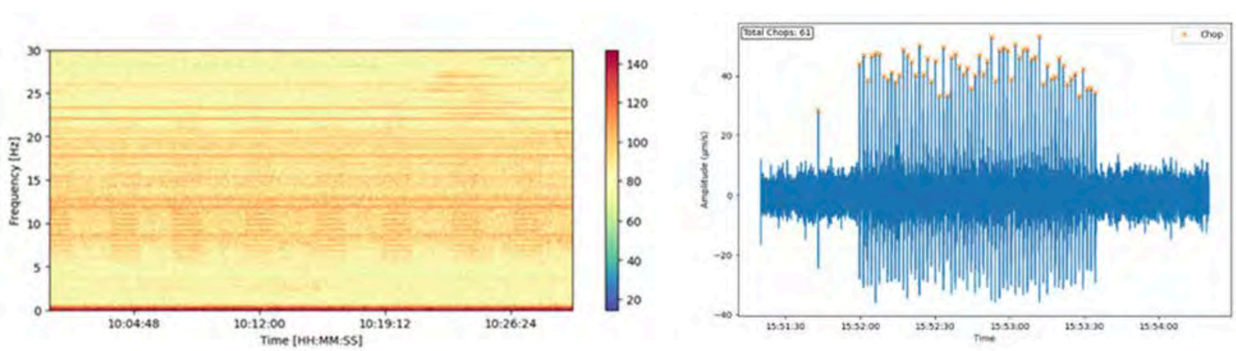
TOTAL APPROVED AMOUNT:
$747,000 over 2 years

PRINCIPAL INVESTIGATOR:
Edna Cárdenas

CO-INVESTIGATORS:
Luis Ocampo Giraldo, INL
Michael Patterson, INL

Innovative seismoacoustic monitoring safeguards nuclear materials.

This project focused on evaluating the capabilities of seismoacoustic detection and monitoring to enhance the safeguarding of nuclear materials within pyroprocessing systems. Pyroprocessing is a chemical method used to recycle nuclear fuel and minimize waste, specifically by separating uranium from other waste products generated in irradiated nuclear fuel. The equipment used in pyroprocessing is confined to heavily shielded hot cells, which present significant challenges to safeguards due to high temperatures, intense radiation, and restricted access. To address these issues, seismoacoustic monitoring was investigated as a potential safeguarding tool. Initial evaluations identified the product element chopper as the most promising target for detection. Monitoring campaigns at INL's Fuel Conditioning Facility involved placing sensors directly outside a hot cell containing an element chopper used for processing sodium-bonded nuclear fuel. Comprehensive signal analysis, corroborated by operator logs, verified the alignment of seismoacoustic signals with the fuel chopping process. Distinct operational features—such as chopping rate, number of chops, different fuel components being chopped, and abnormal events—were identified. A machine learning model was subsequently developed to recognize normal chopping events. The research demonstrated that seismoacoustic monitoring could significantly enhance safeguards in pyroprocessing by verifying chopping operations against records and identifying anomalous activities. This innovative approach offers a robust method to aid in nuclear material accountability and security in pyroprocessing environments.



(a) Spectrogram of seismic signals, most prevalent between 5 Hz and 20 Hz, measured during nuclear fuel chopping at INL's Fuel Conditioning Facility. The signal duration reflects the time taken to segment the fuel into 61 pieces. Harmonic spacing indicates the chopping rate. (b) Individual chops highlighting the initial chop of the fuel spade, which has a lower magnitude than subsequent chops.

TALENT PIPELINE:

- Souleymane Cissokho, student at Rose-Hulman Institute of Technology
- Marcellus Boykin, student at Georgia Institute of Technology
- Melissa Daw, student at College of Eastern Idaho, converted to staff
- Kenton Hummel, postdoc from University of Nebraska-Lincoln

PRESENTATIONS:

- Hummel, K., Hix, J., and Cárdenas, E., "Mounted Accelerometer Frequency Response of Adhesive Products and Aluminum Frame Quick Mounts," Vibration, 8(4), 61 (2025). https://doi.org/10.3390/vibration8040061.
- Ocampo Giraldo, L., Cárdenas, E., and Patterson, M., "Acoustic Monitoring of Pyroprocessing for Safeguards," Global2024, Tokyo, Japan. (October 7, 2024).
- Cissokho, S., and Ocampo Giraldo, L., "Python Processing of an Infrasound mSeed File," Infrasound Technology Workshop, Vienna, Austria. (November 6, 2024) Infrasound Technology Workshop 2024.
- Hummel, K., Cárdenas, E., Ocampo Giraldo, L., Hix, J., and Johnson, J. (September 8, 2025). Seismoacoustic Monitoring of Pyroprocessing Equipment. CTBT: Science and Technology Conference 2025, Vienna, Austria.

AWARD:

- 3rd place winner at the LDRD poster session

Tribonucleation of Gases in Molten Salts

PROJECT NUMBER:
24P1084-028FP

TOTAL APPROVED AMOUNT:
$137,000 over 1 year

PRINCIPAL INVESTIGATOR:
Aditya Moudgal

CO-INVESTIGATORS:
Robin Roper, INL
David Holcomb, INL

Understanding tribonucleation in molten salts opens new pathways for improving fission gas removal in molten salt reactors.

In this study, we conducted tribonucleation experiments aimed at investigating the removal of fission gases from molten salts. Tribonucleation, a process involving the generation of bubbles through the mechanical action of friction, was chosen due to its potential to efficiently extract fission gases, which is critical for the safe and effective operation of molten salt reactors.

To carry out these experiments, we designed and constructed an experimental apparatus tailored for our specific objectives based on a pin-on-disk tribometer. This apparatus was able to simulate the conditions under which tribonucleation might be observed in our candidate molten salts.

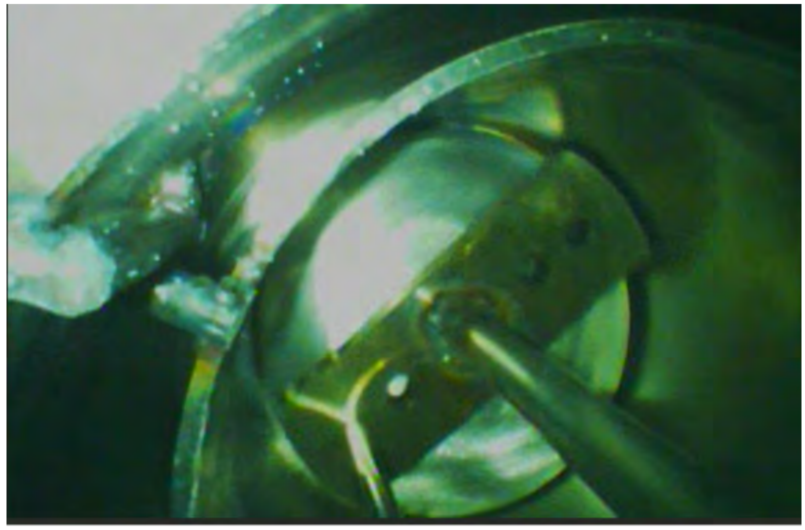
We selected three candidate salts for our tests: a eutectic mixture of lithium chloride and potassium chloride, a nitrate-based mixture of sodium nitrate and potassium nitrate, and a fluoride-based ternary salt mixture that consists of lithium fluoride, sodium fluoride, and potassium fluoride. These salts were chosen due to their relevance and widespread use in nuclear technology and molten salt reactors.

The tests conducted did not yield the desired outcomes. Throughout the series of experiments, we did not observe the formation of any bubbles, indicating that tribonucleation was not successfully induced under the conditions we tested. This lack of bubble generation suggests that either the mechanical action was insufficient to initiate tribonucleation or that the chosen salts and experimental parameters were not conducive to this process. Another significant challenge encountered during the experiments was the difficulty in imaging the rubbing surfaces, which impeded our ability to precisely analyze the tribonucleation process due to the high temperatures (400–550°C). Due to the imaging difficulties, it is also possible that bubbles were formed but were not detectable.

Whether the unsuccessful results are due to experimental conditions or imaging difficulties, the findings highlight the need for further investigation and optimization of experimental conditions. Though no bubbles were observed, the apparatus design itself was successfully tested and demonstrated. This study provides valuable insights and a foundation for future research in the quest to enhance the safety and efficiency of molten salt reactors.

TALENT PIPELINE:

- Aditya Moudgal, postdoc at INL
- Robin Roper, postdoc at INL, converted to staff



High temperature experimental setup to test tribonucleation of bubbles in molten salts.

Advanced Manufacturing of Sol-gel Based Uranium Particles as Reference Materials

PROJECT NUMBER:
24P1089-012FP

TOTAL APPROVED AMOUNT:
$150,000 over 1 year

PRINCIPAL INVESTIGATOR:
Justin Cooper

CO-INVESTIGATORS:
Mathew Snow, INL
Christopher Zarzana, INL
Gregory Eiden, INL

COLLABORATORS:
Critical Materials and Energy Systems Innovation Center

Printing individual uranium oxide particles presents a fast, tunable way to produce uranium reference materials.

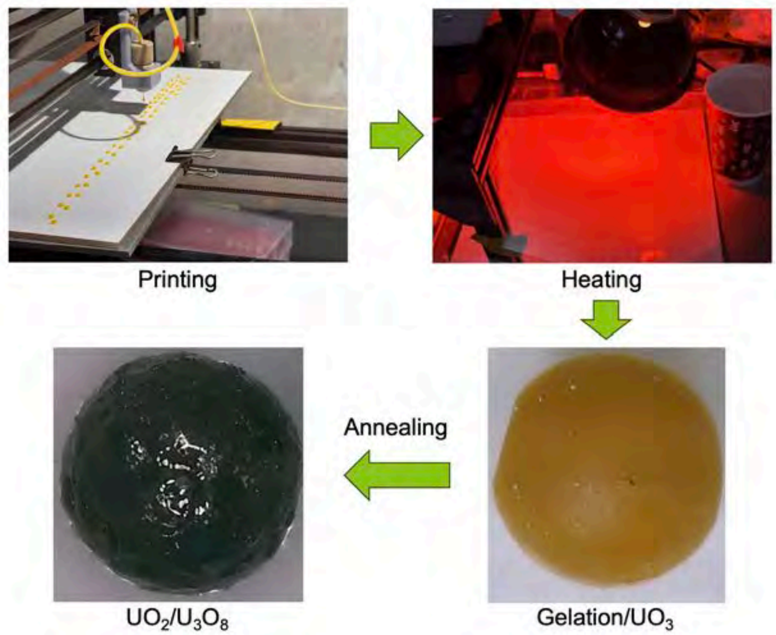
The purpose of this project was to develop and demonstrate a novel method to produce uranium oxide microsphere particles with tunable chemical compositions via a low-temperature sol-gel process using an advanced manufacturing setup. These particles can serve several purposes in research and development as either a forensic training tool or standard reference materials. A key component of the project was to demonstrate an ability to control physical and chemical parameters of the uranium sol-gel precursor material and the subsequent particles created. First, we successfully developed an internal gelation sol-gel method to an automated advanced manufacturing particle printing process to print individual uranium oxide particles of varying sizes. The uranium oxide sol-gel chemical composition and physical integrity were explored as a function of thermal processing temperatures. We also demonstrated the ability to control the secondary matrix composition of the particles by separately incorporating radionuclides of forensic interest into the sol-gel solution. It was observed that a subset of uranium fission products was successfully incorporated and retained in the uranium sol-gel during the gelation process, demonstrating the potential of this technique to generate uranium oxide materials with targeted fission product content with a high degree of precision across a wide range of processing temperatures. Finally, we demonstrated the ability to quantitatively control the isotopic composition of the particles by synthesizing particles with a specific and targeted uranium-237:uranium-238 and neptunium-237:uranium-238 ratios.

TALENT PIPELINE:

- Adelaide Fanner, Master Student University of Idaho
- Kolby Olney, Junior Scientist, INL

PAPER AND PRESENTATIONS:

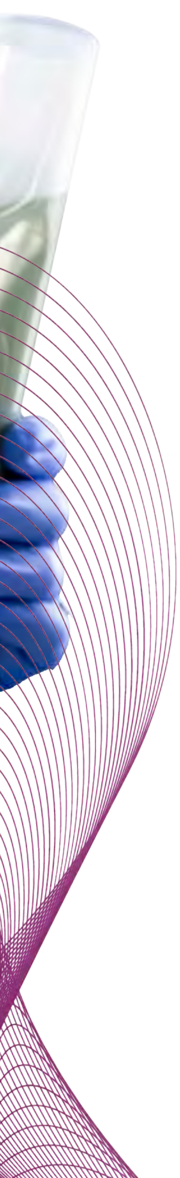
- Cooper, J. T. "Actinide and Fission Product Reference Materials for Nuclear Forensics and Radiological Safety Applications," Presented at FY25 Particle Working Group – Analytical SME Workshop, Los Alamos National Laboratory, Los Alamos, New Mexico, February 5-6, 2025.
- Cooper, J. T. "Recent Advances in Solid Post-Detonation Nuclear Forensic Benchmarking Materials," Presentation at 76th Southeastern and 81st Southwest Joint Regional Meeting of the ACS, Orlando, FL, October 26-29, 2025.



Uranium sol-gel advanced manufacturing process.

WENJUAN BIAN & WEI TONG

INTEGRATED ENERGY SYSTEMS



CORE CAPABILITIES

Applied Materials Science & Engineering

Biological and Bioprocess Engineering

Chemical and Molecular Science

Chemical Engineering

Computational Science

Decision Science and Analysis

Earth and Energy Systems and Infrastructure Analysis and Engineering

Mechanical Design and Engineering

Nuclear Engineering

Power System and Electrical Engineering

Systems Engineering and Integration

We are pioneering innovative technologies that integrate energy generation, storage, and delivery into cohesive, efficient systems. Our multiscale energy systems research combines nuclear and renewable heat with diverse electricity generation sources alongside carbon capture and sequestration to enable US energy dominance while improving grid reliability, resilience, and affordability. Our RD&D spans the innovation spectrum from foundational science to commercial-scale demonstrations. Our Energy Technology Proving Ground features megawatt- and megaton-scale test beds that enable private sector developers to validate new technologies and solutions. These efforts will accelerate advancements in the transportation, chemical, manufacturing, and electric power sectors, driving a cleaner, more resilient energy future.

Development and Demonstration of Versatile Modular Heat Pipe Integrated Thermal Battery for High-Temperature Integrated Energy Systems

PROJECT NUMBER:
22A1059-046FP

TOTAL APPROVED AMOUNT:
$2,189,800 over 4 years

PRINCIPAL INVESTIGATOR:
Sunming Qin

CO-INVESTIGATORS:
Jun Soo Yoo, INL
Daniel Mikkelson, INL
Rami Saeed, INL
Jeremy Hartvigsen, INL
Minseop Song, INL
Konor Frick, INL
Yassin Hassan, Texas A&M University

Innovative heat storage design integrates with any advanced nuclear reactor.

Thermal energy storage transforms heat into a dispatchable energy asset, yet technical challenges, particularly in system interfacing, hinder its commercial-scale deployment in the energy sector, including when integrating thermal energy storage with nuclear energy systems. This project aims to develop an innovative battery-type thermal energy storage design, the heat pipe integrated thermal battery (HITB), which can be seamlessly integrated with emerging microreactor designs. The HITB features high-temperature liquid-metal heat pipes that are displaceable and replaceable, combined with latent- or sensible-heat thermal energy storage technology. These passive heat transfer devices facilitate heat exchange between the HITB and external systems without requiring pumps or separate heat exchangers. Additionally, the thermal energy storage medium within HITB is isolated from external systems, minimizing safety and contamination concerns associated with combining different systems. The HITB comprises four main components: thermal energy storage medium, thermal energy storage container, heat pipes, and heat pipe drive mechanism. The heat pipe drive mechanism operates heat pipes based on thermal energy storage modes: when in charge mode, the heat pipe condenser enters the thermal energy storage medium while the evaporator is exposed to an external heat source, enabling heat transfer to the thermal energy storage medium. In discharge mode, the process is reversed. This innovative battery-type thermal energy storage design is scalable to multiple modules and can be integrated with any thermal energy system, ensuring the optimal use of resilient energy assets alongside advanced nuclear technology.

HITB thermal energy storage facility with insulation in a cargo shipping container located at INL Engineering Demonstration Facility.

TALENT PIPELINE:

- Daniel Orea, student at Texas A&M University
- Hansol Kim, student at Texas A&M University
- Joseph Seo, Senior Research Engineer at Texas A&M University

PAPERS AND PRESENTATIONS:

- Yoo, J., Song, M., Qin, S., Hartvigsen, J. Kim, H., Seo, J., Hassan, Y. (2022). "High-Temperature Latent Heat Storage System using Transportable Heat Pipes for Versatile Integration with Emerging Microreactors." 2022 ANS Winter Meeting and Technology Expo, Phoenix, AZ.
- Song, M., Yoo, J., Qin, S. (2022). "Development of Numerical Model of Metal Foam with PCM for the estimation of effective thermal conductivity." 2022 ANS Winter Meeting and Technology Expo, Phoenix, AZ.
- Kim, H., Seo, J., Hassan, Y. Yoo, J., Song, M., Qin, S., Hartvigsen, J. (2022). "Corrosion evaluation of metal foams in eutectic molten salts for high temperature latent heat energy storage application." 2022 ANS Winter Meeting and Technology Expo, Phoenix, AZ.
- Kim, H., Seo, J., Hassan, Y., Yoo, J., Qin, S., Hartvigsen, J. (2024). "Evaluation and selection of eutectic salts combined with metal foams for applications in high-temperature latent heat thermal energy storage." Journal of Energy Storage. volume 76, 109790.
- Han, J., Yoo, J., Qin, S., and Song, M. (2024) "Numerical Evaluation of Effective Thermal Conductivity of PCM with Metal Foam Incorporating Buoyancy Effects for Thermal Energy Storage." 2024 ANS Annual Conference, Las Vegas, NV.
- Mikkelson, D., Yoo, J., and Qin, S. (2024). "Dynamic Modeling of Latent Heat Thermal Battery." 2024 Pacific Basin Nuclear Conference, Idaho Falls, Idaho.
- Yoo, J., Qin, S., Hartvigsen, J., Mikkelson, D., Saeed, R., Seo, J., Kim, H., and Hassan, A. (2024). "Dynamic Modeling of Latent Heat Thermal Battery." 14th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Operation and Safety (NUTHOS-14), Vancouver, British Columbia, Canada
- Yoo, J., Song, M., and Qin, S. (2025). "Development of a Conduction-Based Model for Analyzing Frozen Startup of Alkali-Metal Heat Pipes." Applied Thermal Engineering, 127475. https://doi.org/10.1016/j.applthermaleng.2025.127475.

EXTERNAL INTELLECTUAL PROPERTY:

- "High-Temperature Latent Heat Thermal Energy Storage System integrated with Transportable Heat Pipes," INL Technology no.: BA-1419, Patent No.: US20240133637A1.

De-risking Preprocessing for the Recovery of Critical Metals from Waste: A Digital Twin Approach

PROJECT NUMBER:
23A1070-017FP

TOTAL APPROVED AMOUNT:
$915,000 over 3 years

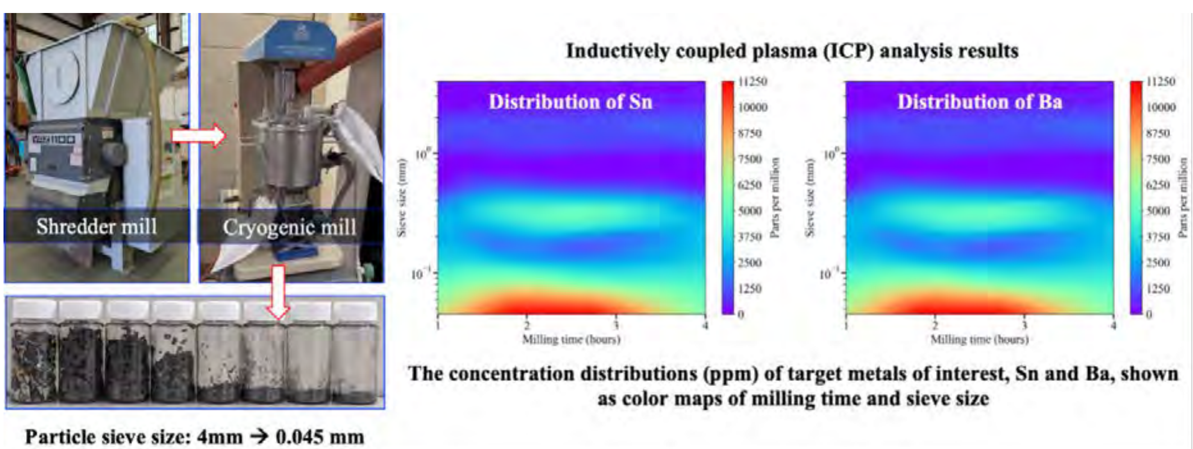
PRINCIPAL INVESTIGATOR:
Yidong Xia

CO-INVESTIGATORS:
Jordan Klinger, INL
Noah Berglund, INL
Vicki Thompson, INL

COLLABORATORS:
University at Buffalo
Clemson University

Digital engineering enhances safe and efficient recovery of valuable metals from electronic waste.

Driven by the increasing demand for electronic devices and their frequent replacement, electronic waste is now the fastest-growing waste stream globally. Printed circuit boards (PCBs) are central constituents in nearly all electronic waste, accounting for about 80% of its intrinsic value. To recover valuable metals from PCBs, industry prefers feedstock streams by component for higher profit margin. This ignores the massive mixed waste PCBs that are fragmented and hard to separate, and that continue to present risks to the living environment. This project explored the potential of valuable metal recovery from abundant low-grade mixed waste PCBs with perspectives from mechanical pretreatment. A two-stage mechanical size reduction process involves shredding and cryogenic milling, with a two-stage elemental composition analysis. This was introduced to investigate the concentrations of select valuable metals. The design of physical methods was guided by computational simulations of the particle milling process and leaching fluid flow in packed particle bed. The developed milling system minimizes airborne fines and reaches over 99% mass retention, ensuring a safe lab environment. The project found that after milling, base metals like copper and aluminum are dominant in mass percentage and concentrated in millimeter-sized particles. Targeted valuable metals, such as barium and tin, are rich in specific sub-millimeter-sized particles. Beryllium is nearly non-detectable. Optimal pretreatment for waste PCBs depends on target metals. The findings suggest the potential of using size-separated milled particles from mixed waste PCBs for targeted metal recovery—i.e., base metals from larger particles and higher-value metals from fine particles. Lead concentration, found to be increasingly high in smaller particles, highlights the necessity of the developed fines-containment method for safe processing. This project benefits DOE missions by addressing the urgent need to recycle massive mixed waste PCBs.



A two-stage comminution process involving shredding and cryogenic milling, with a two-stage elemental composition analysis method, is developed for investigating the concentrations of select valuable metals in mixed waste PCBs.

TALENT PIPELINE:

- Miaosi Dong, student at Carnegie Mellon University
- Zachary Diermyer, student at University at Buffalo, State University of New York
- Tasrif Anwar, student at Utah State University
- Minglei Lu, student at Clemon University
- Luiz Emilio, student at University of Utah

PAPERS AND PRESENTATIONS:

- Yidong Xia, Zachary Diermyer, Ling Ding, Noah Berglund, Jordan Klinger, Vicki Thompson, Jiaoyan Li, Samuel Forrest, Shannon Alford, "The potential of valuable metal recovery from low-grade mixed waste printed circuit boards: Perspectives from mechanical preprocessing." Chemical Engineering Journal Advances 24 (2025): 100846.
- Zachary Diermyer, Yidong Xia, Ahmed Hamed, Jordan Klinger, Vicki Thompson, Zhen Li, Jiaoyan Li, "Mesoscopic flow simulation to understand the percolation through fine-ground electronic waste particle bed." Powder Technology 454 (2025): 120703.
- Yidong Xia, Miaosi Dong, Pengcheng Cao, John E. Aston, Miranda Kunns, Neal Yancey, Jeffrey Lacey, "Mechanical separations of corn stover anatomical fractions in an integrated feedstock preprocessing system: An experimental and data-driven modeling study." Biomass and Bioenergy 202 (2025).
- Minglei Lu, Yidong Xia, Tiasha Bhattacharjee, Jordan Klinger, Zhen Li, "Predicting biomass comminution: Physical experiment, population balance model, and deep learning." Powder Technology 441 (2024): 119830.
- Yidong Xia, Zachary Diermyer, Ling Ding, Noah Berglund, Jordan Klinger, Vicki Thompson, Jiaoyan Li, Samuel Forrest, Shannon Alford, "Selective leaching of electronic waste for valuable metal recovery based on particle size." Proceedings in 2025 REMADE Circular Economy Tech Summit & Conference (2025).
- Y. Xia, N. Berglund, J. Klinger, T. Bhattacharjee, V. Thompson, Z. Diermyer, J. Li (2024). "A Two-Step Size Reduction Method for Fine Milling of Electronic Waste to Improve Recycling," No. 686535, Proceedings of the 2024 AIChE Annual Meeting, San Diego, California, Oct 27-31, 2024.

EXTERNAL INTELLECTUAL PROPERTY:

- Yidong Xia, Tiasha Bhattacharjee, Jordan Klinger. "SPRITE (Smart Preprocessing & Robust Integration Emulator)—An open-source suite of analytical and data-driven models that predict the performance of renewable carbon feedstock preprocessing units and system integration." GitHub address: https://github.com/idaholab/SPRITE Additional Information: https://www.osti.gov/doecode/biblio/116576

Plasma Assisted Catalysis of Ammonia Synthesis Reaction

PROJECT NUMBER:
23A1070-045FP

TOTAL APPROVED AMOUNT:
$1,105,000 over 3 years

PRINCIPAL INVESTIGATOR:
Jeremy Hartvigsen

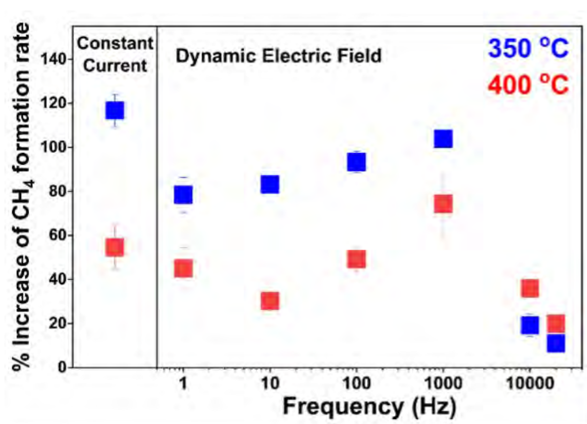
CO-INVESTIGATORS:
Dylan McDowell, INL
Rebecca Fushimi, INL

Electric field enhanced catalytic activity increases ammonia production rate.

The plasma ammonia synthesis project developed a pressurized testbed for electric field assisted ammonia synthesis. The testbed represents a significant capability for voltage, current, and pressure for the testing of electric field catalysts. The stand was built with key safety features to provide state-of-the-art safety as well as performance. Initial test stand validation and commissioning efforts focused on a simpler and safer reaction with key similarities in chemical reaction. Methanation has a thermal catalyst that traditionally uses ruthenium on ceria. The ruthenium on ceria provides an analog for ammonia. Ruthenium is a known catalyst for ammonia synthesis, and ceria is a semi-conduction support, which makes it active for electric field enhanced catalysis. The ruthenium catalyst was also supported on alumina to show the impact from a much-insulating higher dielectric breakdown support. In situ plasma is formed in the catalyst at sufficient voltages in this catalyst and support configuration. Methanation studies showed significant trends and provided insight into the use of ruthenium on different supports. In addition, the use of high frequency electric fields showed a trend compatible with theory. The use of specific frequencies resulted in higher catalyst activity enhancement for a specific energy input. The interaction of the catalyst with the support was characterized, and the catalyst was validated in the Temporal Analysis of Products reactor. Improvements to the catalyst and support for electric fields versus traditional thermal catalysts have been identified.

TALENT PIPELINE:

- Rajagopalan Ranganathan, postdoc at INL



Formation rate increase as a function of frequency.

Characterization of Biomass Fillers, Bio-composites, and Bio-composite Degradation in Harsh Environmental Conditions

PROJECT NUMBER:
23A1070-076FP

TOTAL APPROVED AMOUNT:
$998,800 over 3 years

PRINCIPAL INVESTIGATOR:
Kiyo Fujimoto

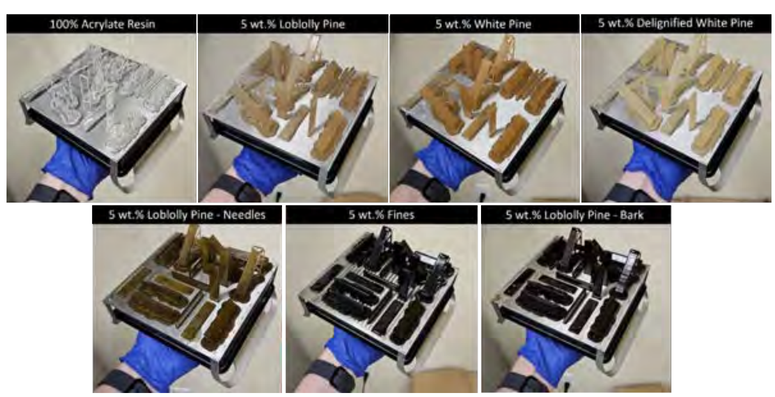
CO-INVESTIGATORS:
Carl Frederik Mikael Karlsson, INL
Brennan Mohr, INL
Luke Williams, INL
Rachel Emerson, INL

Understanding biomass filler/polymer interactions advances composite design for dynamic light processing additive manufacturing.

The project aimed to incorporate biomass materials as fillers into polymeric matrixes by using vat polymerization three-dimensional printing. Biomass fillers, which featured a range of particle sizes and morphologies, were sourced from the Bioenergy Feedstock Library at INL. Composite formulations were developed using biomass materials such as White Pine (*Pinus strobus*) and Loblolly Pine (*Pinus taeda*), with the Loblolly Pine fractionated into various anatomical parts. To evaluate the printability of these formulations, working curves were established to determine the critical exposure parameters for successful layer curing. Additionally, comprehensive characterization of the biomass materials was conducted to understand how their intrinsic properties influence composite performance. This analysis included an evaluation of particle size and morphology, as well as percent whole ash, water-dissolvable extractives, and total extractives. To evaluate the mechanical performance of the resulting composites, dynamic mechanical analysis was performed. This provided key insights into the viscoelastic behavior, stiffness, and structural integrity of the materials under oscillatory loading. When correlated with the biomass characteristics, the dynamic mechanical analysis results demonstrate how filler properties influence the storage and loss modulus, and the transition from linear to nonlinear mechanical behavior. Overall, this work facilitated a comprehensive understanding of both the possibilities and the limitations of using lignocellulosic and agricultural residues to fabricate next-generation, fossil fuel-free composite materials.

TALENT PIPELINE:

- Eliezer Molina, postdoc at INL, converted to staff
- Donovan Ochoa, student at Texas A&M University, Kingsville, converted to staff
- Joel Yazzie, student at Navajo Technical University
- Konnor Cutts, student at Idaho State University, converted to staff



This overview of the printed biomass composites showcasing the range of material formulations and print orientations explored in this study. Shown here are samples printed in standing, 45°, 45° tilted, flat, and longside orientations demonstrates the versatility of the additive manufacturing process with biomass-filled resins.

Radiation-Durable Nanofibers for Sustainable Molecular Hydrogen Production Under Ionizing Radiation

PROJECT NUMBER:
23P1077-005FP

TOTAL APPROVED AMOUNT:
$337,000 over two years

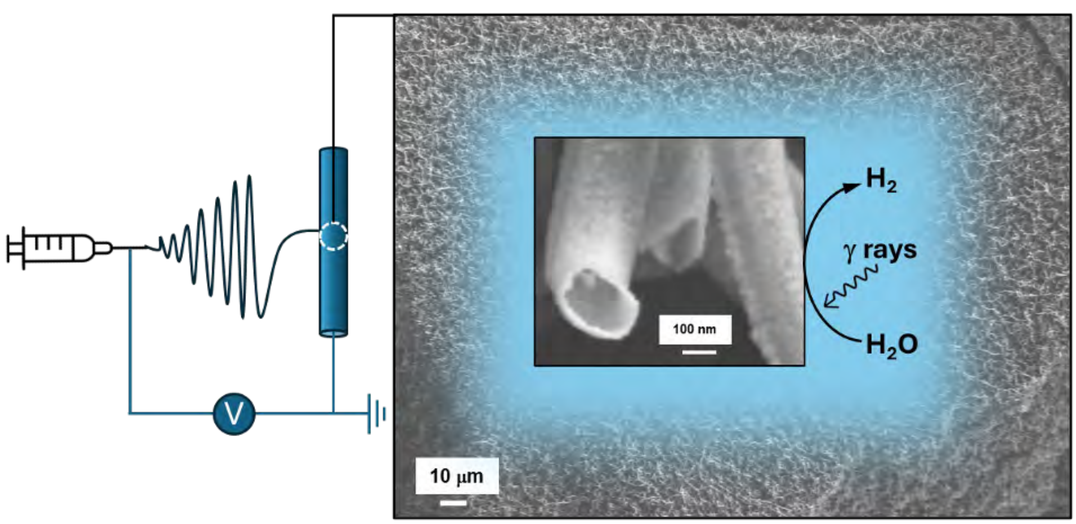
PRINCIPAL INVESTIGATOR:
Hanna Hlushko

CO-INVESTIGATORS:
Jacy Conrad, INL
Bjorn Vaagensmith, INL

COLLABORATORS:
University of Notre Dame

Electrospun zirconium oxide fibers enhance hydrogen generation from water radiolysis.

Water radiolysis decomposes water into various products—including molecular hydrogen—under ionizing radiation. The generation of hydrogen from water radiolysis is enhanced on the surface of zirconium oxide, making it a promising material for hydrogen production using underutilized nuclear energy. We developed a methodology for electrospinning ultrathin zirconium oxide fibers for enhanced water radiolysis and hydrogen production by optimizing electrospinning parameters, such as solution composition, working distance, solution flow rate, and applied voltage. After calcination, the resulting hollow fibers had an average diameter of 159±35 nm and a surface area of 42.6±0.3 m^2/g, composed of crystalline tetragonal zirconium oxide, with some chemisorbed carbon dioxide on the surface. Irradiation at the liquid nitrogen temperature generated radicals tentatively identified as oxygen superoxide while no hydrogen radicals were observed, unlike in commercial oxide powders. Further hydrophilization of fiber surface could improve water adsorption and hydrogen radical generation, consequently resulting in measurable hydrogen generation from radiolysis. Zirconium oxide powder irradiated with highly energetic helium ions quickly saturated with oxygen-centered radicals, indicating that periodic surface regeneration might be needed for reusability of the material as a water decomposition substrate. Accelerator irradiations were conducted through collaboration with the University of Notre Dame Radiation Laboratory. This collaboration will be valuable to carry out efficient radiation studies in future projects. Hanna Hlushko, the principal investigator, has established her research expertise at Idaho National Laboratory and will be converted to a staff member at the end of the project.



The electrospinning process, depicted schematically on the left, produces a fiber mat. On the right, the fiber's morphology after calcination is shown, with an insert depicting enlarged fibers, revealing their hollow structure. The water radiolysis process is shown on the fiber surface, with the goal of producing molecular hydrogen.

TALENT PIPELINE:

- Hanna Hlushko, Russell L. Heath distinguished postdoc at INL, converted to staff

PRESENTATION:

- Hlushko, Hanna, "Interfacial water radiolysis on metal oxide surfaces," 33rd Miller Conference on Radiation Chemistry, October 5-10, 2015, Croatia.

Recycling Critical Raw Materials from Solid Oxide Electrolyzers

PROJECT NUMBER:
24A1081-084FP

TOTAL APPROVED AMOUNT:
$900,000 over 2 years

PRINCIPAL INVESTIGATOR:
Zeyu Zhao

CO-INVESTIGATORS:
John Aston, INL
Luis Diaz Aldana, INL
Meng Shi, INL
Wanhua Wang, INL
Wei Wu, INL

Novel process recycles solid oxide electrolyzers with minimal performance decay.

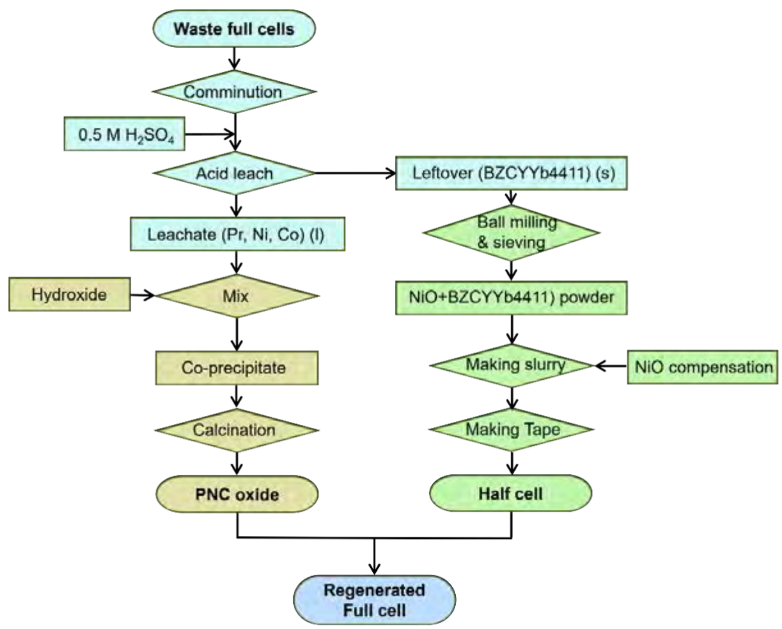
The global shift toward regenerative and eco-friendly energy, with a focus on reducing reliance on fossil fuels and curbing carbon emissions, has led to the rise of hydrogen production via water electrolysis. Proton conducting solid oxide electrolyzers operating at temperatures of 300 – 600°C can use both electrical and thermal energy produced by nuclear power, demonstrating the highest energy efficiency among all electrolysis technologies. However, establishing durable and scalable manufacturing processes for solid oxide electrolyzers faces challenges, including a heavy reliance on critical raw materials, dependence on commercial ceramic composites, and the environmental impact of waste. Therefore, the development of economically viable recycling strategies, even at an early market entry stage, shows the need and opportunity to develop new capabilities in the manufacturing of solid oxide electrolyzers. The limited coverage in the existing literature of solid oxide electrolyzer recycling only focuses on the intrinsic value of recoverable critical materials, disregarding the possibilities of developing a closed-loop approach to recover ceramic composites and catalysts. We developed a physio-electrochemical strategy for recovering and recycling the critical raw materials from end-of-life solid oxide electrolyzer manufacturing waste by integrating INL's capabilities in biomass preprocessing, critical raw material recycling, and solid oxide electrolyzer manufacturing, assisted by technoeconomic and life cycle assessments. This innovative approach achieved over 92% material recovery and an impressive 100% recovery in full cell performance, addressing a significant gap in current manufacturing practices while setting a new standard for the industry. This method led to a 42% cost reduction compared to the conventional process operating at similar scale (25 MW/year). The success of this project provided new insights for future advancements in recycling multifunctional ceramic systems and offered the potential to further reduce costs addressing the Hydrogen Shot's cost target of $1/kg by 2031.

TALENT PIPELINE:

- Wanhua Wang, postdoc at INL

PAPER AND PRESENTATIONS:

- Wu W., Wang W., Berglund N.J., Aston J.E., Shi M., Diaz L.A., Ding D., Stewart F.F., "Advancements in sustainable proton conducting electrochemical cells: Direct recycling of sintered nickel oxide-doped barium zirconate half cells." Resources, Conservation and Recycling. 2024 Oct 1; 209:107782.
- Wang W., Shi M., Berglund N.J., Aston J.E., Ding D., Diaz L.A., and Wu W., "Direct Recycling of Sintered Nickel Oxide-doped Barium Zirconate Proton Conducting Electrochemical Half Cells." ECS, Oct. 2024, Honolulu, HI.
- Wang W., Wu W., Shi M., Aston J.E., Ding D., and Zhao Z., "Direct Recycling of Proton Conducting Electrochemical Cells (PCEC)." ACS Fall, Aug. 2025, Washington, DC.



Processing steps in recycling of solid oxide electrolyzer with physio-electrochemical networks.

Integrated Heterogeneous Structure of High-Entropy-Alloy/Reactor for High-Throughput Chemical Synthesis via in situ Carbon Dioxide Hydrogenation

PROJECT NUMBER:
24A1081-098FP

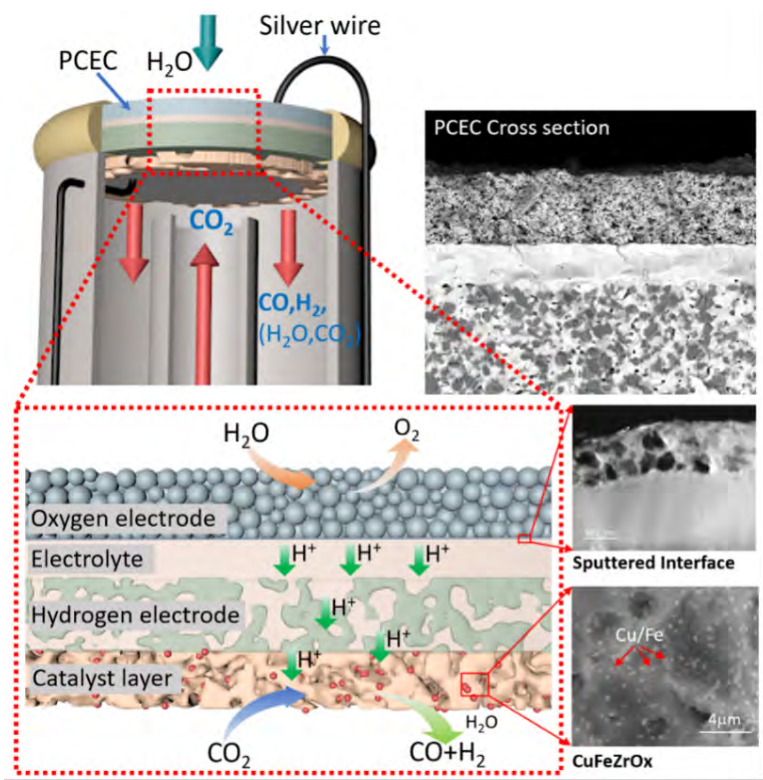
TOTAL APPROVED AMOUNT:
$805,531 over 2 years

PRINCIPAL INVESTIGATOR:
Wenjuan Bian

CO-INVESTIGATORS:
Dong Ding, INL
Hanping Ding, University of Oklahoma
You Qiang, University of Idaho

Controlling the applied current tunes catalytic conversion rates and products.

An integrated heterogeneous structure of electrocatalyst and electrochemical reactor has been proposed to format a new platform to significantly elevate carbon dioxide hydrogenation reaction kinetics and product selectivity. The well-established capabilities in electrocatalyst synthesis and low temperature protonic ceramics were employed to build an integrated structure to establish the synergistic relations between composition, surface atomic ordering, d-band centers, electrochemical proton flux, and conversion, selectivity, and durability for syngas synthesis. The ensemble effect and enhanced electrochemical protonation of the electrocatalyst was studied as primary underlying factors to be linked to increased carbon dioxide conversion with rational understanding on mechanism via systematic characterizations. The study of the electrocatalyst and integrated catalyst and protonic ceramic cells includes: 1) the ratio of syngas produced varies under different current densities when integrating electrocatalysis with the electrochemical cells; 2) systematic material characterizations, including in situ techniques, were employed to investigate the underlying electrocatalytic mechanisms; 3) efforts were made toward mass production and scale-up.



Schematic of electrocatalyst integrated protonic ceramic electrochemical cells and scanning electron microscopy images of oxygen electrode and electrocatalyst.

TALENT PIPELINE:

- Haixia Li, postdoc at INL
- Shuanglin Zheng, student at University of Oklahoma
- Bisheswor Acharya, student at University of Idaho

PAPER AND PRESENTATIONS:

- Shuanglin Zheng, Wenjuan Bian, Hanping Ding, "A robust protonic ceramic fuel cell with a triple conducting oxygen electrode under accelerated stress tests." Materials Advances, 2024, 5, 2296--2305.
- Haixia Li, Wenjuan Bian, Zeyu Zhao, Fan Liu and Dong Ding, "High-valued Chemical Production by Electrochemical CO_2 Conversion through Protonic Ceramic Electrochemical Cells." Oral presentation, 2025 Fall ACS Meeting, Washington, DC, Aug. 17-21, 2025.
- Haixia Li, Wenjuan Bian, Lucun Wang, Wei Wu, and Dong Ding, "Electrochemical CO_2 Conversion to High-Valued Chemicals through a Protonic Ceramic Electrochemical Cell." Oral presentation, PRiME 2024 Electrochemical Society (ECS) Meeting, Honolulu, HI, October 6-11, 2024.

Impurities in Lithium-ion Batteries: Troublemakers or Troubleshooters?

PROJECT NUMBER:
24A1081-101FP

TOTAL APPROVED AMOUNT:
$1,200,000 over 2 years

PRINCIPAL INVESTIGATOR:
Caleb Stetson (First year),
Meng Shi (Second year)

CO-INVESTIGATORS:
Caleb Stetson, INL
Pete Barnes, INL
Bor-Rong Chen, INL
Cody Walker, INL
Daniel Molina Montes de Oca, INL

COLLABORATORS:
TMS International
Optimus Steel, LLC.

Innovative iron, nickel, and cobalt recovery processes maximize critical materials domestic supply chain.

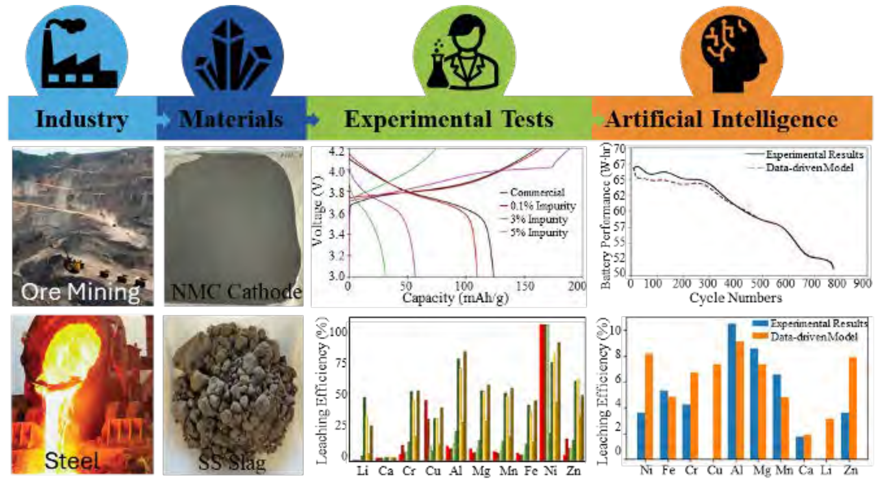
The primary objective of this project was to comprehensively understand and utilize domestic iron, nickel, manganese, and cobalt resources for advanced battery applications. This involved assessing the impact of impurities on electrochemical performance through experimental methods and a machine learning framework and conducting technoeconomic analysis to recommend purity standards for battery metals. Additionally, the project explored the use of stainless steel slag as a potential source of untapped nickel, iron, and cobalt for battery production and aimed to develop a flow diagram for metal leaching and recovery.

The project achieved significant milestones, including the successful analysis of domestic resources and market pricing for nickel and its precursors, specifically nickel sulfate. Impurity-containing cathode materials were synthesized and tested, providing valuable data on their impact on battery performance. A robust machine learning framework was developed to enhance the prediction and optimization of battery performance. The technoeconomic analysis provided critical insights into the energy costs of transition metal purification. A major breakthrough was achieved in the recovery of metals from stainless steel slag, with 100% nickel successfully leached and copper electrodeposited. A comprehensive flowsheet for metal separation and recovery processes was established, incorporating unit operations such as electrochemical leaching, iron precipitation, ion exchange, and electroplating.

The project initiated the Enhanced Validation of Advanced Battery Supply Chains program, funded by the DOE Vehicle Technologies Office. This multiyear research program examined impurities in domestic resource deposits and their impact on lithium-ion battery performance, developing a toolset to enhance both supply and performance. Furthermore, in the study of stainless steel slag, significant efforts were made to build connections with industrial sectors, facilitating the provision of stainless steel slag materials and collaboration on process development. These achievements underscored the progress in understanding and using domestic resources for battery material production, highlighting advancements in resource analysis, impurity impact assessment, and metal recovery processes.

TALENT PIPELINE:

- Aashray Narla, postdoc at INL, converted to staff
- Haeyeon Kim, postdoc at INL
- Farhin Tabassum, student at Stevens Institute of Technology



Integration of materials processing, experimental tests, and artificial intelligence optimization of materials from ore mining and steel industry. This workflow demonstrates the process from raw material extraction to final product enhancement through advanced experimental and artificial intelligence techniques.

Direct Carbon Capture from Seawater by Leveraging Flowing Electrode Capacitive Deionization Strategy Based on Two-Dimensional Materials

PROJECT NUMBER:
24A1081-118FP

TOTAL APPROVED AMOUNT:
$775,000 over 2 years

PRINCIPAL INVESTIGATOR:
Arindam Mukhopadhyay

CO-INVESTIGATORS:
Luis Diaz Aldana, INL
Meng Shi, INL
John R. Klaehn, INL
Dave Estrada, Boise State University

COLLABORATORS:
Boise State University

Capturing dissolved carbon dioxide mineral forms strengthens the global economy.

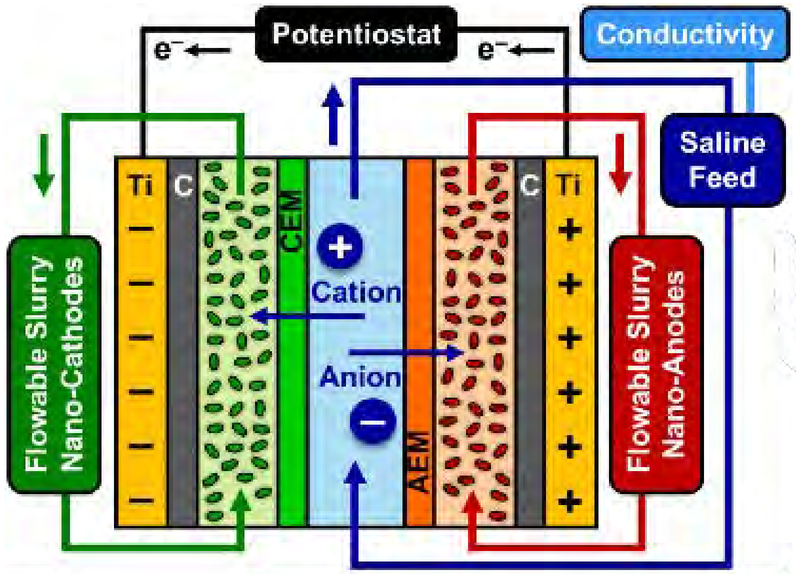
Capturing carbon dioxide from the atmosphere-ocean interface is paramount to minimizing global carbon emission and promoting economic and environmental sustainability. Strategies to capture dissolved inorganic carbon from seawater have recently garnered a surge of research interest. State-of-the-art electrochemical-driven technologies for seawater desalination—e.g., electrodialysis and membrane-based deionization—are inefficient and economically challenging for dissolved inorganic carbon capture due to low separation selectivity for bicarbonate over chloride, non-continuous operation, cross-contamination of effluent, and low process scalability. To overcome these setbacks, we developed in this project an energy-efficient flowing electrode capacitive deionization (FE-CDI) technology for the selective capture of bicarbonate over chloride in simulated seawater feed streams (sodium bicarbonate and sodium chloride; 1 g/L). The performance of titanium carbon MXene ($Ti_3C_2T_X$) and graphene two-dimensional nanostructures were evaluated as pseudo-capacitive slurry electrodes in FE-CDI. Due to lower surface tension and viscosity along with higher zeta potential and conductivity, MXene electrodes featuring hydrophilic heteroatom surface functionalities showed superior desalination performance over hydrophobic graphene electrodes. MXene showed ~10–24 times higher salt capture capacity, ~25–40 times higher charge response, and ~40–60% higher electrode regeneration efficiency than graphene during FE-CDI desalination. The advantage of MXene in FE-CDI for the selective capture of sodium bicarbonate over sodium chloride was demonstrated by >5 times larger specific capacitance, ~2–5 times higher salt capture capacity, and ~2 times lower energy consumption. The non-faradaic, pseudo-capacitive mechanism of reversible and diffusion-limited salt capture by MXene via surface interaction and intercalation of ions was delineated by a combination of in-depth electrochemical, microstructural, and spectroscopic analyses. The molecular rationale for the observed selectivity of MXene in capturing sodium bicarbonate over sodium chloride was garnered from computational simulation via density functional theory, which underscored >10 kcal/mol of thermodynamic energy incentive for interfacial charge transfer and hydrogen bonding of bicarbonate over chloride with the terminal oxygen functionalities of MXene. The observed FE-CDI performance of MXene for sodium bicarbonate desalination was superior to those known for most nanoscale electrodes. The energy consumption of MXene for sodium bicarbonate FE-CDI (~0.38 kWh/kg) was 10–20 times lower than those of state-of-the-art technologies (~4–7 kWh/kg) used in commercial desalination plants. The results essentially highlight the first potential application of MXene nanostructures as superior pseudo-capacitive slurry electrodes in FE-CDI for the selective and energy-efficient capture of dissolved inorganic carbon over major interfering salts from seawater.

TALENT PIPELINE:

- Arindam Mukhopadhyay, postdoc at INL, converted to staff
- Dung Thi Hanh To, postdoc at INL
- Sharmistha Das Karmakar, postdoc at INL
- Hailey Burgoyne, student at Boise State University
- Ajay Pratap, student at Boise State University

PRESENTATION:

- H.; Estrada, D., "Direct CO_2 Capture from Seawater by Leveraging Flowing Electrode Capacitive Deionization based on 2D Nanoscale Materials." 2025 ACS Spring Meeting, San Diego, CA, March 27, 2025.



FE-CDI desalination system leveraging two-dimensional nanoscale materials as flowable electrodes for selective capture of dissolved carbon dioxide mineral forms over major interfering salts in seawater surrogates.

The Development of Aqueous Zinc-Manganese Oxides Batteries for Long-Duration Energy Storage

PROJECT NUMBER:
24A1081-209FP

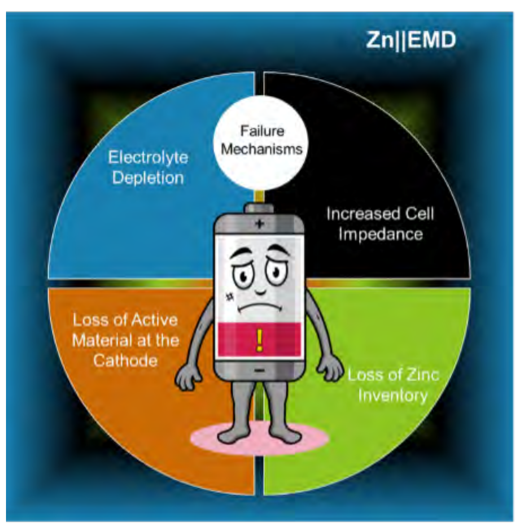
TOTAL APPROVED AMOUNT:
$867,000 over 2 years

PRINCIPAL INVESTIGATOR:
Abderrahman Atifi

CO-INVESTIGATORS:
Meng Li, INL
Pete Barnes, INL
Eric Dufek, INL

Electrolyte-engineered control of interfacial solvation drives next-generation zinc batteries.

This project advanced the design and understanding of zinc batteries by integrating electrochemical performance studies, interfacial spectroelectrochemical characterization, and computational modeling into a unified research framework. The work addressed critical challenges limiting zinc battery performance, including capacity fade, interfacial instability, and dendrite formation, which arise from poorly understood electrolyte-electrode interactions and uncontrolled zinc ion solvation chemistry. Electrochemical investigations in zinc electrolytic manganese oxide established how electrolyte composition and loading govern early capacity loss and identified electrochemical fingerprints for the rapid, nondestructive diagnosis of failure mechanisms. Preliminary in situ interfacial spectroelectrochemical studies provided a molecular level illustration of how ionic liquid additives would restructure the interfacial speciation, suppress water activity, and mitigate side reactions that drive hydrogen evolution and dendrite growth. Computational studies using molecular dynamics simulations revealed how protic and aprotic additives modulate zinc ion solvation, water hydrogen-bond networks, and ion transport, pinpointing additive chemistries and concentrations that balance interfacial stability with efficient zinc ion mobility. Together, these efforts produced a coherent molecular- to device-level understanding of zinc battery degradation pathways and electrolyte design principles. The project trained three postdoctoral researchers—two experimentalists and one computational—while yielding high-impact publications and disseminating findings at national conferences. These outcomes not only advance fundamental insights into zinc battery chemistry, but also establish a strong foundation for competitive proposals in energy storage research, consolidating INL expertise in electrochemical energy systems, interfacial science, and computational materials design.



TALENT PIPELINE:

- Eugene Engmann, postdoc at INL, converted to staff
- Sharmistha Das Karmakar, postdoc at INL
- Jeanne N'Diaye, postdoc at INL

PAPER AND PRESENTATIONS:

- E. Engmann, P Barnes, L. V. Montoto, A. Atifi, "The Role of Catholyte Modulation in Suppressing the Initial Capacity Fade of Zinc Electrolytic Manganese Dioxide Coin Cells." ACS Omega 2025, 10, 9, 9096–9105.
- E. Engmann, P. Barnes, E. J. Dufek, A. Atifi, "Nondestructive electrochemical diagnosis of failure mechanisms in aqueous zinc batteries." Energy Storage Materials 77 (2025) 104190.

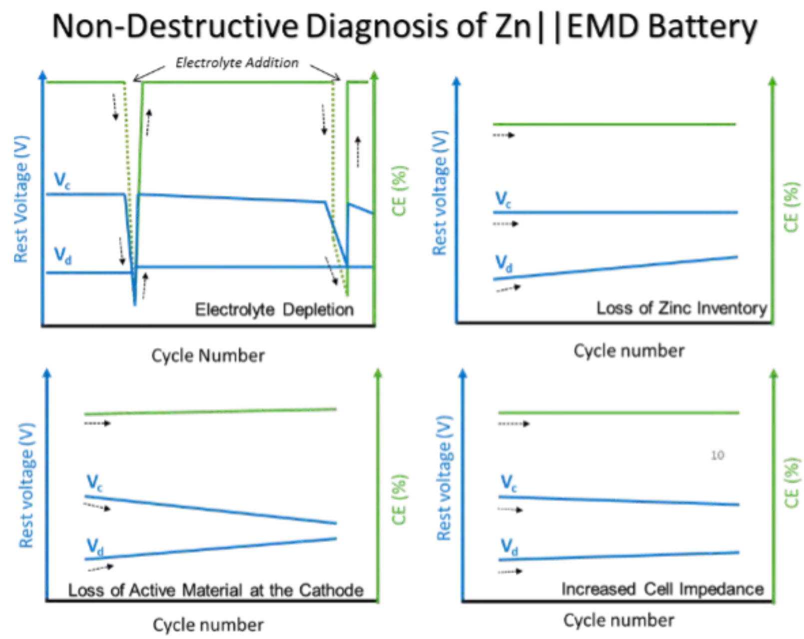


Illustration of nondestructive electrochemical diagnosis of failure mechanisms in aqueous zinc electrolytic manganese oxide batteries.

Grid-Forming Control for Unbalanced Distributed Microgrids

PROJECT NUMBER:
24P1089-016FP

TOTAL APPROVED AMOUNT:
$150,000 over 1 year

PRINCIPAL INVESTIGATOR:
Yemi Ojo

CO-INVESTIGATORS:
Soumyadeep Nag, INL
Temitayo Olowu, INL
Kurt Myers, INL

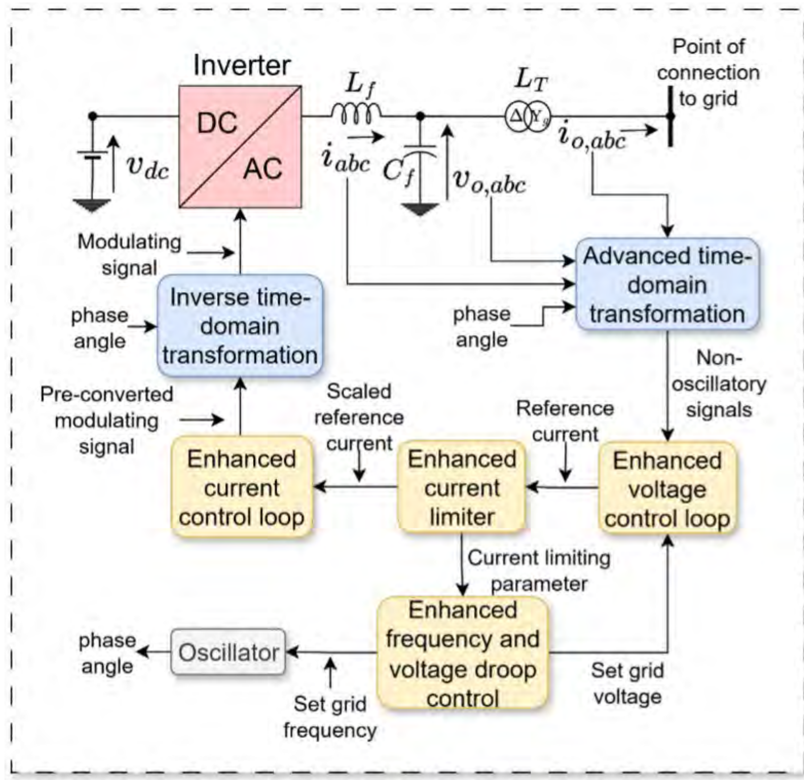
Time-domain transformation and grid-forming control for inverter-based microgrids expand access to electricity in isolated areas.

Expanding access to electricity in isolated areas and providing backup power to critical facilities requires low and medium voltage inverter-based microgrids that can operate independent from the grid. These networks are often unbalanced due to unbalanced phase loading and faults, causing oscillatory responses in grid-forming control designed for balanced conditions. This project addressed this problem by developing advanced grid-forming control that is effective under unbalanced conditions and meets universal interoperability for grid-forming inverter specifications by setting and regulating grid frequency and voltage, sharing active power proportionally, injecting negative sequence current, and enabling fault ride-through. The controller design is achieved by developing advanced time-domain transformation that enables the conversion of unbalanced currents and voltages to non-oscillatory signals. Real-time tests on an isolated Institute of Electrical and Electronics Engineering 123 distribution network on the Real-Time Digital Simulator showed that the proposed transformation and grid-forming control are effective under unbalanced conditions and support off-grid operations. The solution developed can be deployed in any inverter-based asset, including mobile/immobile microgrids, battery storage systems, energy management systems, fuel cells, smart inverters, as well as INL's Microgrid-in-a-Box and Energy Proving Ground's inverter-based assets, supporting utilities and developers in buying down risk and demonstrating technological benefits.

TALENT PIPELINE: NONE

PRESENTATION:

- Y. Ojo, S. Nag, and T. O. Olowu, "Enabling Grid-forming Control Under Unbalanced Conditions." 2025 IEEE Energy Conversion Congress and Exposition, October 19 – 23, 2025.



Three-phase inverter using the advanced time-domain transformation and grid-forming control featuring enhanced frequency and voltage droop control, current and voltage control loops, and enhanced current limiter.

Bridging the Divide Between the Real and Simulated Worlds: Operations-informed Models to Facilitate Widespread Deployment of Zero-emissions Buses

PROJECT NUMBER:
25A1103-002FP

TOTAL APPROVED AMOUNT:
$103,000 over 1 year

PRINCIPAL INVESTIGATOR:
Torrey Lyons

CO-INVESTIGATORS:
Steven Schmidt, INL
Kang Ching "Jean" Chu, INL
Kevin Meudt, INL
John Smart, INL
Paden Rumsey, INL

State-of-the-art energy consumption simulation model predicts the capabilities of medium and heavy-duty electric vehicles.

Many efforts have been made to simulate energy consumption of battery electric buses to optimize their deployment into existing fleets. The models produced, however, are rarely validated against real-world consumption data, limiting their generalizability and widespread application to fleets around the US. Furthermore, a major concern specific to battery electric buses is the effects of harsh climates on their performance. We build upon the state-of-the-art energy consumption modeling techniques developed for battery electric buses and apply them to a unique geographic context and a unique electrified vehicle. This geography, climate, and vehicle further the existing understanding of the factors affecting medium- and heavy-duty electric vehicles by allowing for new relationships to be tested and by assessing the generalizability of known relationships to new contexts. We find that temperature is less predictive of energy consumption for the battery electric motorcoach in the case study environment than it is for battery electric buses in other studies. A mitigating factor that we presume to be working on the relationship between temperature and energy consumption is the fact that the battery electric motorcoach route does not stop between origin and destination to exchange passengers, and in turn, condition cabin air. Our model also incorporates wind speed and direction relative to travel, which is a novel contribution of our methodology. Results from our study are helpful for transit service planners and fleet operators, improving their ability to predict performance of potential deployments of medium- and heavy-duty electric vehicles into existing fleets.

Charging demonstration at the Central Facilities Area.

CALVIN DOWNEY

ADVANCED MATERIALS AND MANUFACTURING FOR EXTREME ENVIRONMENTS

Creating advanced materials that perform well in extreme environments is essential for US energy dominance. The lab is changing the paradigm from traditional design methods to digital design and manufacturing, focusing on nuclear fuels, lightweight materials, and advanced survivability materials. By combining expertise in metallurgy, materials science, and multiphysics modeling with innovations in advanced manufacturing and artificial intelligence, we predict how materials perform at different scales under various harsh conditions.

CORE CAPABILITIES

Advanced computer science, visualization, and data

Applied Materials Science & Engineering

Computational Science

Mechanical Design and Engineering

Nuclear Engineering

Lattice Structure Design of Low-density Resilient Materials for Advanced Reactors

PROJECT NUMBER:
23A1070-030FP

TOTAL APPROVED AMOUNT:
$1,545,800 over 3 years

PRINCIPAL INVESTIGATOR:
Calvin Downey

CO-INVESTIGATORS:
Boone Beausoleil, INL
Asa Monson, INL
Lynn Munday, INL
Cameron Howard, INL
Wen Jiang, North Carolina State University
Carolyn Seerpersad, Georgia Institute of Technology

Advanced modeling, coupled with mechanical characterization, optimizes complex lattice structure designs.

The Topology Reverse Optimization Universal Tool (TROUT) optimizes structures for specific loading conditions, exemplified by a 4-point bend test setup. The design region, a rectangular prism, was optimized for maximum stiffness while it was minimized for material volume. Pseudo-density represents relative density within the design, where color gradients indicate varying densities. The optimized topology can be converted into desired lattice structures using Q-bit for fabrication and testing. The effectiveness of the method—solid isotropic material with penalization—for bulk compliance reduction is noted, but finer scale modeling is required for lattice structures to account for local stress concentrations. A projection-based reduced order model was employed for more precise solutions, using higher-order elemental basis for continuous modeling at interfaces, enabling faster and more accurate calculations.

The fabrication of refractory alloys and lattice structures was completed using digital light processing, powder bed fusion, direct laser metal sintering, and laser engineered net shaping. Digital light processing and direct laser metal sintering can fabricate high-resolution lattice components while directed energy deposition systems are better suited for refractory metal fabrication. Challenges like cracking during debinding and sintering in digital light processing were addressed with custom resin recipes and refined processing profiles. The development of a heated build plate for laser engineered net shaping allowed for the fabrication of refractory multi-principal element alloys with process parameters optimized for bulk builds.

Lattice structures were characterized using stainless steel 316L due to available mechanical property data. Tensile bars with various strut thicknesses were fabricated and tested using in situ x-ray computed tomography tensile testing. The results indicated differences in mechanical performance based on fabrication orientation, with vertically fabricated samples showing more consistent and stronger properties. Compression testing of lattice cubes provided insight into compressive strength and failure modes, with the 0.7-mm strut thickness samples exhibiting behavior akin to bulk material.

Micromechanical testing of tensile bars fabricated from lattice struts and joints revealed differences in yield strength and ultimate tensile strength, attributed to variations in grain size and morphology. The optimized lattice structures for 4-point bend testing were fabricated and tested to validate the TROUT optimization. Experimental results showed that vertically built specimens performed better under loading conditions, with the optimized model demonstrating improved performance over a non-optimized, homogeneous density model.

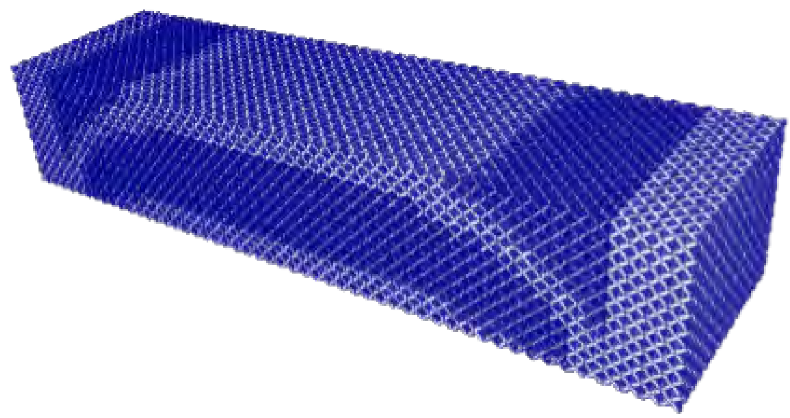
Overall, the TROUT tool effectively optimized lattice structures for specific loading conditions, with fabrication and characterization efforts providing valuable data for verification and validation. Future work aims to refine models and fabrication techniques to further enhance the optimization and performance of lattice structures.

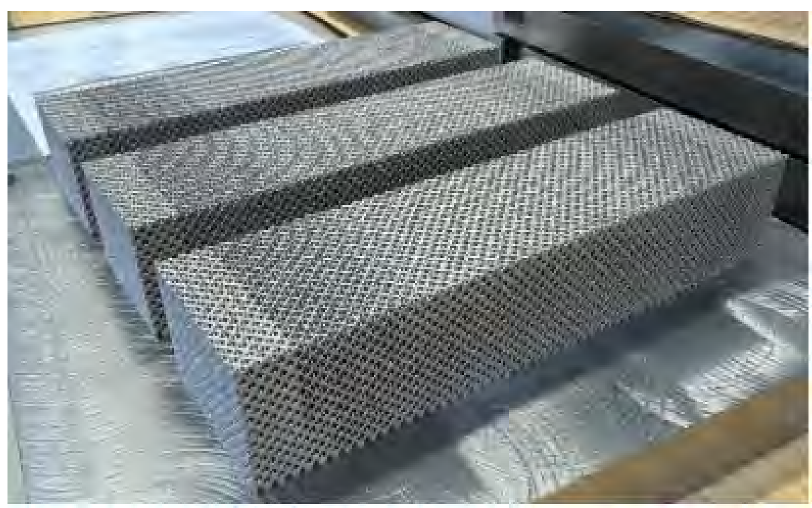
TALENT PIPELINE:

- Jacques Wang, student at Georgia Institute of Technology
- Jakub Toman, postdoc at INL
- Swapnil Morankar, postdoc at INL

PAPERS AND PRESENTATIONS:

- Downey, C., M. Nezdyur, L. Munday, S. Morankar, C. Howard, J. Toman, C. Seepersad, G. Beausoleil, "Multiscale Characterization and Development of SIMP Topology Optimized SS316L Lattice Structured Architectures for Lightweighting Applications." Materials Science and Technology conference, October 6–9, 2024.
- Wang, J. and C. Seepersad, "Design of a Heated Build Plate for Printing Refractory Alloys using Powder Bed Fusion." Solid Freeform Fabrication Symposium, 2024.





Unlocking the Power of Microreactors with Biomimicry and Additively Manufactured Nuclear Fuel

PROJECT NUMBER:
23A1070-037FP

TOTAL APPROVED AMOUNT:
$2,830,000 over 3 years

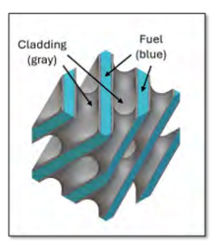
PRINCIPAL INVESTIGATOR:
Nicolas Woolstenhulme

CO-INVESTIGATORS:
Adam Zabriskie, INL
Austen Fradeneck, INL
Joshua Zelina, INL
Nicolas Martin, INL
Silvino Balderrama Prieto, INL
Terry Morton, INL
Joshua Gess, Oregon State University
Mark Anderson, University of Wisconsin

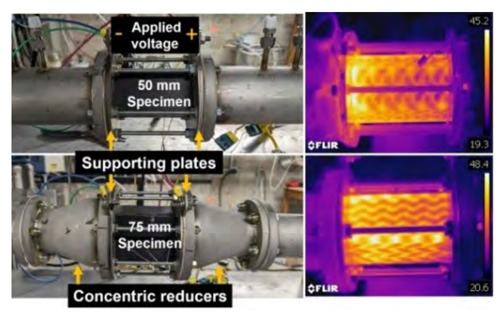
COLLABORATORS:
Massachusetts Institute of Technology
University of Central Florida
StarHagen Aerospace Components, LLC

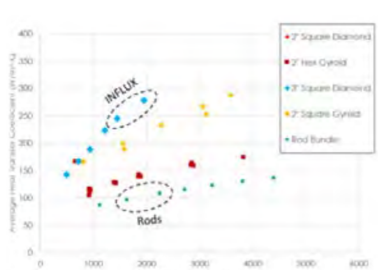
Nature-inspired lattice designs improve nuclear fuel performance.

Nuclear reactors are essentially heat exchangers. Not surprisingly, classical reactor designs resemble traditional tube-in-tank heat exchangers. Progress in advanced manufacturing has spurred a new era of compact heat exchanger research in other energy markets. These designs mimic efficiencies found in nature to significantly improve thermal performance and compactness. This project hypothesized that these same principles would greatly enhance the performance of nuclear fuel by using intertwined lattice geometries based on continuously curved triply periodic minimal surfaces. New methods were pioneered for discretizing and modeling triply periodic minimal surface geometries for nuclear physics, thermal hydraulics, and fuel performance predictions. Innovative approaches were created to perform thermal hydraulic experiments for self-heated triply periodic minimal surface specimens. Novel manufacturing methods were researched using advanced manufacturing to create multi-material lattices with uranium compounds inside. Example reactor design predictions were pursued to compare the performance gains possible using this radical new approach to nuclear fuel design. While much work remains to carry this concept through an applied research and development enterprise, this project was successful in confirming the hypothesis that biomimicry and advanced manufacturing can be used to immensely improve nuclear fuel technology. The key conclusion from this research is that intertwined nuclear fuel lattices offer the potential for dramatic gains in the power output possible from future reactors alongside benefits in nuclear physics optimization and system versatility.



One INFLUX unit cell, can be "tiled" in 3D to create fuel assemblies & reactor cores





Overview of the Intertwined Nuclear Fuel Lattice for Uprated heat eXchange (INFLUX) design and experiments showing dramatic improvements in heat transfer.

TALENT PIPELINE:

- Andrew Ostrowski, student at University of Central Florida
- Beau Ballard, student at University of California, Berkely
- Brett Prussack, student at University of Wisconsin
- Dade George, student at Pennsylvania State University
- Erik Pagenkopf, student at University of Wisconsin
- Paul Ferney, postdoc at INL, converted to staff
- Silvino Balderrama Prieto, postdoc at INL, converted to staff
- Smruti Sanjaykumar Shah, student at Texas A&M University
- William Fritsch, student at University of Tennessee Knoxville
- Youyeon Choi, student at Massachusetts Institute of Technology
- Zander Ray, student at Oregon State University

PAPERS AND PRESENTATIONS:

- N. Martin, S. Seo, S. Balderrama Prieto, C. Jesse, N. Woolstenhulme, "Reactor physics characterization of triply periodic minimal surface-based nuclear fuel lattices." Progress in Nuclear Energy, 165, 104895, November 2023.
- Ferney, Paul Alexandre and Martin, Nicolas Pierre, "Implementation of Triply Periodic Minimal Surfaces in OpenMC." Available at SSRN: https://ssrn.com/abstract=5179133
- Silvino A. Balderrama Prieto, Nicolas P. Martin, Brett A. Prussack, Austen D. Fradeneck, Nicolas E. Woolstenhulme, Mark H. Anderson, "CFD modeling of turbulent air flow in self-heated gyroid TPMS structures: Thermal hydraulic performance and validation." Applied Thermal Engineering, Volume 279, Part E, 2025, 127682, ISSN 1359-4311.
- N. Woolstenhulme, N. Martin, C. Jesse, J. Zelina, M. Anderson, B. Prussack, "The Prodigious Potential of Intertwined Nuclear Fuel Lattices." Proceedings of the TopFuel 2024 conference.
- Brett Prussack, Ian Jentz, Tiago A. Moreira, Nicolas Woolstenhulme, Casey Jesse, Greg Nellis, Mark Anderson, "Thermal and hydraulic performance of volumetrically heated triply periodic minimal surface heaters." Applied Thermal Engineering, 2024, 123291, ISSN 1359-4311.
- Brett Prussack, Erik Pagenkopf, Silvino Balderrama Prieto, Austen Fradeneck, Adam Zabriskie, Josh Zelina, Ray Zander, Joshua Gess, Cheng-Kai Tai, Jeffrey Reed, Nicolas Woolstenhulme, Greg Nellis, Mark Anderson, "Thermal hydraulic and neutronic performance characterization of triply periodic minimal surface lattices." Proceedings of the TopFuel 2025 conference.
- Brett Prussack, Ian Jentz, Tiago A. Moreira, Erik Pagenkopf, Nicolas Woolstenhulme, Greg Nellis, Mark Anderson, "Local heat transfer measurement in a volumetrically heated TPMS lattice using distributed optical fiber thermal sensing." Applied Thermal Engineering, Volume 269, Part B, 2025, 126101, ISSN 1359-4311.
- Nicolas E. Woolstenhulme, Nicolas P. Martin, Joshua Zelina, Paul A. Ferney, Austen D. Fradeneck, Adam Zabriskie, Mark H. Anderson, Brett Prussack, Koroush Shirvan, Youyeon Choi, Jeffrey L. Reed, Kai Tai, "Progress Toward Revolutionary Reactor Designs using Nature-Inspired Nuclear Fuel." Proceedings of the TopFuel 2025 conference.

EXTERNAL INTELLECTUAL PROPERTY:

- INL Software, & Martin, N. (2024), "Triply Periodic Minimal Surface Geometry Builder." Software https://inlsoftware.inl.gov/product/triplyperiodicgeometry
- Calvin M. Downey, Joshua T. Hanophy, Nicolas E. Woolstenhulme, Max N. Nezdyur, Silvino A. Balderrama Prieto, Joshua N. Zelina, "Nuclear Fuel System, Method of Operating a Nuclear Fuel System, and Method of Fabricating a Nuclear Fuel Assembly," 63/843,802 07/14/2025.
- Joshua N. Zelina, Nicolas E. Woolstenhulme, "Fabrication of Articles Having Different Materials and Fabrication of Nuclear Fuel Assemblies through Hot Isostatic Pressing and Additive Manufacturing," 63/778,231 03/26/2025.

AWARD:

1st place winner at the LDRD poster session

Computationally Informed Design and Manufacturing of Damage Tolerant Materials

PROJECT NUMBER:
23A1070-057FP

TOTAL APPROVED AMOUNT:
$1,275,000 over 3 years

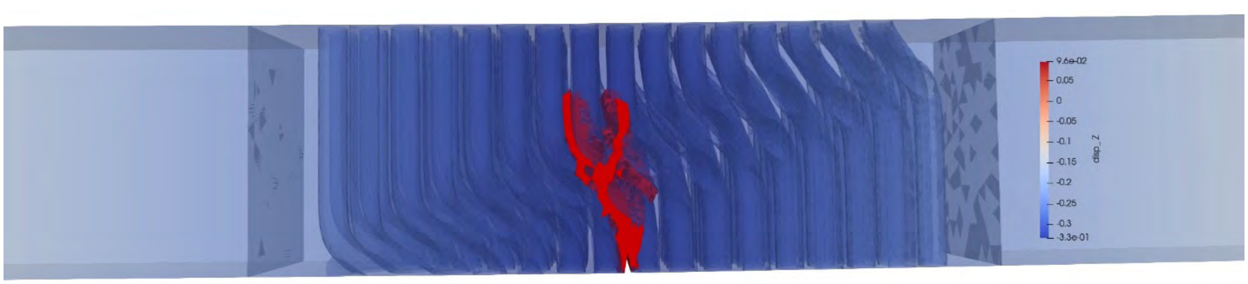
PRINCIPAL INVESTIGATOR:
Donna Post Guillen

CO-INVESTIGATORS:
Bradley Huddleston, INL
Adrian Wagner, INL

COLLABORATORS:
Argonne National Laboratory
Lawrence Berkeley National Laboratory
University of Washington
Purdue University
Rocky Mountain Scientific

Dental enamel microstructures inspire damage tolerant ceramics design.

Our project addressed the critical issue of low fracture toughness in modern ceramics by designing microstructures and composites inspired by dental enamel. Despite its high mineral content, dental enamel exhibits remarkable fracture toughness due to its intricate nanostructure, which effectively deflects cracks and dissipates energy. We aimed to replicate these mechanisms in ceramic materials using advanced characterization and digital reconstruction techniques. Synchrotron studies on mammalian enamel samples revealed rods arranged in bands with a decussated structure. Using synchrotron micro- and nano-computed x-ray tomography, we elucidated the microstructural assembly of enamel rods and characterized decussation bands. The resulting three-dimensional printed ceramic structures serve to guide crack propagation, with cracks becoming more tortuous around the rods, which dissipated fracture energy. We successfully developed a novel ceramic composite by integrating additively manufactured yttria stabilized zirconia rods into an alumina matrix. To evaluate the mechanical performance of these composites, we designed and validated a custom ball-on-ring testing apparatus. This apparatus accurately measures rupture strength by inducing a biaxial flexural stress state, thereby avoiding the edge-induced stress concentrations common in traditional bend tests. Using microwave debinding, rather than conventional thermal debinding furnaces, we were able to achieve a 70% energy savings. By integrating electromagnetic and heat transfer modules within MOOSE, we accurately predicted temperature gradients and prevented temperature spikes, thereby enhancing process efficiency during microwave debinding. In summary, our accomplishments include developing bioinspired ceramic composites, validating novel testing methods, and achieving significant energy savings in microwave debinding processes. These findings contribute to the advancement of ceramic materials for high-temperature and high-stress applications, aligning with the interests of DOE and the Department of Defense in high-performance materials.



Example of crack branching behavior in rodded composite material predicted by finite element simulations.

TALENT PIPELINE:

- Gabriel Thompson, student at Colorado School of Mines
- Konner Cutts, student at Idaho State University, converted to staff
- Bradley Huddleston, postdoc at INL, converted to staff

PAPERS AND PRESENTATIONS:

- Marsico, C., Grimm, J. R., Renteria, C., Guillen, D. P., Tang, K., Nikitin, V., Arola, D. D., "Characterizing the Microstructures of Mammalian Enamel by Synchrotron Phase Contrast microCT." Acta Biomaterialia 178, 208-220 (2024)
- Guo, Z., Guillen, D.P., Grimm, J.R., Renteria, C., Marsico, C., Nikitin, V., Arola, D., "High Throughput Automated Characterization of Enamel Microstructure using Synchrotron Tomography and Optical Flow Imaging." Acta Biomaterialia, 181, 263-271 (2024).
- C. Marsico, C. Renteria, J. R. Grimm, J. Fernandez-Arteaga, D. Guillen, and D. Arola, "A Machine Learning Approach to Quantitative Analysis of Enamel Microstructure from Scanning Electron Microscopy Images." Small Structures 6(5), 2400510 (2025).
- Guillen, D. P., DeChant, C. S., Cutts, K. S., Tucker, D., "Microwave Debinding of Ceramics Produced by Additive Manufacturing." Presented at IMPI's 59th Annual Microwave Power Symposium, Edmonton, Alberta, Canada, June 2025.

EXTERNAL AWARDS:

1st place, Argonne National Laboratory, Art of Science contest, 2024.

A Hybrid Physics-informed Reduced Order Model Embedded with Process-informed Fluctuations for Quality Control in Directed Energy Deposition

PROJECT NUMBER:
23A1070-096FP

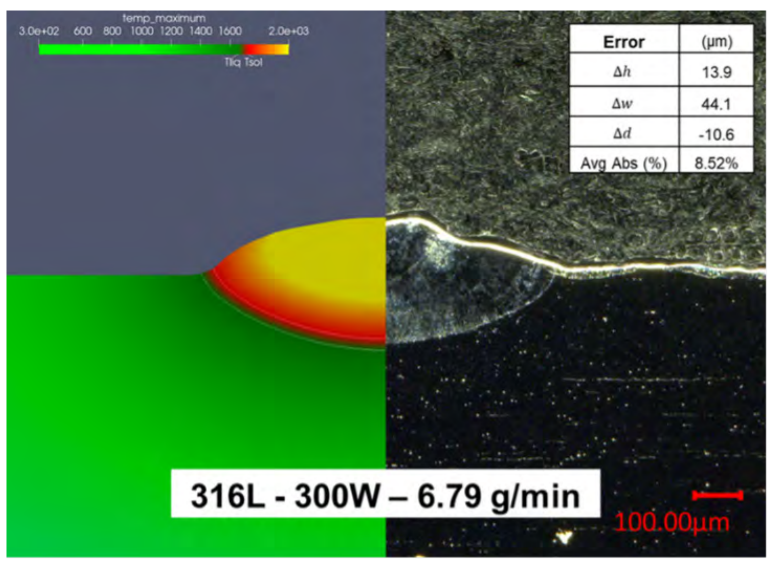
TOTAL APPROVED AMOUNT:
$1,300,000 over 3 years

PRINCIPAL INVESTIGATOR:
Dewen Yushu

CO-INVESTIGATORS:
Asa Monson, INL
Rongjie Song, INL
Wen Jiang, INL
Yifeng Che, INL
Anant Raj, Purdue University
Hany Abdel-Khalik, Purdue University

Advanced modeling improves additive manufacturing quality control.

This project aims to enhance the quality of additive manufacturing materials by developing physics-informed reduced order models with process-informed fluctuations for the directed energy deposition process. Throughout the project, we have achieved several significant scientific milestones. First, enhancements were made using ray tracing to accurately account for laser reflection and absorption among particles. Meanwhile, a cellular automata finite element model was developed, showing promise in simulating grain growth and morphology during directed energy deposition. Second, the laser and powder efficiency of the melt pool model were validated through a machine learning based approach using experimental measurements. Third, the collection of microstructural data from directed energy deposition samples produced under varying process parameters and corresponding microstructural analysis have been completed. Fourth, the reduced order model solver demonstrated efficiency for the heat equation within the MOOSE framework and was applied to the multiphysics melt pool model. Finally, machine learning approaches were explored to create reduced order models, providing an alternative method for fast and accurate predictions of melt pool temperature, velocity, pressure, and level set variables. Beyond supporting existing projects and additive manufacturing related research programs, this project achieved several significant outcomes and impacts. It supported the academic pursuits of a former INL intern, a former INL distinguished postdoctoral researcher, and a former computational scientist. Additionally, the project established close collaborations with North Carolina State University and Purdue University and supported two graduate students in their studies.



Example of calibrated bead geometry.

TALENT PIPELINE:

- Luis Nuñez, postdoc at INL
- Max Nezdyur, staff at INL
- Tsu-Chun Teng, student at North Carolina State University
- Yifeng Che, Russell L. Heath distinguished postdoc at INL, assistant professor at Georgia Institute of Technology
- Anant Raj, postdoc at Purdue University, staff at Oak Ridge National Laboratory
- Charles Reynolds Owen, student at Purdue University, research assistant at University of Texas Austin

PAPER AND PRESENTATIONS:

- A. Raj, H. Abdel-Khalik, L. Nuñez, Y. Che, W. Jiang, R. Song, "Physics-informed reduced order model for directed energy deposition simulations in MALAMUTE." TMS Fall Meeting, October 2023.
- W. Jiang, D. Yushu, H. Oh, "Multiphysics modeling of melt pool with Raytracing in the open-source MALAMUTE software." TMS, March 2024.
- D. Yushu, S. Pitts, S. Biswas, P. German, S. Dhulipala, M. Moorehead, L. Aagesen, A. Jokisaari, "Advanced manufacturing qualification through multiscale multiphysics modeling, validation, reduced order modeling, and process-informed optimization." SIAM Conference on Materials Science, May 2024.
- T. Teng, D. Yushu, L. Nuñez, W. Jiang, "Integrating CAFE with MOOSE for Microstructure Evolution Analysis in 316L Stainless Steel 3D Printing Process." TMS, March 2025.
- W. Ji, O. Muransky, M.C. Messner, W. Jiang, T. Hu, M. Smith, "Development, validation, and verification of multi-pass thermomechanical welding simulations using the open-source MOOSE framework: NeT TG4 benchmark weldment." International Journal of Pressure Vessels and Piping, 2025, 105560.

Melt Wires Analyzed via Wireless Radio Frequency Identification Techniques

PROJECT NUMBER:
24P1084-021FP

TOTAL APPROVED AMOUNT:
$125,000 over 1 year

PRINCIPAL INVESTIGATOR:
James Smith

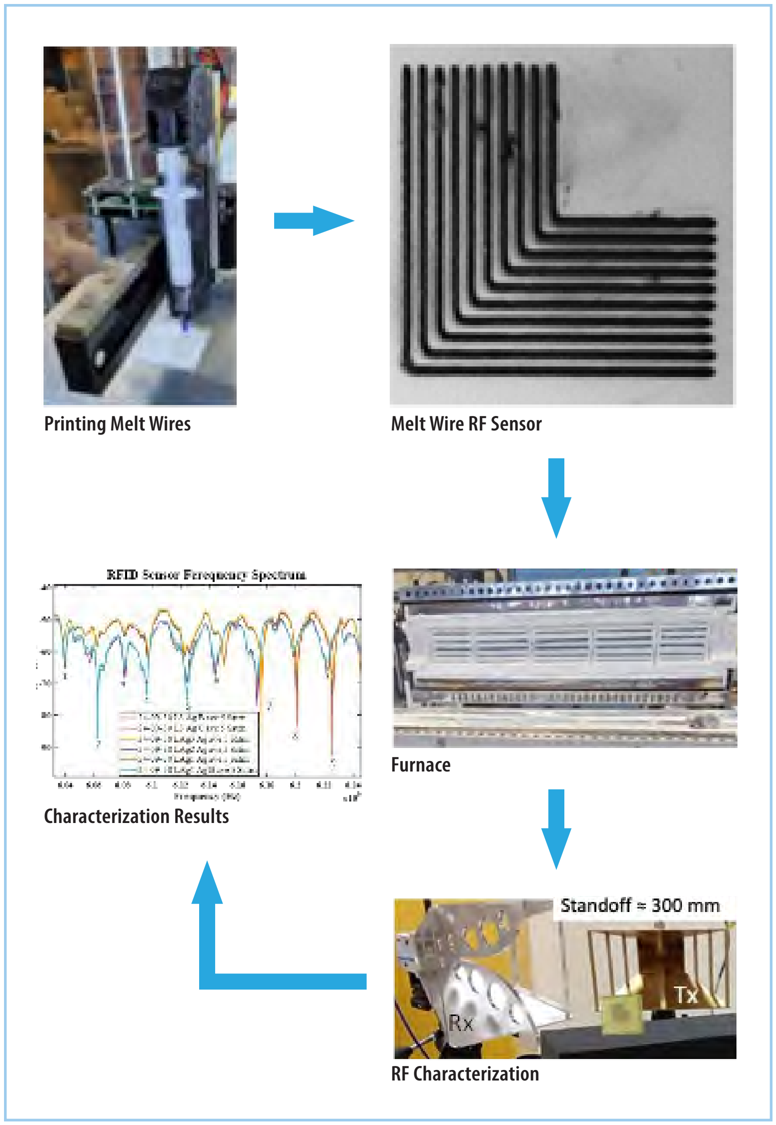
CO-INVESTIGATORS:
Joshua Daw, INL
Kiyo Fujimoto, INL
Konner Cutts, INL

Novel technique reduces cost and improves accuracy and reliability of irradiation testing temperature measurements.

Current passive temperature monitors have been in use for many decades in irradiation testing experiments. The simplest method of measuring the maximum temperature during an irradiation experiment is with melt wires. Melt wires are metallic wire segments which are encapsulated and installed within an experiment. As the melting temperatures of the included wires are carefully characterized, the peak temperature can be estimated by determination of whether a wire has melted during an experiment. A capsule containing wires of varied compositions improves the estimate as some wires melt and others do not. Using melt wires is common because they are inexpensive and passive, needing no pressure vessel penetrations. However, post experiment analysis of the melt wire is complicated by the need for a person to visually inspect the quartz capsule and determine which melt wires have and have not melted. This is not a trivial task and can be subjective at times because the quartz capsule can be obscured and the melt wires may deform but not be completely melted. An innovative methodology based on additive manufacturing and a radio frequency identification sensor has been investigated to simplify and accelerate melt wire characterization with greater precision. Ultimately, the additive manufacturing inks can be mixed to tailor alloys that will melt at specific temperatures. The ability to tailor the ink compositions to melt at specific temperatures addresses the limited temperature resolution of currently available melt wire materials. The radio frequency identification sensor addresses the need to increase melt wire reading expediency, accuracy, and reliability.

TALENT PIPELINE:

- Konner Cutts, student at Idaho State University, converted to staff



The process to fabricate, heat and characterize the radio frequency melt wire sensor is shown.

SECURE AND RESILIENT CYBER-PHYSICAL SYSTEMS

CORE CAPABILITIES

Advanced Computer Science, Visualization, and Data

Applied Mathematics

Applied Materials Science and Engineering

Condensed Matter Physics and Material Science

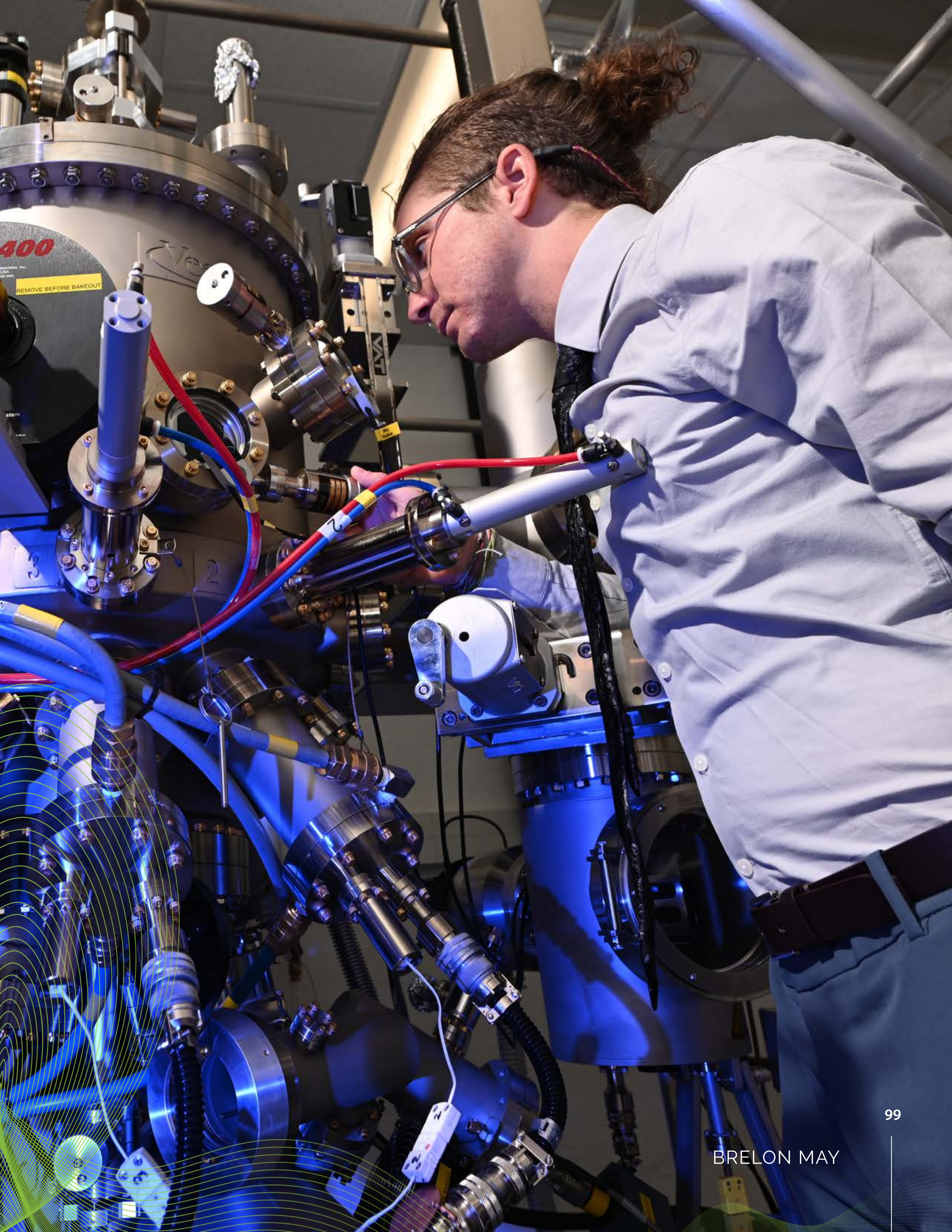
Cyber and Information Science (or Cyber and Information Sciences)

Decision Science and Analysis

Microelectronics

Systems Engineering and Integration

The lab is enhancing the nation's critical infrastructure's resilience against complex and dynamic cyber threats, adapting to a wide range of hazards and environmental changes. With rapid energy expansion each year, the bulk electric system faces more unprotected connections. Additionally, US government officials are increasingly worried that foreign state-sponsored cyber actors may prepare for disruptive or destructive cyberattacks on US critical infrastructure during major crises or conflicts. INL has already developed new test beds and simulators for critical infrastructure resilience R&D and created a new range for testing next generation mission critical communications. Over the next five to ten years, we will help industries, government, and academia adopt cyber-informed engineering principles and innovate new ways for civilian and government entities that provide essential services to protect themselves against cyberattacks.



BRELON MAY

Provable Security and Resilience for Critical Infrastructure

PROJECT NUMBER:
22P1067-004FP

TOTAL APPROVED AMOUNT:
$5,475,000 over 3 years

PRINCIPAL INVESTIGATOR:
Gregory Shannon

CO-INVESTIGATORS:
Lance Joneckis, INL

COLLABORATORS:
Kry10
University of Pittsburgh
Iowa State University
Cyber Manufacturing Innovation Institute

Formal verification methods improve cyber-physical systems protection and development efficiency by several orders of magnitude.

This project developed a formal methods-based approach to ensure the security and resilience of cyber-physical systems for critical infrastructure (CPS-CI), with the goal of enhancing operational protection efficacy and development efficiency. Formal methods-based approaches use mathematical techniques to specify, design, and verify software and hardware, providing proof-based evidence of correctness while preventing errors that often surface after deployment. CPS-CI require strong guarantees of operational correctness, resilience, and security because they control physical processes, where failures can cause equipment damage, injury, or loss of life. Additionally, CPS-CI are increasingly targeted by cyberattacks as advanced technologies are integrated to facilitate remote operations, administration, and maintenance. Current approaches rely on engineering best practices, imprecise application of technical controls, and corrective threat and incident response procedures, which are insufficient for mission and safety critical CPS-CI.

To overcome these limits, this project leveraged the formally verified seL4 microkernel, whose implementation was proven to meet its specification, ensuring functional correctness. It also enforces confidentiality, integrity, and availability through security proofs. By collaborating with Kry10, this project developed the Assured Reserve Modes Architecture (ARMA) on the seL4-based Kry10 operating system. ARMA enables systems to transition to predefined, secure reserve modes during failures or cyberattacks. This sustains continuous operation without impacting system performance with automated threat and incident responses. ARMA was demonstrated on a representative industrial control system and on Open Radio Access Networks, detecting simulated incidents and transitioning the system into appropriate reserve modes to contain and mitigate the impacts.

To ensure safe and secure communication between processes, this project developed the Dynamically Assured Typed Universal Messaging (DATUM) framework, which formalizes protocol specifications using refined multiparty session types. The refined multiparty session types were formally specified and verified in the interactive theorem prover F* and compiled into OCaml for runtime verification during system operations. DATUM was demonstrated on ground control station – unmanned aerial vehicles communications that prevented stealthy attacks against the MAVLink mission subprotocol.

Finally, this project developed a framework for integrating fully homomorphic encrypted digital control systems deployed in CPS-CI. This framework established end-to-end privacy by using a fixed-point learning with error-based encryption scheme, which encrypts sensitive sensor measurements and system parameters and performs computations on the encrypted data without the need to decrypt. This project demonstrated the framework on linear control systems, Kalman filters, and in a hardware-in-the-loop approach for an advanced nuclear reactor.

TALENT PIPELINE:

- Arthur Amorim, student at University of Central Florida
- Beau Smith, student at Iowa State University
- Daniel Cole, professor at University of Pittsburgh, appointed as INL faculty researcher
- Henry Ray Olvera Jr., student at University of Texis Rio Grande Valley, converted to staff
- Karem Elmaaroufi, student at University of California, Berkeley
- Maxwell Taylor, student at The Ohio State University, converted to staff
- Robert Lois, student at University of Pittsburgh
- Sara Logsdon, student at University of Georgia
- Sebastion Vera, student at California State University Monterey Bay, converted to staff
- Tracy La Van, student at Iowa State University
- Trevor Kann, student at Carnegie Mellon University
- William Harrison, professor at University of Missouri, appointed to INL faculty researcher

PAPERS AND PRESENTATIONS:

- A. Amorim, T. Kann, M. Taylor, and L. Joneckis, "Toward Provable Security in Industrial Control Systems Via Dynamic Protocol Attestation." in 2024 Annual Computer Security Applications Conference Workshops, Honolulu, HI, 2024.
- A. Amorim, M. Taylor, T. Kann, W.L. Harrison, G.T. Leavens, and L. Joneckis, "Enforcing MAVLink Safety & Security Properties via Refined Multiparty Session." NASA Formal Methods: 17th International Symposium, NFM 2025, Williamsburg, VA, 2025.
- L. Joneckis, "A High Assurance Protection Stack for Critical Infrastructure." AFRL Space Cyber Summit, October 2023.
- L. Joneckis and W. Harrison, "Extensions of SysML Using Category Theory for Structured Analysis." Workshop on Mathematical Formalized Assurance for National Security," April 2024.
- L. Joneckis and I. Kuz, "Assured Reserve Modes in Action." 2024 seL4 Summit, Sydney, AUS, 2024.
- R.S. Lois, and D.G. Cole, "Designing secure and resilient cyber-physical systems using formal models." 2022 Resilience Week (RWS) IEEE, Washington D.C., 2022.
- R.S. Lois, and D.G. Cole, "Encrypted Control Using Modified Learning with Errors-based Schemes." International Federation of Automatic Control, Modeling, Estimation, and Control Conference, Chicago, IL, 2024.
- R.S. Lois, and D.G. Cole, "Employing a Hardware-in-the-Loop Approach to Realize a Fully Homomorphic Encrypted Controller for a Small Modular Advanced High Temperature Reactor." 2025 ANS Annual Conference, Chicago, IL, 2025.

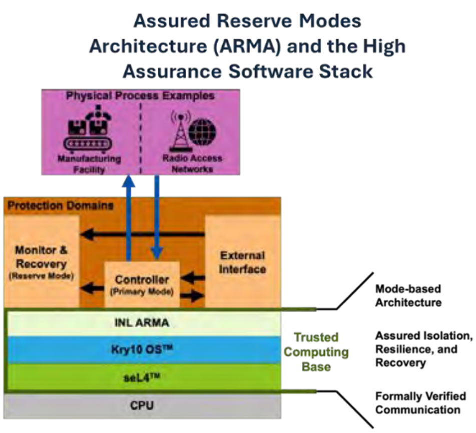
EXTERNAL INTELLECTUAL PROPERTY:

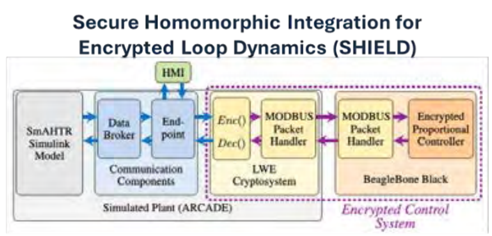
R. Lois, L. Joneckis, D. Cole, G. Shannon, "Homomorphic Encryption to Protect Cyber-Physical Interfaces and Related Apparatuses, Systems, and Methods." BEA Docket No. BA 1458 Draft Provisional Patent Application.

EXTERNAL AWARDS:

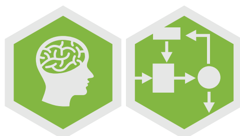
First Place, Best Student Paper, R. Lois, "Employing a Hardware-in-the-Loop Approach to Realize a Fully Homomorphic Encrypted Controller for a Small Modular Advanced High Temperature Reactor." NPIC & HMIT 2025.

The high assurance software stack for cyber-physical systems that consists of ARMA and its trusted computing base foundations. The DATUM framework for formally verified protocols and runtime anomaly detection. The Secure Homomorphic Integration for Encrypted Loop Dynamics (SHIELD) framework for integrating fully homomorphic encryption into control systems, providing confidentiality for critical control signals and parameters.





Augmented Machine Intelligence for Critical Infrastructure



PROJECT NUMBER:
23A1070-061FP

TOTAL APPROVED AMOUNT:
$1,000,000.00 over 3 years

PRINCIPAL INVESTIGATOR:
Eduardo Trevino

CO-INVESTIGATORS:
Shiloh Elliott, INL
Matthew (Ross) Kunz, INL
Ashley Shields, INL

COLLABORATORS:
University of Utah

Advanced multi-modal artificial intelligence frameworks strengthen national security.

Critical infrastructure analysis is essential for ensuring resilient operations of US energy, water, transportation, and healthcare systems under uncertain and evolving operational conditions. Current machine learning approaches present significant limitations: they are statistical, highly specialized, and confined to well-defined problem sets within narrow application domains. These characteristics result in products that are brittle and at risk of failure in national security contexts, where critical safety performance must be maintained under unknown operational conditions.

A fundamental technical challenge lies in simultaneously characterizing and contextualizing critical infrastructure entities, operations, and systems. The existing human-based decision-making process relies on manual analysis of sparse and disparate datasets, requiring causal inference for reasoning to reduce decision uncertainty. This approach is error-prone, brittle, quickly becomes obsolete, and fails to scale or adapt to emerging national security challenges.

Recent advances in data science offer promising solutions by developing methods inspired by human analytical capabilities, incorporating reasoning, multidisciplinary ensemble techniques, and fusion methods. This project proposes a novel ensemble modeling approach that implements data fusion techniques, leverages diverse datasets, and employs advanced machine learning methods to construct a robust data fusion framework. This framework will enable accurate decision-making while adapting to unknown operational conditions.

The proposed solution goes beyond standard content-only machine learning by delivering an analytical framework capable of both characterizing and contextualizing critical infrastructure entities, operations, and systems. The framework will integrate reasoning capabilities that mirror human analytical processes while providing the scalability and adaptability required for evolving national security needs.

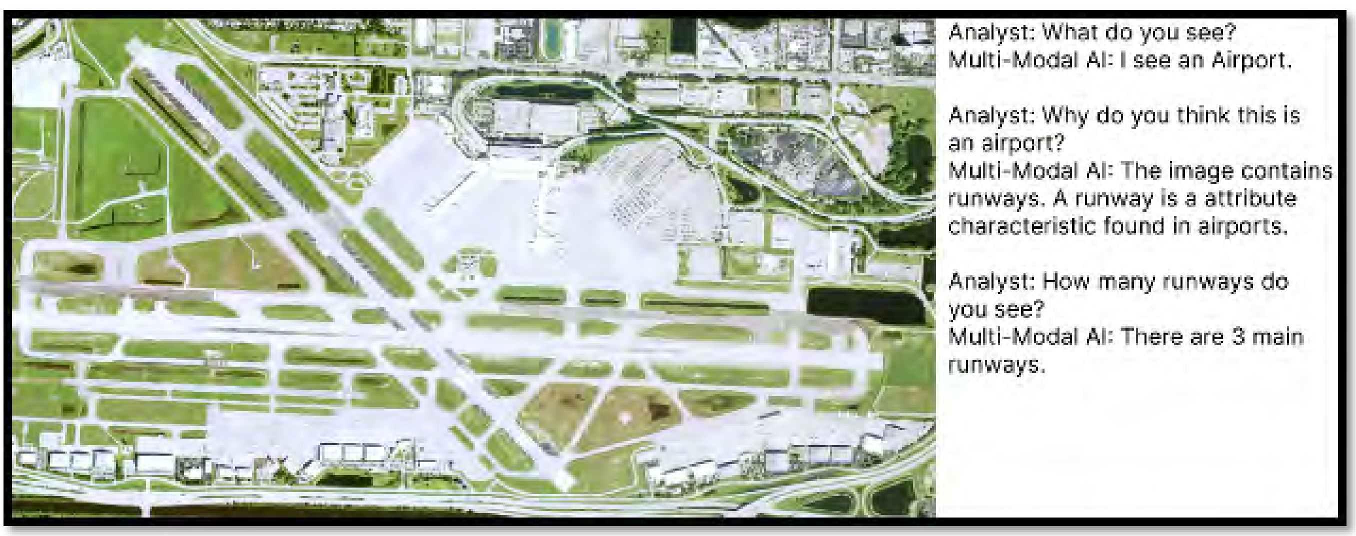
Successful implementation would establish a methodology achieving decision-making performance comparable to human-based critical infrastructure characterization and contextualization. More importantly, it would provide reasoning capabilities that can scale effectively with emerging national security requirements, addressing the critical gap between current brittle systems and the dynamic needs of infrastructure security. This advancement would significantly enhance the nation's ability to protect and maintain critical infrastructure under increasingly complex and unpredictable threat landscapes.

TALENT PIPELINE:

- Joseph Anthony Coco, student at Illinois Institute of Technology
- Laura Ziegler, student at University of Utah

PRESENTATION:

- Ziegler et al., (2023, March 19-23) “Scaling Microstructure-dependent Mechanical Properties to Bulk Material Properties using 3D Convolutional Neural Networks.” [Poster Presentation]. TMS 2013 Conference, San Diego, CA.



Human-like Conversational Reasoning. This example demonstrates the model’s ability to identify an asset and to explain its reasoning. The model correctly identifies the image as an airport and justifies its conclusion by pointing to a key visual feature, the runways (though it appears that the number of runways is incorrect). This showcases the model's capacity for contextual understanding, mirroring a human analyst's thought process.

Evidence-Based Zero Trust Data Analytics Toolkit for Industrial Internet of Things Systems to Fuel Cyber Strategies for Security and Reliability

PROJECT NUMBER:
23A1070-086FP

TOTAL APPROVED AMOUNT:
$1,194,000 over 3 years

PRINCIPAL INVESTIGATOR:
Shaya Wolf

CO-INVESTIGATORS:
Rita Foster, INL
Bryan Beckman, INL
Manuel Maestas, INL
Manuel Vazquez, INL
May Chaffin, INL
Jed Haile, INL
Michael Cutshaw, INL
Sin Ming Loo, Boise State University
Hao Chen, Boise State University
Mike Borowczak, University of Central Florida

Zero trust data analytics strengthen cybersecurity and reliability of industrial Internet of Things systems, cloud environments, and embedded networks.

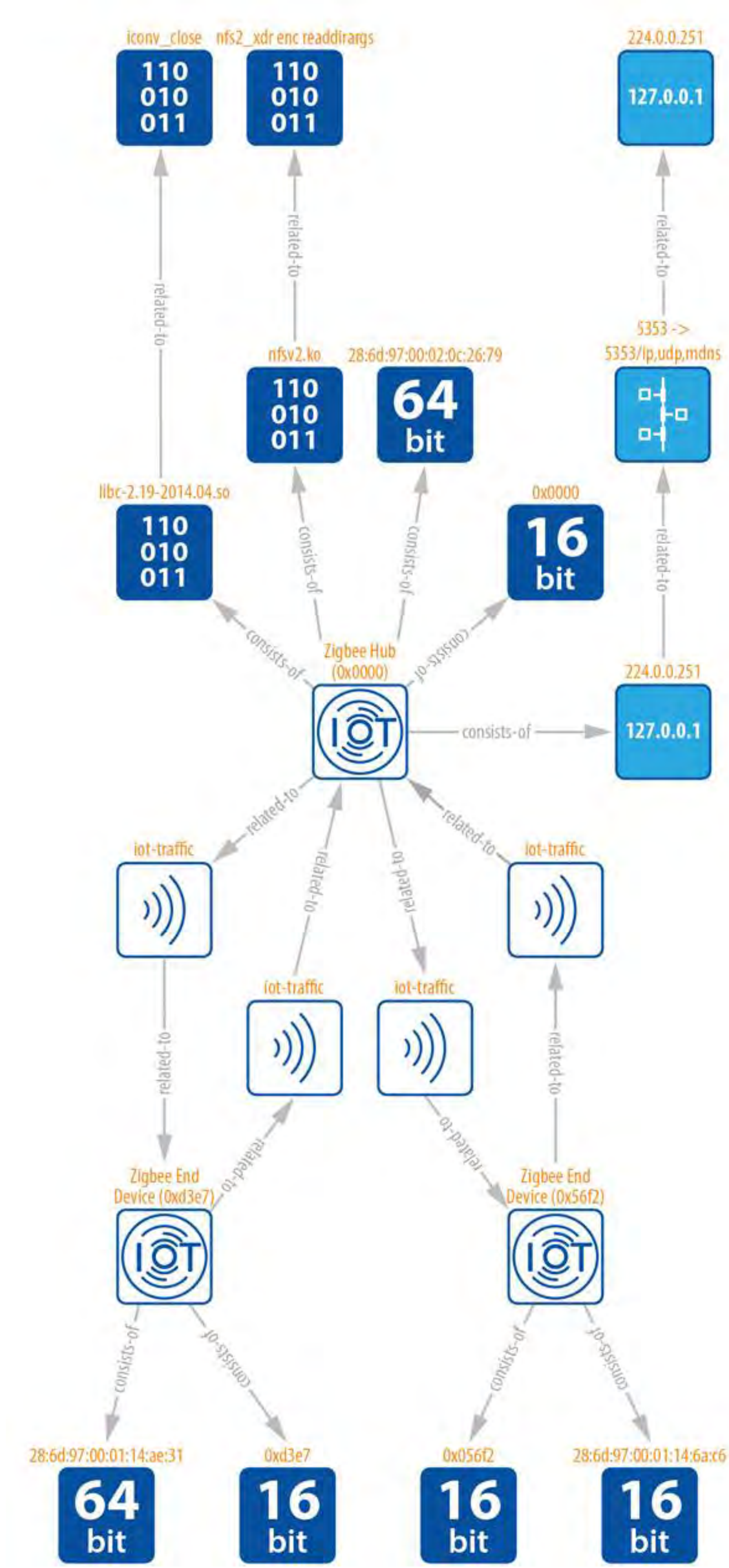
The Zero Trust project for industrial Internet of Things (IIoT) devices investigated zero trust principles and found that while many claim compliance with concepts like "never trust, always verify", these principles have not been extended to devices, cloud environments, embedded architectures, and specialized networks. The Zero Trust research team built two testbeds to investigate zero trust principles, one at INL and one at Boise State University, consisting of typical smart building technologies that are widely used and nearly ubiquitously trusted. Throughout this project, visibility was increased for mesh networks, cloud environments and IIoT systems. Three major contributions were made including:

- Creation of enduring codified attack surface capabilities tailored to zero trust concepts and IIoT devices, including identification of cloud environments and meshed networks, which allows asset owners to take control of emerging threats and vulnerabilities over full life cycles and included enhanced data quality standards,
- Verification of visibility into IIoT through performance impacts of mesh networks under system changes, finding that such impacts cannot be properly analyzed on IIoT devices due to lack of visibility, and leading to other methods including specification analysis to identify the internals of embedded architectures and analysis of pulled firmware, and
- An investigation into the difficulties of firmware analysis capabilities on IIoT devices which showed a lack of transparency in IIoT devices with the firmware being problematic to pull and difficult to analyze using reverse engineering tools.

Supporting this effort included the development of three tools. First, EVAL (short for evaluation), extended from the INL Scoring Threat Object Analysis Tool, was created to examine the quality of the system information provided through the generated attack surface graphs. The second tool, EEV (standing for enrich, enforce, and validate) enriches attack surface graphs by adding associated weaknesses, vulnerabilities, and attack patterns to the graphs; enforces high quality data standards by applying various common fixes and checking for errors; and validates that attack surfaces are compliant with data formatting rules for these types of graphs. The third tool, Zapiary, enabled better understanding of network communications between the testbed devices regardless of their use of Zigbee and ZWave technologies which do not follow typical protocol formats.

TALENT PIPELINE:

- Adithya Chantala, student at University of Texas, Dallas
- Alyssa Taylor, student at University of Idaho
- Braxton Marlatt, student at University of Idaho
- Claire Westby, student at University of Idaho
- Clara Ness, student at University of Tulsa
- Darrin Lea, student at Louisianan State University, converted to staff
- Faith Coslett, student at the University of Wyoming, converted to staff
- Gio Roberts, student at Albany State University
- Grace Lytle, student at Boise State University
- Jason Wharton, student at University of California, Los Angeles
- Joey Krejchi, student at Iowa State University
- Jorge Cortez, student at Idaho State University
- Karina Permann, student at University of Idaho, converted to staff
- Kevin Guerra, student at University of Texas, El Paso
- Mark Tachick, student at Boise State University
- Michael Ades, student at Texas A&M University
- Paul-Ann Francis, student at University of Southern Florida
- Sam Ofiaza, student at University of Texas, Dallas
- Taylor McCampbell, student at the University of Wyoming



An attack surface graph in Structure Threat Intelligence eXpression (STIX). Created using Zapiary and the other Zigbee/ZWave capabilities.

Detecting Unclassified Electromagnetic Signals for Secure Wireless Communication Using Open Set Recognition

PROJECT NUMBER:
24A1081-049FP

TOTAL APPROVED AMOUNT:
$800,000 over 2 years

PRINCIPAL INVESTIGATOR:
Anna Quach

CO-INVESTIGATORS:
Daniel Wells, INL
Nicholas Kaminski, INL
Randall Reese, INL
Dola Saha, University at Albany, SUNY

Enhanced open set recognition models improve the security of wireless communications.

We developed multiple machine learning methods for the detection and classification of new wireless communication waveforms, which is critical for targeted attacks in wireless networks and electronic warfare. Our machine learning models are capable of dynamically detecting security threats in near real time through our advanced open set recognition approach. This model has demonstrated significant improvements in the detection of unknown waveforms, thereby enhancing the security and reliability of mission critical communications.

Our approach to detecting uncertain security threats is novel; we advanced open set recognition techniques by incorporating multiple domain representations of wireless signals. Specifically, we combined time and frequency domain model features to enhance the model's performance. Utilizing an open set recognition approach eliminates the need for training data to be distributed similarly to the deployment environment and removes the requirement for the training set to contains all possible threat classes, which is pertinent due to the inability to anticipate all possible signals without prior knowledge.

Our models were trained on simulated data, generated in partnership with the University at Albany, State of New York. The dataset contained a diverse array of wireless signals, including those with additive white Gaussian noise and multipath signals, with and without line of sight. This comprehensive training set allowed us to optimize our models to detect unknown waveforms under various challenging scenarios, such as low signal-to-noise ratios. By training on various waveforms, varying signal-to-noise ratio, experimenting with different combinations of known data classes, and different sample sizes under normal conditions, our models were fine tuned to perform effectively in challenging environments.

TALENT PIPELINE:

- Sushmita Sarker, student at University of Nevada, Reno
- Oshadhi Rajapakshe, student at University at Albany, SUNY
- Getaneh Tarekegn, postdoc at University at Albany, SUNY
- Xue Wei, student at University at Albany, SUNY

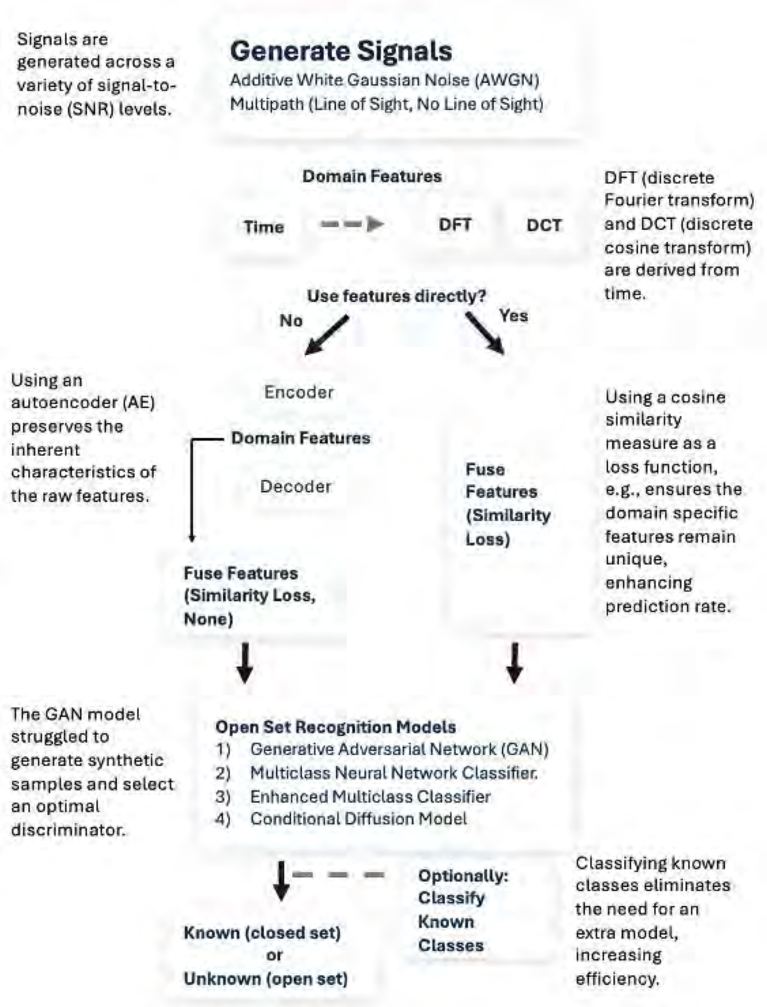
PRESENTATIONS:

- X. Wei, D. Saha, and A. Quach, "Exploiting multi-domain features for detection of unclassified electromagnetic signals." MILCOM 2024—2024 IEEE Military Communications Conference (MILCOM), 2024.
- X. Wei, A. Quach, D. Wells, and D. Saha, "Contrasting Time-Frequency Representations for Unknown Waveform Detection." ICC 2025—2025 IEEE International Conference on Communications, 2025.

EXTERNAL AWARDS:

MILCOM 2024 ComSoc Student Travel Grant

Overall workflow outlining the data generation, preprocessing steps, and the sequential development of models for the open set recognition task. Initially, data was generated and preprocessed before being fed into various model architectures. The first model, a generative adversarial network, utilized autoencoder features representing three domain features but did not classify known classes. The second model employed a discriminative neural network architecture, leveraging fused time and discrete Fourier transform features with a cosine similarity loss. The third model advances this architecture to handle an expanded and diverse set of wireless signal types (multipath with and without line-of-sight). Through systematic optimization, we determined that raw feature inputs outperformed enhanced autoencoder features (which provide native complex number support and phase preservation), and that Manhattan distance for minimizing loss across time and frequency domain features yielded optimal performance in classifying unknown wireless signals. Finally, a conditional diffusion model was developed, operating directly on time and frequency domain data.



AskSoftly: Combining Multiple Language Models with External Information Storage to Increase Binary Software Analysis Capabilities at Scale

PROJECT NUMBER:
24A1081-220FP

TOTAL APPROVED AMOUNT:
$542,000 over 2 years

PRINCIPAL INVESTIGATOR:
Rafer Cooley

CO-INVESTIGATORS:
Michael Cutshaw, INL
Zachary Priest, INL

Locally hosted large language models combined with secure knowledge retrieval and hallucination mitigation tools enable scalable, private, and accurate software analysis across sensitive computing environments.

The AskSoftly project explored how large language models can be securely and effectively integrated into software analysis workflows to accelerate research across the DOE complex. The project focused on developing a locally hosted, privacy preserving framework that enables researchers to interact with large language models using natural language while maintaining full control over their data and computational environment.

To achieve this, the team implemented a modular retrieval augmented generation system that allows large language models to access and reason over domain-specific knowledge without requiring fine tuning. Instead, the system uses semantic embeddings and vector databases to retrieve relevant information from curated local datasets. This approach enables rapid, context-aware responses to research queries while ensuring that sensitive data never leaves the secure environment.

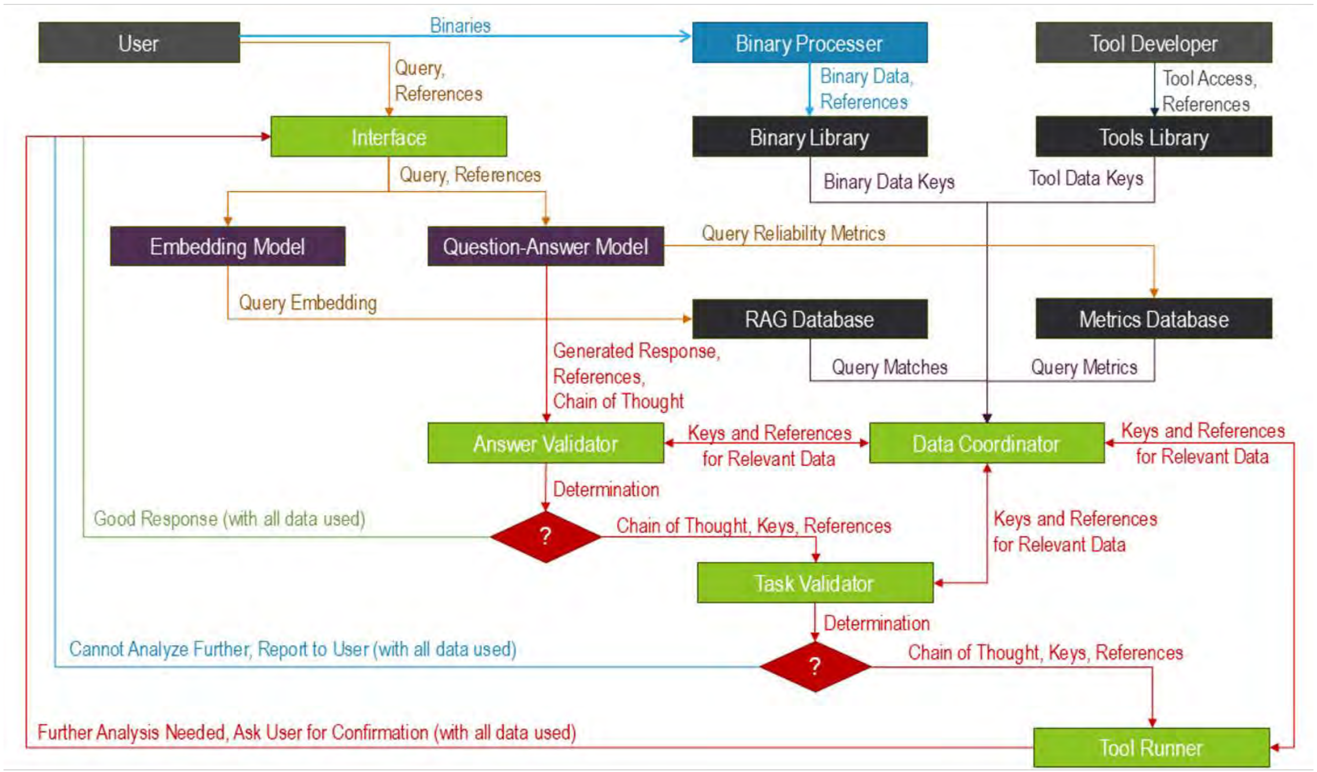
A key innovation of the project was the integration of hallucination mitigation and detection mechanisms. These included structured reasoning techniques such as chain-of-thought and self-reflection prompting, as well as statistical tools that assess the confidence and semantic alignment of model outputs. These safeguards help ensure that large language model generated insights are both accurate and trustworthy.

The project also developed proof-of-concept agentic artificial intelligence workflows that allow large language models to perform multi-step tasks, such as analyzing cyber threat intelligence or reverse engineering software binaries. These workflows integrate with tools like Neo4j, Ghidra, and Binary Ninja, enabling researchers to automate complex reasoning tasks and accelerate discovery.

All components of the system were deployed using Docker and Kubernetes, providing a scalable and portable solution that can be adopted by other DOE research teams. The resulting framework is already in use by multiple projects at INL, supporting secure, artificial intelligence-assisted research in cybersecurity, software analysis, and beyond.

TALENT PIPELINE:

- Samuel Ofiaza, student at University of Texas, Dallas
- Adithya Chintala, student at University of Texas, Dallas
- Darrin Lee, student at Louisiana State University, converted to staff
- Dalton Diez, student at Louisiana State University
- Shelby Heins, student at University of Tulsa, converted to staff
- John Tran, student at Notre Dame University



AskSoftly retrieval-augmented generation system diagram illustrating the software analysis proof-of-concept workflow.

Creation and Verification of Shadow Masked Patterns

PROJECT NUMBER:
24P1087-021FP

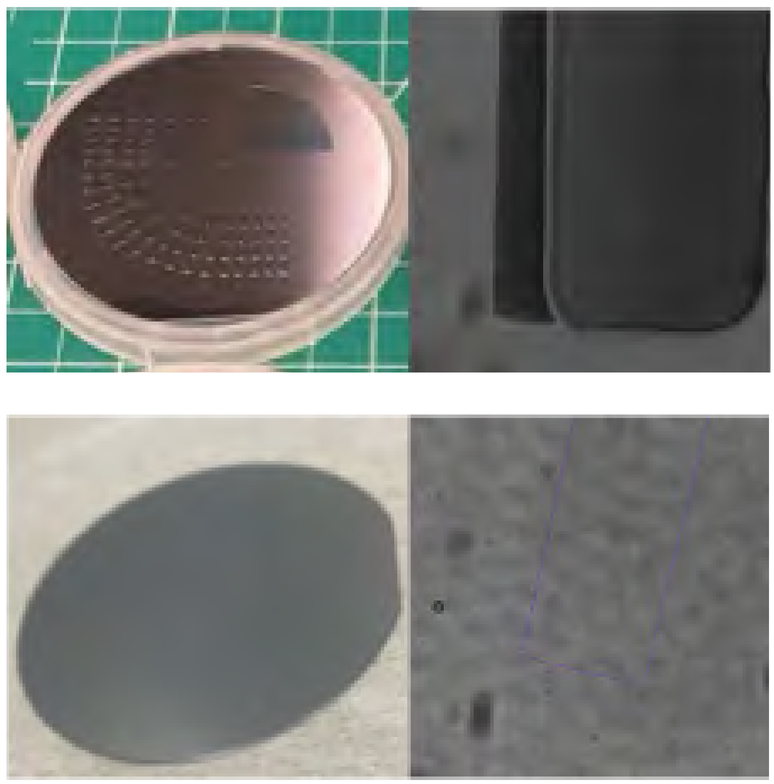
TOTAL APPROVED AMOUNT:
$229,000 over 1 year

PRINCIPAL INVESTIGATOR:
Brelon May

CO-INVESTIGATORS:
Thomas Walters, INL
Joel Johnson, INL

Custom imaging and deposition techniques advance covert marking technology.

The purpose of this project was to employ shadow masks to make and detect patterns on a substrate which are invisible to the human eye. A mask was strategically designed to test multiple parameters simultaneously and leverage asymmetry in the mask and deposition chamber and fabricated in house. Modeling of reflectance curves of various materials showed how thick a layer needs to be to become perceptible. Tests with metallic, and nominally transparent thin films on silicon substrates show slight distortion from the anticipated shape due to wrinkles in the mask and a slightly different color to the substrate. Raman spectroscopy worked as a method for visualizing patterns which were nearly invisible to the human eye, but long acquisition times were required. To circumvent this issue, a custom modular imaging system was developed for viewing in the nonvisible wavelength ranges, which yielded better results, including real-time viewing.



Photos of an entire three inch sample and single feature taken with the custom imaging system where the deposited shadow masked pattern is (a) clearly visible and (b) invisible to the human eye.

Resilient Wireless Security Communications Against Modern Electronic Warfare

PROJECT NUMBER:
24P1088-021FP

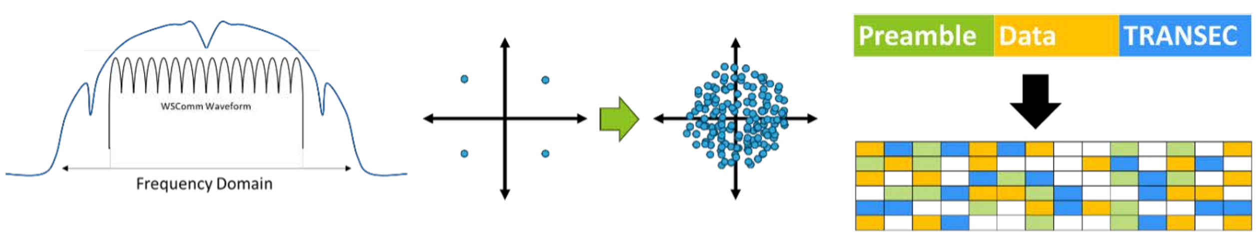
TOTAL APPROVED AMOUNT:
$150,000 over 1 year

PRINCIPAL INVESTIGATOR:
Brian LeNeave

CO-INVESTIGATORS:
John Capson, INL

Advanced waveform transmission security techniques safeguard next-generation wireless communications against modern electronic warfare threats.

In response to modern electronic warfare threats, INL undertook a multi-faceted approach to enhance the security of advanced waveforms. Initially, the team explored using artificial intelligence to characterize and classify signals in a radio frequency environment. They developed an initial architecture capable of identifying known signals, thereby enabling the obfuscation of their own signals and adding an additional layer of protection to the waveform. Following this, the team investigated unitary braid division multiplexing as an alternative method for enhancing signal security. Unitary braid division multiplexing randomizes the complex phase and amplitude of modulated signals, making it nearly impossible to decipher transmitted symbols. While both the signal characterization and unitary braid division multiplexing approaches show preliminary promise, further research is required for full integration and optimization. Finally, the team implemented a transmission security scheme designed to randomize every packet, thus protecting the wireless security communications waveform against low power replay attacks. This transmission security-enhanced version of wireless security communications has proven effective in mitigating disruptions that previously compromised communications. These efforts collectively advanced the understanding and capabilities in securing advanced waveforms against modern electronic warfare attacks. The initial transmission security work was pivotal, laying the foundation for a recently awarded $1.8 million project with the US government. This project has significantly contributed to the development of resilient communication technologies.



Making waveforms resilient through obfuscation, modulation transform, and transmission security.

CHEMICAL AND MOLECULAR SCIENCE

INL's chemical and molecular science capability explores fundamental research in nuclear science and radiation and actinide chemistry and addresses important challenges in energy supply, conversion, and storage as well as national security. Our scientists use this capability to advance basic research in energy delivery systems, advanced and critical materials, clean water, renewable chemicals, transient kinetic analysis, and chemical separations.

CORE CAPABILITIES

Chemical and Molecular Science

Chemical Engineering

Computational Science

Nuclear and Radio Chemistry

CHLOE TOLBERT

Transient Species Reaction Fundamentals

PROJECT NUMBER:
23A1070-112FP

TOTAL APPROVED AMOUNT:
$1,430,000 over 3 years

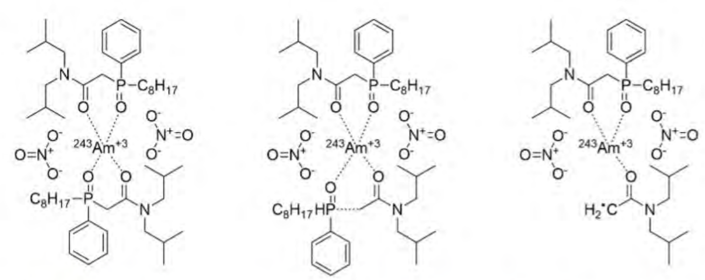
PRINCIPAL INVESTIGATOR:
Christopher Zarzana

CO-INVESTIGATORS:
Brittany Hodges, INL
Corey Pilgrim, INL
Cristian Celis-Barros, Oak Ridge National Laboratory
Thomas Albrecht, Colorado School of Mines

COLLABORATORS:
Free Electron Lasers for Infrared eXperiments (FELIX) Laboratory, Radboud University

Transient metal-ligand complexes reveal unexpected electron density rearrangements during fragmentation, advancing understanding of metal transport and coordination chemistry.

The transport of metal ions across a boundary from an aqueous to an organic phase is a critical step in nuclear fuel reprocessing and critical material recovery. Because the initial metal coordination environment is significantly different from the final, the metal must transition through a series of transient species as it passes from one phase to another. The chemistry of these transition species is critical to the overall chemistry of transport. This project investigated the difference in behavior between actinides and lanthanides in gas phase complexes that are representative of species involved in transport of metals across liquid phase interfaces using a new capability at Idaho National Laboratory for studying gas phase transuranic chemistry. The transient nature of these transition species makes them especially challenging to study. Our approach was to produce, stabilize, manipulate, and study species that can serve as models of transient species using trapping mass spectrometry. This allowed the investigation of the intrinsic behavior of these transient species in a controlled fashion. These gas phase measurements were complimented with computational quantum chemistry. Significantly, we have shown that during fragmentation of these species, the electron density can rearrange in ways that change the metal-ligand interaction in unexpected ways. This suggests that the dynamics of such non-equilibrium processes as radiolysis and hydrolysis could play an important role in overall transport. This coupling of intrinsic behavior with theoretical methods provided insight into the fundamentals of metal-ligand coordination in transport across phase boundaries, which can strengthen the theoretical underpinnings of nuclear fuel reprocessing, critical material recovery, and other processes that rely on metal transport across phase boundaries.



a. Intact complex — b. P—C bond cleavage — c. P=O fragment eliminated

Bond	Electron density ρ: a. Intact complex	Electron density ρ: b. P—C bond cleavage	Electron density ρ: c. P=O fragment elimination	Delocalization: a. Intact complex	Delocalization: b. P—C bond cleavage	Delocalization: c. P=O fragment elimination
Am—O=P	0.3628	0.3327	--	0.3434	0.3145	--
Am—O=C	0.3432	0.4352	0.4157	0.3102	0.4156	0.3961
P—C	1.0584	0.1670	--	0.7380	0.3975	--

Collisional activation of the americium nitrate (N,N-diisobutylcarbamoylmethyl)phenyloctylphosphine oxide complex results in loss of a fragment containing the phosphoryl (P=O) bond, which is unexpected, as it is more strongly bound to the americium than the carbonyl (C=O)-containing fragment. However, as fragmentation occurs, the electron density rearranges, weakening the americium phosphoryl oxygen bond and strengthening the americium carbonyl oxygen bond, causing the formerly weaker bound side of the molecule to be retained.

TALENT PIPELINE:

- JungSoo Kim, postdoc at INL, converted to staff
- Madeline Martelles, student at Colorado School of Mines

PAPER AND PRESENTATIONS:

- Hodges, B. D. M.; Kim, J.; Berden, G.; Martens, J.; Zarzana, C. A., "Investigation of Uranyl Perchlorate Anion Complexes in the Gas Phase via Infrared Multiphoton Dissociation and Collision-Induced Dissociation." Rapid Communications in Mass Spectrometry 2025, 39 (20), e10106.
- Zarzana, C. A.; van Wieringen, T.; Schuurman, J.; Hodges, B. D. M.; Berden, W. C. M.; Kim, J.; "Investigation of the Collision-Induced Dissociation Mechanism of Protonated TODGA with IRIS." American Society for Mass Spectrometry (ASMS) 73rd Annual Conference on Mass Spectrometry and Allied Topics, Baltimore, Md, USA, June 1st-5th, 20245.
- Zarzana, C. A.; Kim, J.; Pilgrim, C. D.; Albrecht, T.; Hodges, B. D. M.; Martelles, M.; Celis-Barros, C.; "Collision-induced dissociation mass spectrometry for small quantity actinide-ligand interaction studies." 13th International Conference on Methods and Applications of Radioanalytical Chemistry, Kona, HI, March 23rd-28th.
- Zarzana, C. A.; Kim, J.; Hodges, B. D. M.; Martelles, M.; Martens, J.; Berden, G.; Celis-Barros, C.; Albrecht-Schoenzart, T.; "Gas Phase Coordination of Phosphine-Chalcogenides to the Uranyl Cation." American Society for Mass Spectrometry (ASMS) 72nd Annual Conference on Mass Spectrometry and Allied Topics, Anaheim, CA, USA, June 2nd-6th, 2024.
- Hodges, B. D. M.; Zarzana, C. A.; Kim, J.; Martens, J.; Berden, G.; Oomens, J.; "Investigation of Uranyl Perchlorate Anion Complexes in the Gas Phase via Infrared Multiphoton Dissociation and Collision-Induced Dissociation." American Society for Mass Spectrometry (ASMS) 72nd Annual Conference on Mass Spectrometry and Allied Topics, Anaheim, CA, USA, June 2nd-6th, 2024.
- Kim, J; Zarzana, C. A.; Hodges, B. D. M.; Pilgrim, C.; "Comparison of Gas Phase Fragmentation Behaviors of Nuclear Fuel Cycle Ligands in Lanthanide and Americium Metal Ligand." American Society for Mass Spectrometry (ASMS) 72nd Annual Conference on Mass Spectrometry and Allied Topics, Anaheim, CA, USA, June 2nd-6th, 2024.
- Celis-Barros, C.; Zarzana. C. A.; Hodges, B. D. M.; Kim, J.; "Impact of the Electronic Properties of Chalcogenide Ligands in their Complexation with Uranyl Nitrate Complexes." 46th Actinide Separations Conference, Idaho Falls, ID, USA, May 16th-18th, 2023.
- Hodges, B. D. M.; Kim, J.; Zarzana, C. A.; "Investigation of Transient Species through Metal Clusters of Triphenylphosphine Chalcogenides With Sodium." American Society for Mass Spectrometry (ASMS) 71st Annual Conference on Mass Spectrometry and Allied Topics, Huston, TX, USA, June 4th-8th, 2023.

Development of a Predictive Model for Organic Diluent Radiolysis

PROJECT NUMBER:
24A1081-012FP

TOTAL APPROVED AMOUNT:
$563,000 over 2 years

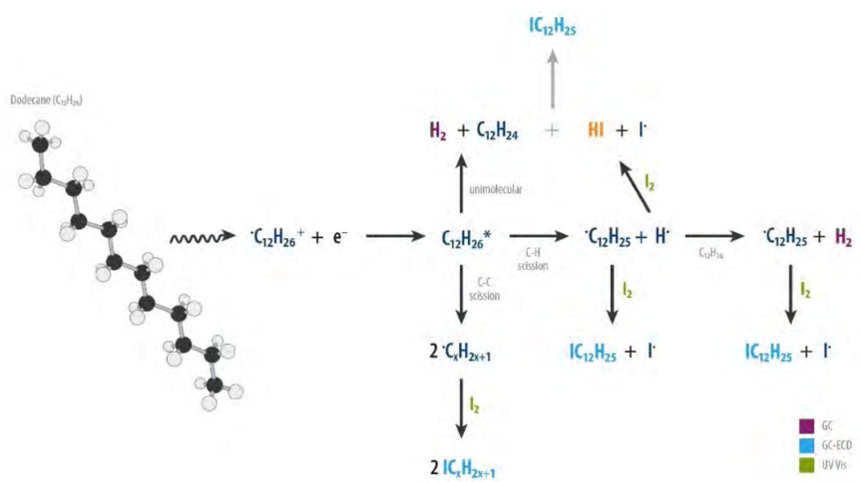
PRINCIPAL INVESTIGATOR:
Jacy Conrad

CO-INVESTIGATORS:
Gregory Holmbeck, INL
Stephen Mezyk, California State University, Long Beach

COLLABORATORS:
Brookhaven National Laboratory
University of Notre Dame

Predictive modeling and experimental studies of radiation-induced chemistry enable improved strategies for nuclear waste management.

This project investigated radiation-induced degradation of n-dodecane, a key solvent used in nuclear fuel reprocessing, to enhance understanding of the underlying chemical processes that occur in organic diluents under ionizing radiation. By employing a combination of experimental techniques, including pulsed electron radiolysis, gamma irradiation, radical scavenging studies, advanced spectroscopic methods, and gas chromatography, the research team quantified the yields of electrons, excited states, carbon-centered radicals, and hydrogen atoms produced during the irradiation of n-dodecane. Significant accomplishments included the successful measurement of yields for different bond scission mechanisms from excited state n-dodecane, including unimolecular hydrogen elimination, providing essential data for understanding the relative importance of various radiation-induced degradation pathways. Additionally, temperature-dependent reaction rates were measured for the solvated electron with dissolved oxygen and diglycolamide ligands proposed for minor actinide removal from used nuclear fuel. Collaborations with Brookhaven National Laboratory and the University of Notre Dame enriched the project by incorporating time-resolved picosecond pulsed electron radiolysis and electron paramagnetic resonance spectroscopy, allowing for more detailed insights into radical formation. These findings have laid the groundwork for future studies aimed at modeling organic diluent radiolysis, optimizing nuclear waste management strategies, and addressing the challenges resulting from radiation exposure in organic media.



A schematic map of the dominant radiation-induced degradation pathways for n-dodecane, as determined from gamma irradiation studies using molecular iodine as a carbon-centered radical scavenger.

TALENT PIPELINE:

- Michaela R. Bronstetter, student at Michigan State University
- Hanna Hlushko, Russell L. Heath Distinguished Postdoc at INL

PAPERS:

- Conrad, J. K.; Hlushko, H.; Cook, A. R., "Kinetics for the reaction between the solvated electron and dissolved oxygen in n-dodecane from 2.5 to 40°C." Radiation Physics and Chemistry, 230, 112587-112590 (2025).
- Bronstetter, M. R.; Horne, G. P.; Cook, A. R.; Mezyk, S. P.; Wilbanks, J. R.; Layne, B.; Gaiser, A.; Conrad, J. K., "Impacts of molecular architecture on the radiation-induced degradation and reaction kinetics of hydrophobic diglycolamides with the solvated electron and the dodecane radical cation." Physical Chemistry Chemical Physics, 27, 16254-16263 (2025).
- Conrad, J. K., Anderson, K. R., Sosulin, I., Wilbanks, J. R., Klaehn, J., Pilgrim, C. D., Lisouskaya, A., Horne, G. P., "Radiation-induced chemical yields of carbon-centered radicals and hydrogen atoms from the gamma irradiation of n-dodecane." The Journal of Physical Chemistry A. DOI: 10.1021/acs.jpca.5c06414 (2025).

Predicting Radiation-Induced Plutonium Redox Chemistry Using Multiscale Modeling Methods

PROJECT NUMBER:
24A1081-050FP

TOTAL APPROVED AMOUNT:
$858,000 over 2 years

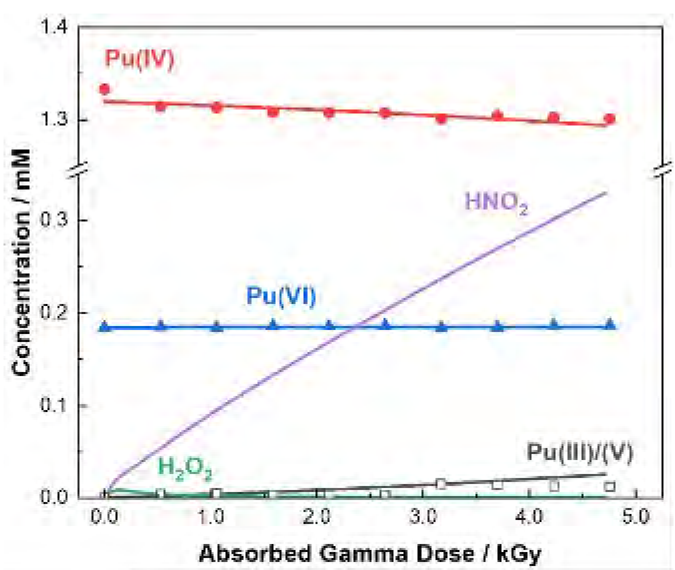
PRINCIPAL INVESTIGATOR:
Gregory Holmbeck

CO-INVESTIGATORS:
Travis Grimes
Amy Kynman

COLLABORATORS:
Brookhaven National Laboratory

Multiscale modeling of alpha and gamma-induced plutonium redox chemistry reveals key mechanisms governing actinide behavior in nuclear fuel reprocessing systems.

Plutonium plays a key role in global actinide science research and nuclear fuel cycle technologies, and yet, our fundamental understanding of its inherent radiation-induced chemical behavior is limited. These radiation-induced processes cannot simply be "switched off" and have a significant impact on the steady-state oxidation state distribution of other less chemically complex actinide elements. In this study, an experimentally validated, predictive multiscale computer model was developed to enhance our understanding of the radiation-induced mechanisms underpinning the complex molecular level behavior of plutonium ions in aqueous solution. By using a combination of in situ alpha, from the radioactive decay of actinide ions, and ex situ cobalt-60 gamma irradiation techniques, the oxidation state distribution of plutonium ions was quantitatively established in nitric acid, a solvent relevant to used nuclear fuel reprocessing. Additionally, time-resolved electron pulse radiolysis techniques were employed to determine the chemical kinetic reactivity between specific plutonium oxidation states and oxidizing radicals from the radiolysis of aqueous solutions. These new kinetics were incorporated into a multiscale computer model to elucidate the redox mechanisms underpinning experimental alpha and gamma irradiation observations. The calculations revealed that the apparent "radiation-resistance" of plutonium's predominant oxidation states (+4 and +6) is due to several radiation-driven redox cycles that predominantly regenerate the initial oxidation state distribution. The new knowledge gained is essential to advance actinide science and support technological innovation in global nuclear energy and non-proliferation efforts.



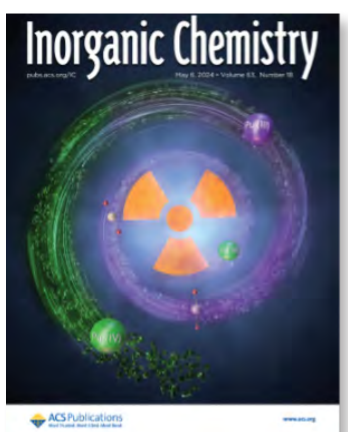
Concentration of plutonium oxidation states [Pu(III), Pu(V), Pu(IV), and Pu(VI)], and significant (≥ 1 µM) radiolysis products (hydrogen peroxide and nitrous acid) as a function of absorbed dose from the cobalt-60 gamma irradiation of Pu(IV,VI) in aerated, aqueous 6.0 M nitric acid solution. Open symbols were determined by mass balance. Solid curves are predicted values from multiscale modeling calculations.

TALENT PIPELINE:

- Amy Kynman, Glenn T. Seaborg distinguished postdoc at INL, converted to staff
- Samantha Kruse, INL Glenn T. Seaborg distinguished postdoc at INL

PAPER AND PRESENTATIONS:

- A.E. Kynman, T.S. Grimes, J.K. Conrad, S.M. Pimblott, and G.P. Horne, "Multiscale Modeling of Plutonium Radiation Chemistry in Nitric Acid Solutions. 1. Cobalt-60 Gamma Irradiation of Pu(IV)." Inorganic Chemistry 2024, 63(18), 8092.
- G.P. Holmbeck (Invited Talk), "The Role of Radiation-Induced Non-Equilibrium Plutonium Oxidation States in Solution." Materials Research Society (MRS) Spring Meeting & Exhibit—Actinide Materials Symposium, Seattle, Washington, April 2024.
- G.P. Holmbeck (Invited Seminar), "The Role of Transient Radiation-Induced Non-Equilibrium Actinide Species in Solution." Los Alamos National Laboratory Invited Seminar Series, Los Alamos, New Mexico, May 2024.
- G.P. Holmbeck (Invited Talk), "The Role of Transient Radiation-Induced Non-Equilibrium Actinide Species in Solution." 4th International Conference on Ionizing Processes, Notre Dame, Indiana, August 2024.
- G.P. Holmbeck (Invited Keynote Lecture), "Elucidating the Radiation-Induced Redox Chemistry of Plutonium Under Used Nuclear Fuel Reprocessing Conditions." ATALANTE 2024 – Nuclear Chemistry for Sustainable Fuel Cycles, Avignon, France, September 2024.
- A.E. Kynman (Invited Talk), "Predicting Radiation-Induced Plutonium Redox Chemistry using Multiscale Modeling Methods." Plutonium Futures—The Science, Charleston, South Carolina, September 2024.
- G.P. Holmbeck (Invited Seminar), "Unraveling the radiation-induced redox chemistry of plutonium ions." iDREAM EFRC, Pacific Northwest National Laboratory, Washington, March 2025.
- G.P. Holmbeck, "Unravelling the radiation-induced redox chemistry of plutonium ions in aqueous solution poster." Gordon Research Conference 2025—Inorganic Reaction Mechanisms, Pomona, California, March 2025.
- T.S. Grimes, "The Impact of Alpha and Gamma Irradiations on the Redox Distribution of Plutonium in Acidic Media." MARC XII, Hawaii, March 2025.
- G.P. Holmbeck (Invited Seminar), "Unraveling the radiation-induced redox chemistry of plutonium ions." RAD-CERT, Berkely, California, May 2025.



EXTERNAL AWARDS:

- Back cover art on Inorganic Chemistry, volume 63, issue 18, 2024.

Fundamental Exploration of the Magnetophoretic Nature of Lanthanides Applied to Separations

PROJECT NUMBER:
24P1088-029FP

TOTAL APPROVED AMOUNT:
$150,000 over 1 year

PRINCIPAL INVESTIGATOR:
Chloe Tolbert

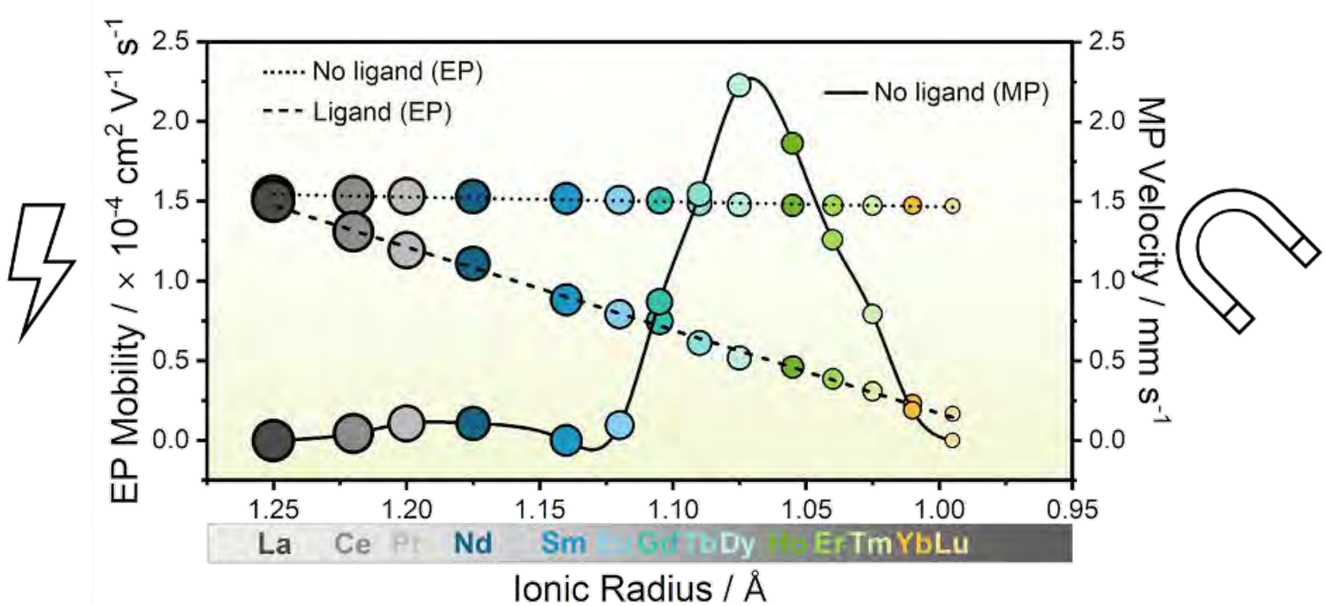
Magnetophoretic properties of lanthanides can be exploited to enhance critical material recovery.

Critical materials such as the lanthanides have become increasingly important over the past several years due to their vital role in a wide range of technological spaces, including permanent magnets, electronics, and defense weapons systems. As the demand for highly pure lanthanides increases, efforts have been directed toward the identification of suitable complexing agents that aid in more efficient lanthanide isolation. While considerable advancements have been made in this area, only incremental improvements in separation modalities have been demonstrated to date. The conventional modality for lanthanide separation is solvent extraction, which is capital intensive, spatially demanding, and generates large volumes of organic waste, thereby imparting a significant environmental footprint. It is therefore pertinent to explore alternative areas that provide pathways for lanthanide separation. This study focused on determining the feasibility of exploiting lanthanide paramagnetism as an additional modality for separations.

Studies were conducted to characterize the magnetophoretic behavior of lanthanides and evaluate the separability of binary mixtures using only a permanent magnet. Magnetophoretic velocities of various lanthanide droplets in the presence of a magnetic field gradient were recorded at variable concentration in different viscous media. The additive effect of paramagnetism was further explored with binary lanthanide mixtures using different percent compositions of each respective lanthanide. Lanthanides with large differences in their effective magnetic moment demonstrated comparably large differences in magnetophoretic velocity, indicating that exploitation of the magnetophoretic properties of lanthanides for separations is feasible. Information collected from this study will be used in a finite element model to determine the conditions necessary for magnetophoretic separation.

TALENT PIPELINE:

- Chloe Tolbert, postdoc at INL, converted to staff



Transport properties of lanthanide nitrates measured under variable conditions including the presence of an electric field with (black dashed line) and without (black dotted line) ligands (left axis, EP = electrophoretic), and the presence of a magnetic field gradient (black solid line) (right axis, MP = magnetophoretic) which may be exploited for separations.

Intrinsic Characterization of Active Site Population Under Dynamic Reaction Conditions

PROJECT NUMBER:
25A1092-001FP

TOTAL APPROVED AMOUNT:
$300,000 over 1 year

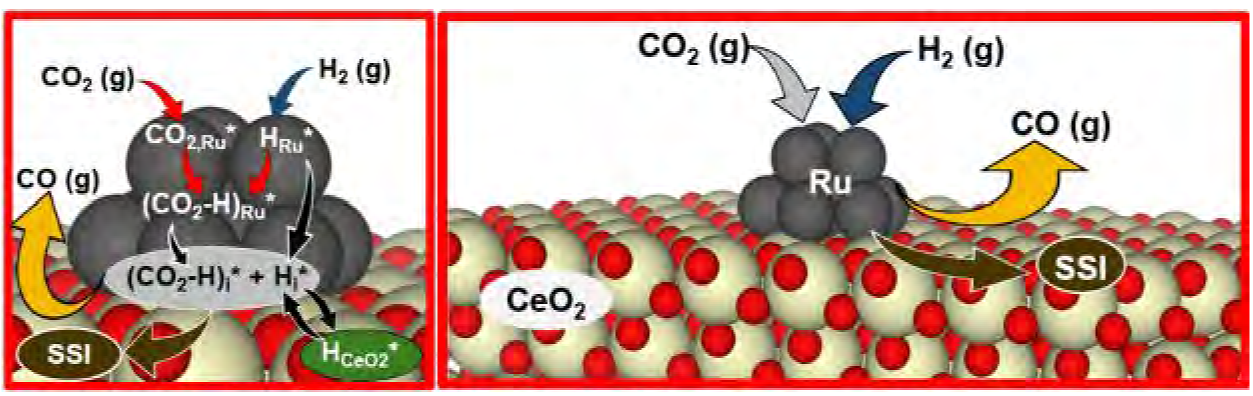
PRINCIPAL INVESTIGATOR:
Debtanu Maiti

Quantitative analysis of dynamic active sites and surface intermediates guides more efficient catalytic system designs.

Ruthenium supported on ceria is widely recognized as an efficient catalyst for carbon dioxide conversion. However, a persistent challenge lies in the accurate quantification of active catalytic sites and the dynamic nature of surface adsorbed intermediates that critically influence performance. In this work, we investigate the mechanistic role of dynamic surface species by systematically modulating H feed to control the coverage of hydrogenated intermediates under an intrinsic, transport-limitation-free regime. Transient kinetic measurements over 1–3 wt.% ruthenium-ceria catalysts at different temperatures (300, 400, 500, and 600°C) enable direct quantification of transient populations of key adsorbed species. These dynamic populations were correlated with variations in intrinsic rate constants and activation energies, thereby establishing a fundamental link between surface coverage dynamics and catalytic activity. The results reveal that hydrogen feed modulation significantly alters the availability and reactivity of surface intermediates, dictating the overall carbon dioxide conversion pathways on ruthenium-ceria and provides mechanistic insights essential for rational design of next-generation catalysts for efficient carbon dioxide repurposing.

TALENT PIPELINE:

- Han K. Chau, postdoc at INL



Carbon dioxide conversion on ruthenium-ceria catalysts through a series of surface reactions that forms a dynamic population of surface adsorbed species.

Forced Dynamic Control of Reaction During Photocatalytic Ammonia Decomposition and Synthesis

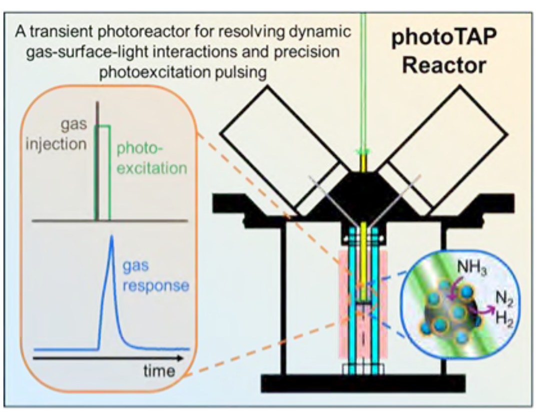
PROJECT NUMBER:
25A1092-002FP

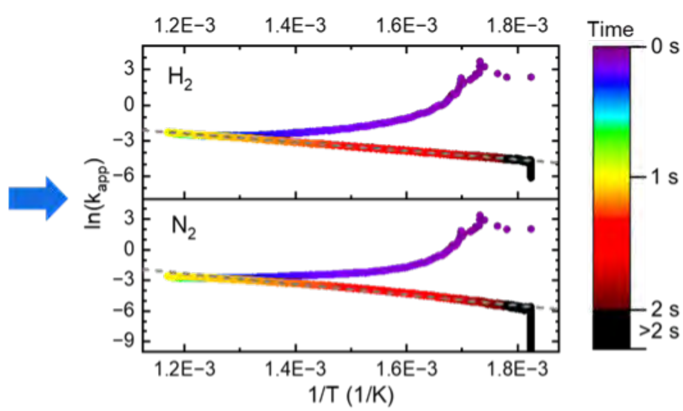
TOTAL APPROVED AMOUNT:
$224k over 1 year

PRINCIPAL INVESTIGATOR:
Jason Malizia

A novel transient photokinetic reactor enables dynamic control of chemical reactions.

Dynamic operation of photocatalytic processes can enable extraordinary productivity, efficacy, and resilience in chemical manufacturing processes. The challenge is that the current tools for photocatalytic reaction characterization operate under steady-state conditions and do not report the detailed kinetics required for realizing dynamic operation of these systems. Transient experiments that can decouple gas, light, and surface kinetic processes are needed to fully understand the physics behind these systems and pave the way to develop the next generation of photonically powered reactions. This project developed a one-of-a-kind transient photokinetic reactor capable of dynamic gas and light pulsing to study the complex reaction network of heterogeneous plasmonic photocatalysts. This photokinetic reactor was then applied to advanced studies of ammonia photodecomposition over a supported copper catalyst decorated with ruthenium. Critical insights into the photoactive reaction mechanism were learned through comparison of the reaction in the dark and under illumination, revealing how light cleans the catalyst surface to prevent saturation and facilitate further reaction. The novel precision light-gas pulsing capability of the photokinetic reactor was used to disentangle the role of light-induced heating from photoexcited hot electrons during ammonia decomposition and revealed that light can invoke metastable transformations of the catalyst surface that further alter the reaction pathway relative to operation in the dark. It was demonstrated that dynamic illumination can change the reaction kinetics during ammonia photodecomposition.





(a) The transient photokinetic reactor developed during this project, dubbed the "photoTAP" reactor. (b) Arrhenius plot of product formation during ammonia photodecomposition, collected with the photoTAP reactor during dynamic light/gas pulsing. The photoexcitation is turned on for 1 s concomitant with gas injection at 0 s.

Synthesizing Heterometallic Uranium Single Crystals to Understand the Influence of the Secondary Metals on Uranyl Axial Bond Strength

PROJECT NUMBER:
25A1092-010FP

TOTAL APPROVED AMOUNT:
$283,000 over 1 year

PRINCIPAL INVESTIGATOR:
Ashini Jayasinghe

COLLABORATORS:
Colorado School of Mines
University of Notre Dame

Fundamental chemistry enables novel lanthanide and actinide materials design.

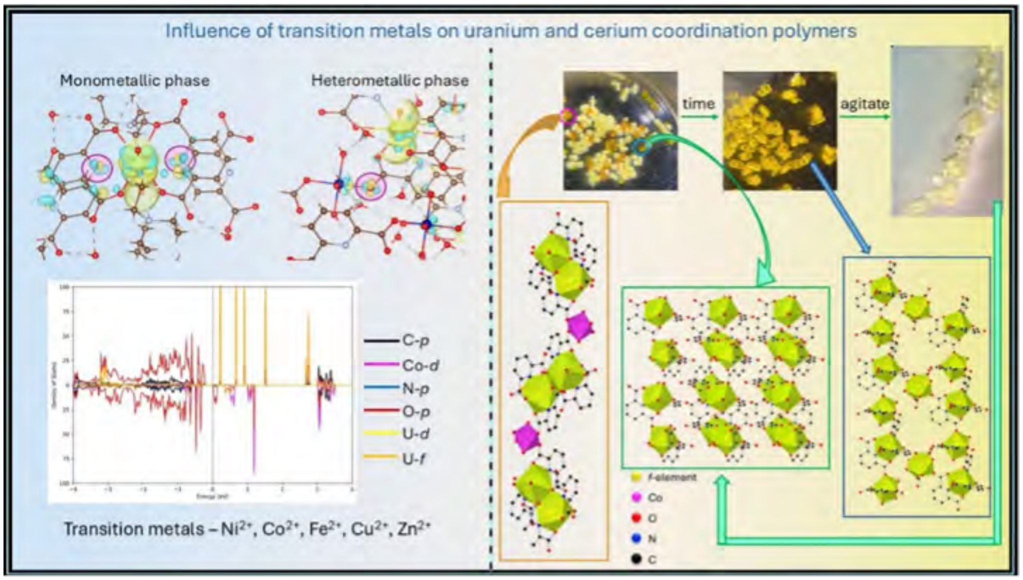
Understanding how transition metals influence the chemistry of lanthanide and actinide materials is critical to advance separation technologies, materials design, and coordination chemistry. This project examined how incorporating first-row transition metals affected the structural and spectroscopic properties of lanthanide and actinide coordination polymers. In uranium(VI)-based systems synthesized with 2,6-pyridinedicarboxylic acid (PDC) ligands, single-crystal x-ray diffraction and Raman spectroscopy revealed that the presence of transition metals shortened the uranyl axial bond and induced a blue shift in its symmetric stretching vibration—evidence of increased bond strength. Electronic structure analysis, including density of states calculations using density functional theory, revealed altered orbital overlaps and highlighted the role of transition metal *d*-orbitals in modulating bonding. Raman modes were modeled using truncated structural fragments in collaboration with the University of Notre Dame, and although the predicted frequencies were lower than experimental values, they remained within expected ranges. In parallel, similar experiments with cerium (Ce) in the presence of cobalt (Co) and PDC demonstrated multistep single-crystal to single-crystal transformations, a behavior not observed in the uranium systems. Initial products included light yellow, orange, and polycrystalline materials. Single-crystal x-ray diffraction studies, conducted in collaboration with the Colorado School of Mines, identified the yellow phase as monometallic $Ce(PDC)_2(H_2O)_2 \cdot 4H_2O$ and the orange phase as heterometallic $Ce_2Co(PDC)_4(H_2O)_6$. After standing in solution for one week, both phases fully transformed into a dark yellow crystalline phase, $Ce_3(PDC)5(H_2O)8].6(H_2O)$. Remarkably, this transformation was reversible—disturbing the equilibrium by removing the crystals or shaking the vial caused reversion to the initial $Ce(PDC)_2(H_2O)_2 \cdot 4H_2O$ phase, highlighting dynamic behavior. All three structures were previously unreported. Solid-state ultraviolet-visible and Raman spectroscopy further distinguished these phases, revealing ligand-to-metal charge transfer involving cerium and characteristic d–d transitions from Co(II). The precise mechanism driving these transformations remains unclear; however, pH-dependent experiments confirmed that the transformation did not occur when the pH decreased. Overall, the project demonstrated that transition metals could be employed to tune bonding interactions, structural dimensionality, and optical properties in lanthanide and actinide materials, establishing new pathways for designing functional heterometallic systems. The work resulted in several novel structural discoveries and fostered productive collaborations with the University of Notre Dame and the Colorado School of Mines.

TALENT PIPELINE:

- Ben Valley, student at Colorado School of Mines
- Heather Culbertson, student at University of Notre Dame
- Keerthan Raghavendra Rao, postdoc at INL
- Tyler Hines, student at Colorado School of Mines

EXTERNAL PRESENTATIONS:

- Jayasinghe, A. S., Rao, K. R., Culbertson, H. J., Holmbeck, G. P., Zalupski, P., "Exploring the influence of transition metals on uranyl bonding." ACS National meeting, Washington, DC, 19 August 2025.



This project highlights two complementary systems built on the PDC ligand. In uranium–transition metal–PDC systems, density of states and charge density analyses revealed how transition metals modulate uranyl bonding. In cerium–cobalt–PDC systems, dynamic single-crystal-to-single-crystal transformations provided new insight into how transition metals direct lanthanide coordination chemistry.

PARIKSHIT BAJPAI

COMPUTATIONAL SCIENCE

CORE CAPABILITIES:

Applied Materials Science & Engineering

Applied Mathematics

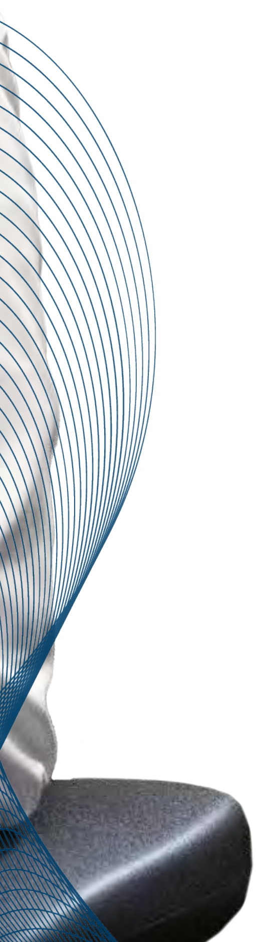
Chemical Engineering

Computational Science

Condensed Matter Physics and Materials Science

Nuclear Engineering

INL's computational science capability connects applied mathematics, computer science, and domain-specific expertise to conduct multiscale, multiphysics modeling across energy, materials, nuclear, and national-security systems. Using high performance computing platforms, INL researchers simulate reactor cores, fuel performance in harsh environments, sensor-driven digital twins, uncertainty quantification in complex systems, and so on. This capability enables INL to reduce experiment burden and accelerate advanced reactor RD&D.



Accelerated Nuclear Materials Thermochemistry Through Active Learning Surrogate Models

PROJECT NUMBER:
23P1077-004FP

TOTAL APPROVED AMOUNT:
$345,000 over 2 years

PRINCIPAL INVESTIGATOR:
Parikshit Bajpai

CO-INVESTIGATORS:
Daniel Schwen, INL

Thermochemistry surrogate modeling accelerates nuclear reactor design.

Accurate prediction of material behavior is essential to advance nuclear materials modeling and reactor simulations. Thermochemical properties such as Gibbs energies, chemical potentials, heat capacities, phase evolution, and speciation are critical to understand how materials respond under diverse operating conditions. The Computer Coupling of Phase Diagrams and Thermochemistry (CALPHAD) method provides a rigorous approach, combining experimental measurements with ab initio calculations to predict thermodynamic and kinetic properties of complex material systems. Despite its accuracy, CALPHAD has been computationally prohibitive for direct use in multiphysics frameworks such as the MOOSE, limiting its application and forcing reliance on simplified empirical correlations with restricted validity.

This project developed a computational thermochemistry surrogate modeling capability to overcome this barrier. By leveraging machine learning and barycentric interpolation from cached high-fidelity calculations, we created efficient surrogates for CALPHAD calculations that capture essential thermodynamic relationships while significantly reducing computational cost. This enabled fully coupled thermodynamically informed simulations in MOOSE without sacrificing predictive fidelity. The approach accelerated source-term analyses and depletion-driven thermochemistry calculations for molten salt reactor systems, providing a foundation for more accurate assessments of reactor safety and performance. In addition, the methods were extended to support microstructural corrosion modeling of structural materials in contact with molten salts, a key challenge for reactor longevity. The accomplishments of this project demonstrate how computational thermochemistry surrogate modeling can enable faster, more accurate prediction of thermodynamic behavior, establishing a path for broader integration of thermochemistry into nuclear reactor design and analysis.

TALENT PIPELINE:

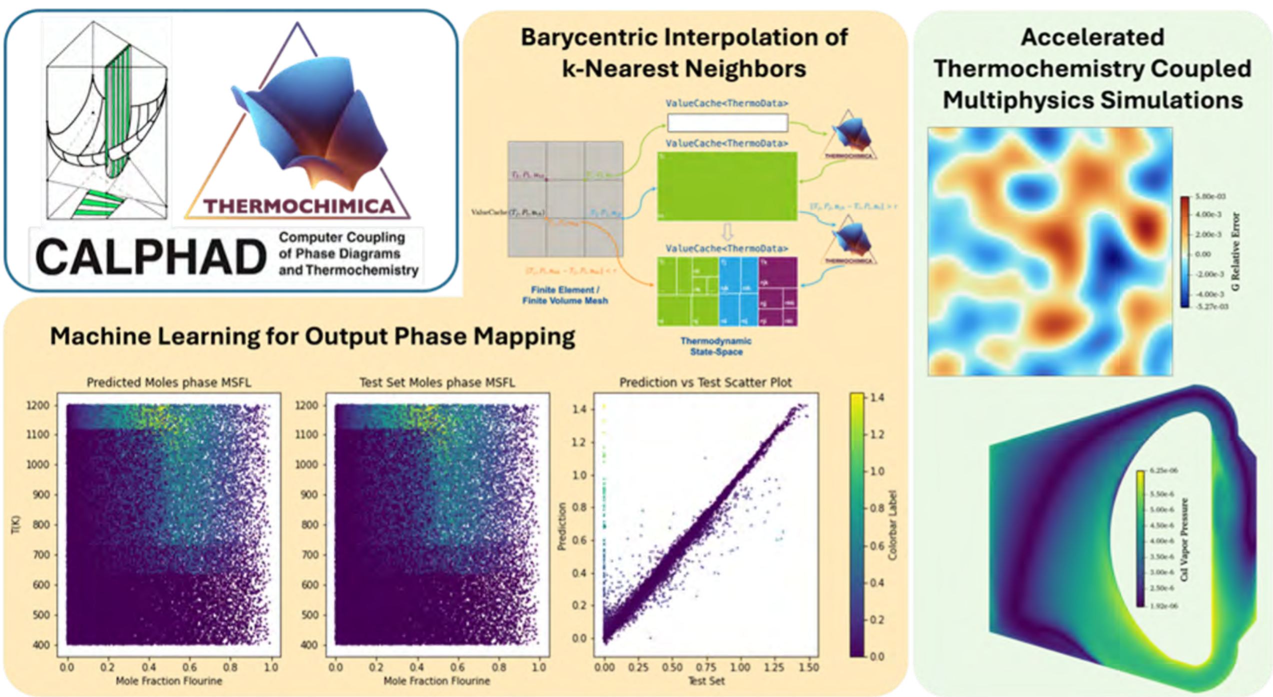
- Andrew Kitterman, student at University of Colorado Denver
- Parikshit Bajpai, Russell L. Heath distinguished postdoc, converted to staff

PRESENTATIONS:

- Bajpai, P., & Schwen, D., "Accelerating thermochemical equilibrium calculations for nuclear reactor applications," 51st International Conference on Computer Coupling of Phase Diagrams and Thermochemistry, Mannheim, Germany. May 26–31, 2024.
- Bajpai, P., & Schwen, D., "Surrogate Models for Accelerating CALPHAD-Informed Materials Simulations in MOOSE," TMS 2025 Annual Meeting & Exhibition, Las Vegas, March 23–27, 2025.
- Bajpai, P., Bhave, C.V. & Schwen, D., "Accelerated Nuclear Materials Thermochemistry in MOOSE through Surrogate Modeling," MS&T Technical Meeting and Exhibition (MS&T 2025), Columbus, September 28–October 1, 2025.

AWARD:

- 2nd place winner at the LDRD poster session



Thermochemistry acceleration pipeline and its application to multiphysics simulations of spinodal decomposition in iron-chromium alloy and off-gassing simulation in molten salt fast reactor. The acceleration capability, highlighted in yellow, combines a k-d tree-based caching capability with machine learning algorithms to reduce the computational cost of full thermochemical equilibrium calculations within multiphysics simulations using the MOOSE framework providing speedups of up to twenty times compared to fully coupled simulations.

Development of a Graphics Processing Unit Enabled Spectral Solver Integrated into the Multiphysics Object-Oriented Simulation Environment

PROJECT NUMBER:
24P1087-011FP

TOTAL APPROVED AMOUNT:
$150,000 over 1 year

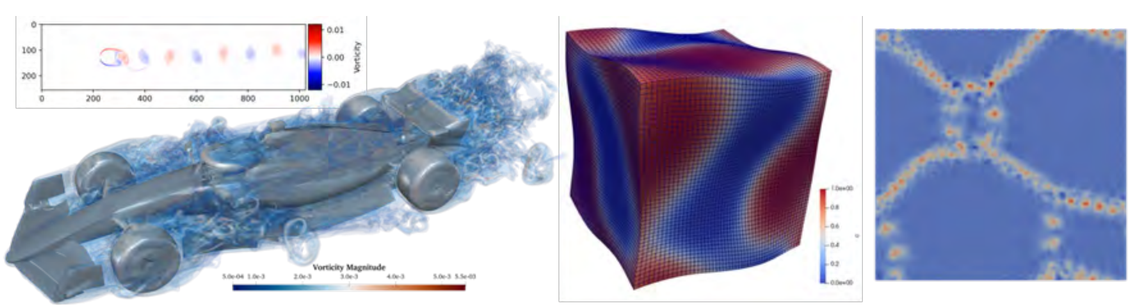
PRINCIPAL INVESTIGATOR:
Daniel Schwen

CO-INVESTIGATORS:
Chaitanya Bhave, INL

COLLABORATORS:
University of Wyoming
University of Florida

Fourier spectral and lattice Boltzmann application enables scalable, extensible mesoscale modeling of energy-relevant materials and thermal-fluid systems.

This project delivered Marlin, a device independent Fourier spectral and lattice Boltzmann application built on the MOOSE framework and powered by libTorch. Over the performance period, we designed, implemented, and open-sourced a tensorcentric architecture (Domain, TensorBuffers, TensorComputes, TensorSolver) that expressed physics as dependency resolved operator graphs executing on central processing units or graphics processing units with identical code paths. We integrated distributed and single node fast Fourier transforms, asynchronous extensible data model and format tensor output and MOOSE multiapp/transfer coupling for grid↔mesh data exchange, enabling high graphics processing unit utilization and scalable workflows. Physics capabilities included fast Fourier transform based gradient and semi-implicit time integration for phase field and pattern forming models (e.g., Cahn-Hilliard, Swift-Hohenberg) and a lattice Boltzmann module with Bhatnagar-Gross-Krook / Multiple Relaxation Time / Smagorinsky collision models, complex boundary conditions, force terms, and unit conversion. The code supported Compute Unified Device Architecture and Apple Metal Performance Shaders with automatic precision handling, device selection, and optional slab domain decomposition for parallel fast Fourier transforms. We supplied exemplars covering canonical flows (Hagen-Poiseuille, Kármán vortex, Rayleigh-Bénard), microstructure evolution, and mechanics, plus documentation and installation guidance. The software matured from concept to a usable, extensible capability that interoperated with the broader MOOSE ecosystem, lowering time to solution for mesoscale simulations and unlocking largescale sampling, uncertainty quantification, and Bayesian inference. The effort also catalyzed a new academic collaboration: a two-time INL intern transitioned to a Ph.D. at the University of Wyoming using Marlin's lattice Boltzmann capabilities as a foundation. Overall, Marlin advanced INL's graphics processing unit ready mesoscale modeling and strengthened INL's open, portable high-performance computing tools.



From top left to right: Vortex shedding around a cylinder computed using the lattice Boltzmann method, aerodynamic analysis of a Formula 1 car run on a single A100 graphics processing unit, coupled phase field and mechanics solve of a two-component alloy demixing with different Eigenstrains, and a Swift-Hohenberg crystal phase field simulation showing boundaries between multiple grains.

TALENT PIPELINE:

- Nijat Rustamov, student at University of Wyoming
- Thompson Igunma, student at University of Florida

PRESENTATION:

- D. Schwen, C. Bhave, N. Rustamov, T. Igunma, "Swift—A MOOSE based GPU accelerated spectral solver framework." 18th US National Congress on computational mechanics, Chicago, Illinois, July 2025. (Swift has since been renamed Marlin).

EXTERNAL INTELLECTUAL PROPERTY:

- D. Schwen, C. Bhave, N. Rustamov, "Marlin—a device independent spectral and lattice Boltzmann solver." 2025. https://github.com/idaholab/marlin.

SHUXIANG ZHOU

CONDENSED MATTER PHYSICS AND MATERIALS SCIENCE

CORE CAPABILITIES

Applied Materials Science & Engineering

Computational Science

Condensed Matter Physics and Materials Science

INL's condensed matter physics and materials science capability focuses on developing a comprehensive, atomic-to-bulk understanding of material behavior in extreme environments. By advancing our understanding of material behavior at the atomic level, researchers can develop new materials and technologies that enhance the efficiency, safety, and sustainability of nuclear reactors. This foundational knowledge is essential to overcome challenges associated with quadrupling nuclear energy production by 2050.

Phonon Transport in Superior Heat Conductors Under Irradiation

PROJECT NUMBER:
23A1070-064FP

TOTAL APPROVED AMOUNT:
$750,000 over three years

PRINCIPAL INVESTIGATOR:
Shuxiang Zhou

CO-INVESTIGATORS:
Kaustubh Bawane, INL
Zilong Hua, INL
Tianli Feng, the University of Utah

COLLABORATORS:
University of Texas, Dallas
University of Houston
University of Michigan
Texas A&M University

First principles and experimental investigations of radiation-induced defects guide radiation-tolerant thermal conductor design.

Recent advancements have transitioned several novel materials with ultra-high thermal conductivity, such as boron arsenide, cubic boron nitride, and cubic boron phosphide, from theoretical concepts to experimental validation. These materials, characterized by unique phonon and thermodynamic properties, hold significant promise for enhancing thermal conductivity in nuclear fuels. However, a comprehensive understanding of radiation-induced defects is crucial for their effective application. This research investigates the impact of radiation on phonon transport in boron arsenide, aiming to develop materials with both ultra-high thermal conductivity and strong radiation damage tolerance. The study focuses on two primary objectives: understanding defect formation and thermal transport properties under irradiation.

For the first objective, first principles calculations were performed to determine the formation energies of charged intrinsic defects in boron arsenide and cubic boron nitride. The results indicate that boron arsenide tends to form antisite pairs while cubic boron nitride is prone to form vacancies. Additionally, density functional theory was employed to explore the impact of point defects on doping in boron arsenide, revealing that certain impurities significantly affect the electronic structures for both p- and n-type doping.

The second objective examines the thermal transport properties of boron arsenide under irradiation. The accuracy of different exchange-correlation functionals and the impact of isotope and point defects on thermal conductivity were evaluated. The findings highlight the limitations of certain computational methods and the significant effect of isotopes on phonon transport. Experimental measurements on irradiated boron arsenide samples were conducted to validate theoretical predictions. This research provides critical insights into developing advanced materials for nuclear applications, combining high thermal conductivity with robust radiation tolerance.

TALENT PIPELINE:

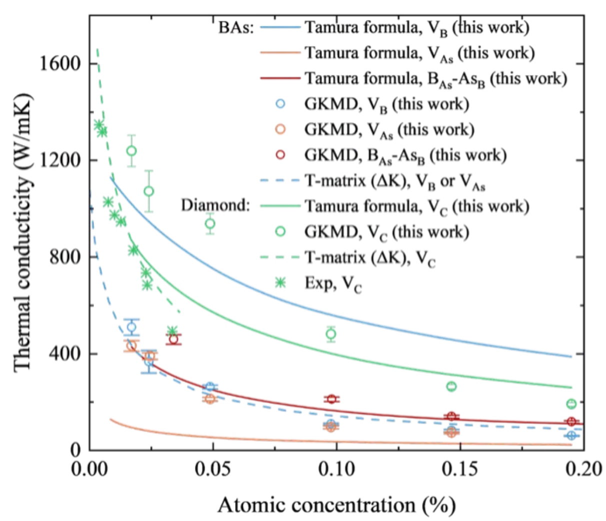
- Hao Zhou, student at University of Utah

PAPERS AND PRESENTATIONS:

- H. Zhou, S. Zhou, Z. Hua, K. Bawane, and T. Feng, "Extreme sensitivity of higher-order interatomic force constants and thermal conductivity to the energy surface roughness of exchange-correlation functionals." Applied Physics Letters. 123, 192201 (2023).
- H. Zhou, S. Zhou, Z. Hua, K. Bawane, and T. Feng, "Impact of classical statistics on thermal conductivity predictions of BAs and diamond using machine learning molecular dynamics." Applied Physics Letters, 125, 17 (2024).
- S. Zhou, Z. Hua, K. K. Bawane, H. Zhou, and T. Feng, "Impacts of point defects on shallow doping in cubic boron arsenide: A first principles study." Computational Materials Science, 247, 113483 (2025).
- Hao Zhou, "Accurate prediction of lattice thermal conductivity with defects." International Mechanical Engineering Congress & Exposition (IMECE), November 2023.
- Hao Zhou, "Impact of classical statistics on thermal conductivity predictions of BAs and diamond using machine learning molecular dynamics." IMECE, November 2024.
- Hao Zhou, "Extreme sensitivity of higher-order interatomic force constants and thermal conductivity to the energy surface roughness of exchange-correlation functionals." IMECE, November 2024.
- Shuxiang Zhou, "Impacts of point defects on shallow doping in cubic boron arsenide." MRS Fall Meeting, December 2024.

EXTERNAL AWARDS:

- The journal paper, H. Zhou et al., Applied Physics Letters. 123, 192201 (2023), was chosen as a featured article and included in the 2024 Applied Physics Letters Rising Stars Collection.



Thermal conductivity of boron arsenide and diamond as a function of atomic defect concentration for point defects, computed using three methods: Tamura formula and T-matrix method, both based on density functional theory, and Green-Kubo molecular dynamics at 300 K with machine learning interatomic potentials.

Unraveling Fundamental Mechanisms of Elemental Segregation Using Integrated Experimental and Multiscale Modeling Approach

PROJECT NUMBER:
23A1070-092FP

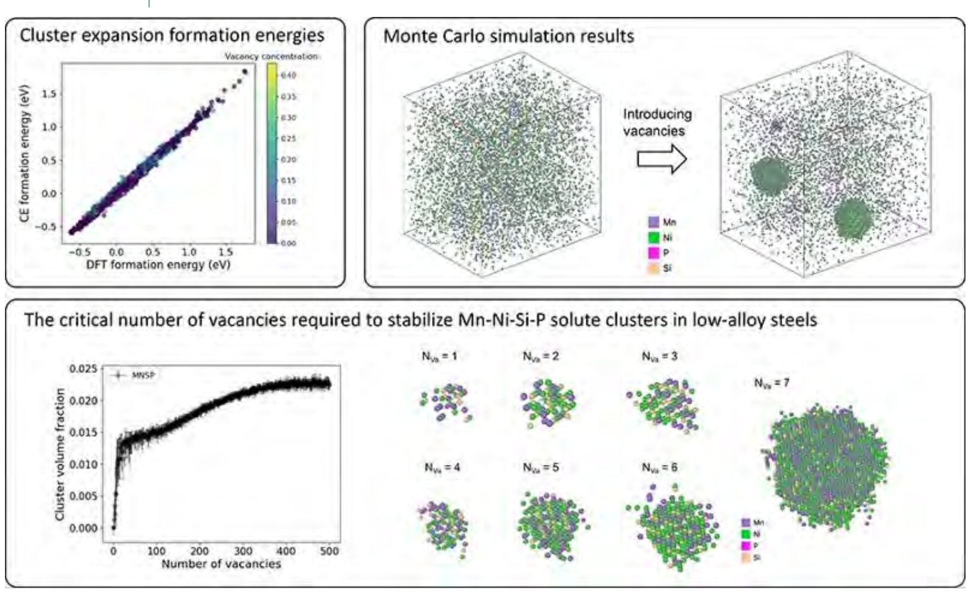
TOTAL APPROVED AMOUNT:
$1,263,500 over 3 years

PRINCIPAL INVESTIGATOR:
Mukesh Bachhav

CO-INVESTIGATORS:
Boopathy Kombaiah, INL
Jia-Hong Ke, INL
Sourabh Kadambi, INL
Lin Shao, Texas A&M University

Integrated multiscale modeling and experimental characterization enable predictive design of radiation-resistant materials.

The fundamental understanding of radiation-induced segregation in structural materials with various non-dilute compositions of solute species depended on the evolution of defects. To that end, we developed an integrated multiscale predictive modeling approach validated and correlated with experimental characterization to systematically understand and unravel radiation-induced segregation mechanisms in binary and ternary iron-chromium-nickel alloys. Atomistic calculations using density functional theory and molecular dynamics, aided by state-of-the-art interatomic potentials and regression approaches, were employed to obtain a local environment-specific property database. A novel phase field model that described bulk and interfacial processes was employed to simulate the effect of multiple radiation-induced segregation mechanisms. We also worked with an atomistic fitting approach to generate phase field radiation-induced segregation predictions. Some of these predictions were validated against a correlated chemical segregation-structure experimental analysis using atom probe tomography and scanning transmission electron microscopy. The integrated model was assessed for sensitivity and uncertainty to diverse radiation-induced segregation mechanisms, including dominant, synergistic, and competitive radiation-induced segregation modes. Surrogate (ion) irradiation was performed on binary model alloys of nickel-based and iron-based alloys at different temperatures to elucidate how the distribution of defects (interstitials and vacancies) was affected. Additionally, a rate-theory model was developed to consider the production bias and dislocation sink bias on radiation-induced segregation in dilute iron-chromium alloys.



Stability and morphology of nano-size coherent solute clusters with excess vacancies in low-alloy steels examined using density functional theory, cluster expansion, and lattice-based Monte Carlo simulations.

TALENT PIPELINE:

- Sourabh Kadambi, postdoc at INL, converted to staff
- Yasir Mahmood, student at Clemson University
- Sohail Shah, postdoc at INL, converted to staff
- Russell Oplinger, student at Texas A&M University
- Benjamin Diaz, student at Texas A&M University

PAPERS:

- S. Shah, C. Howard, B. Kombaiah, S. Dasari, F. Teng, Y. Wang, J. Daniel, M. Bachhav, "Correlating microstructure and mechanical properties of harvested high dose Zorita light water reactor internals." Journal of Nuclear Materials, Volume 599, 2024, 155241.
- P. Wang, B. Kammenzind, R. Smith, A. Motta, M. Aumand, D. Kaczorowski, M. Bachhav, G. Was, "Discerning the effect of various irradiation modes on the corrosion of Zircaloy-4." Journal of Nuclear Materials, Volume 604, 2025, 155505.
- S. Shah, M. Pena, Y. Li, M. Bachhav, X. Zhang, N. Thomas, C. Sun, F. Garner, M. Nastasi, L. Shao, "Irradiation-induced formation of G-phase precipitates and M2X carbides in self-ion irradiated HT-9." Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Volume 563, 2025, 165703.
- J. Rittenhouse, M. Bachhav, S. Shah, L. Hawkins, C. Howard, D. Frazer, N. Cinbiz, T. Yao, H. Wen, "Post Neutron Irradiation Characterization of the Effects of Grain Size on Microstructural Evolution and Mechanical Properties in an FeCrAl Alloy." Microscopy and Microanalysis, Volume 31, Issue Supplement 1, July 2025.
- S. Shah, M. Bachhav, P. Wang, "Investigating the Nanoscale Distribution of Alloying Elements in Zircaloy-4 Using High Resolution Characterization Techniques." Microscopy and Microanalysis, Volume 31, Issue Supplement 1, July 2025.
- J.-H. Ke, A. Kamboj, M. Bachhav, "The role of excess vacancies in stabilizing solute clusters in low-alloy steels." Scripta Materialia, Volume 267, 2025, 116797.

EXTERNAL INTELLECTUAL PROPERTY:

- "FeCr free energy material based on CALPHAD assessment in Marmot." https://github.inl.gov/ncrc/marmot/pull/922

Emergent Topological Phenomena in Antiperovskite Nitrides at Surfaces and Interfaces

PROJECT NUMBER:
23A1070-153FP

TOTAL APPROVED AMOUNT:
$1,210,000 over 3 years

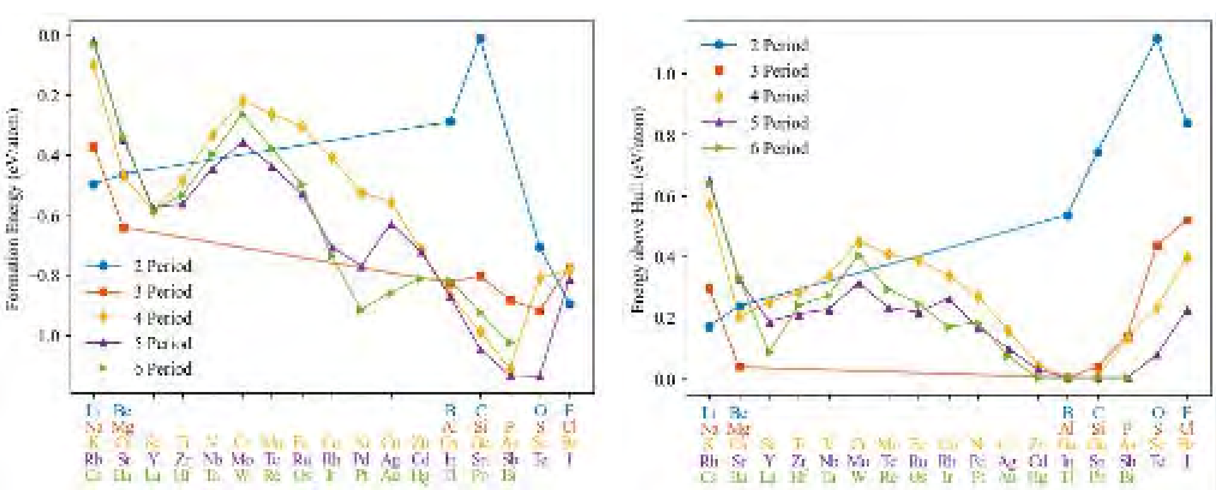
PRINCIPAL INVESTIGATOR:
Krzysztof Gofryk

CO-INVESTIGATORS:
Kevin Vallejo, INL
Shuxiang Zhou, INL

COLLABORATORS:
University of Central Florida

Epitaxial synthesis and quantum-level modeling advance discovery of quantum materials with tunable electronic properties.

Antiperovskites are intermetallic materials with a perovskite crystal structure that exhibit a wide range of tunable physical properties, including superconductivity, giant magnetoresistance, and the topological Hall effect. This project focused on the synthesis and fundamental investigation of the electronic and magneto-transport properties of selected nitrogen-based antiperovskite epitaxial films and heterostructures, grown via molecular beam epitaxy. Special emphasis was placed on exploring topological quantum phenomena governed by strong spin-orbit interactions and non-collinear magnetism. Incorporating f-electron elements into the antiperovskite structure not only enhanced spin-orbit coupling, critical for band inversion and the emergence of non-trivial electronic structures, but also introduced localized non-collinear magnetic ordering, which is essential for the formation of surface states and the topological Hall effect. Additionally, density functional theory was applied for high-throughput screening to predict promising candidate materials for experimental synthesis and characterization.



(a) formation energy (b) energy above hull of antiperovskite Ce3XN computed by generalized gradient approximation calculations.

TALENT PIPELINE:

- Iftakhar Bin Elius, student at University of Central Florida, hired as postdoc at Los Alamos National Laboratory
- Volodymyr Buturlim, *Glenn T. Seaborg distinguished postdoc* at INL, converted to staff
- Kevin Vallejo, *Russell L. Heath distinguished postdoc* at INL, converted to staff
- Sabin Segmi, postdoc at INL
- Shuxiang Zhou, *Glenn T. Seaborg distinguished postdoc* at INL, converted to staff

PAPERS AND PRESENTATIONS:

- Sabin Regmi, Iftakhar Bin Elius, Anup Pradhan Sakhya, Milo Sprague, Mazharul Islam Mondal, Nathan Valadez, Volodymyr Buturlim, Kali Booth, Tetiana Romanova, Krzysztof Gofryk, Andrzej Ptok, Dariusz Kaczorowski, and Madhab Neupane, "Electronic structure in a rare earth based nodal line semimetal candidate PrSbTe." Phys. Rev. Mater. 8, L041201 (2024).
- O.A. Salas, Y. Getahun, H.C. Mandujano, F. Manciu, M Castellanos, J. Lopez, R.G. Hernandez, V.B., Buturlim, K. Gofryk, D. Bairwa, S. Elizabeth, H.S. Nair, "Resilience of the Aurivillius structure upon La and Cr doping in a $Bi_5Ti_3FeO_{15}$ multiferroic." Dalt. Trans. 53 (2024) 6423–6435.
- Kanika Parashar, Zheng Zhang, Volodymyr Buturlim, Jie Jiang, Alexander Roseborough, May Nyman, Krzysztof Gofryk, Ruth Pachter, and Bayram Saparov, "Structural and physical properties of two distinct 2D lead halides with intercalated Cu(ii)." J. Mater. Chem. C. 12, 9372–9384 (2024).
- Brelon J. May, Sabin Regmi, Amey R. Khanolkar, Volodymyr Buturlim, Zachery E. Cresswell, Kevin D. Vallejo, Krzysztof Gofryk, and David H. Hurley, "Molecular beam epitaxy of superconducting zirconium nitride on GaN substrates." AIP Advances 14, 125327 (2024).
- K. D. Vallejo, Z. E. Cresswell, V. Buturlim, B. S. Newell, K. Gofryk, and B. J. Ma, "Synthesis of Samarium Nitride Thin Films on Magnesium Oxide (001) Substrates Using Molecular Beam Epitaxy." Crystals 14(9), 765 (2024).
- K. D. Vallejo, Z. Cresswell, A. S. Messecar, R. Makin, S. M. Durbin, M. F. Muñoz, T. Adel, A. R. Hight-Walker, K. K. Bawane, B. Kombaiah, J.-S. Lee, C.-T. Kuo, V. Buturlim, K. Gofryk, and B. J. May, "Synthesis and Physical Properties of Manganese Chromium Nitride Thin Films Grown via Molecular Beam Epitaxy." J. Phys. Chem. C, 129(10), 5237—5244 (2025).
- Z. Cresswell, V. Buturlim, S. Regmi, K. Vallejo, N. Fessler, T. Garrett, K. Bawane, A. Kamboj, P. J. Simmonds, B. Kombaiah, K. Gofryk, and B. May, "Epitaxial integration of superconducting nitrides with cubic GaN." APL Mater. 13, 031106 (2025).
- Bin Elius, J. F. Casey, S. Regmi, V. Buturlim, A. P. Sakhya, M. Sprague, M. I. Mondal, N. Valadez, A. K. Kumay, et al., "Electronic structure of a nodal line semimetal candidate TbSbTe." Phys. Rev. Materials 9, 064202 (2025).
- Kevin Vallejo (Invited Talk), "Thin film synthesis of rare earth and actinide nitrides using molecular beam epitaxy." American Association of Crystal Growers and Epitaxy West Meeting 2024.
- Buturlim Volodymyr, "Magnetoelastic Properties of 5f Ferromagnet UCu_2P_2." AVS 69th International Symposium & Exhibition 2023.

Self-Learning Kinetic Monte Carlo Simulations of Radiation Damage in Nuclear Fuels

PROJECT NUMBER:
24A1081-015FP

TOTAL APPROVED AMOUNT:
$590,000 over 2 years

PRINCIPAL INVESTIGATOR:
Chao Jiang

CO-INVESTIGATORS:
Chris Marianetti, Columbia University

Machine learning advances the understanding of radiation damage evolution in nuclear fuels.

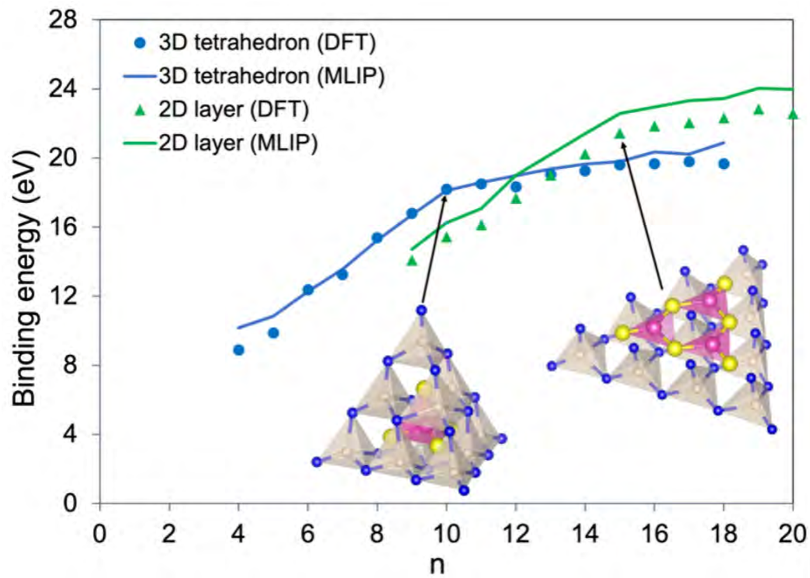
Understanding how irradiation affects the thermophysical and mechanical properties of nuclear materials—such as thermal conductivity degradation in fuels and embrittlement of structural components—is critical to the safety and efficiency of nuclear reactors. To a large extent, these effects are governed by the formation and evolution of atomic-scale point defects and defect clusters. Due to their small sizes, however, these defects are largely invisible under high-resolution scanning transmission electron microscopy. This project aims to fill this experimental knowledge gap by employing kinetic Monte Carlo simulations to predict long time evolution of irradiation-induced defects in such nuclear fuels as uranium dioxide and uranium mononitride. Machine learning interatomic potentials were developed for thorium dioxide and thorium mononitride, which are f-electron-free isostructural surrogates for uranium dioxide and uranium mononitride, respectively. Due to their lack of f-electrons, both thorium dioxide and thorium mononitride are amenable to traditional density functional theory functionals. For thorium dioxide, machine learning interatomic potentials based on both Behler-Parrinello neural network and graph neural network can accurately capture interactions up to the fifth order, with the graph neural network displaying particularly compelling agreement with density functional theory. For thorium mononitride, a Behler-Parrinello neural network-based machine learning interatomic potential was first trained using a large density functional theory dataset and then employed as a high-fidelity, yet computationally efficient surrogate model for density functional theory to accelerate the search for the most energetically favorable ground state configurations of small point defect clusters. In addition, a computer code implementing the activation-relaxation technique and the Lanczos algorithm was developed for autonomous first-order saddle point search. It was employed to explore possible migration pathways of point defects and defect pairs in thorium mononitride. Finally, a one-body reduced density-matrix functional theory of the multi-orbital Hubbard model was developed in this project. This has potential to be ubiquitously applied to f-electron bearing nuclear materials. These efforts lay the groundwork for predictive simulations of radiation damage evolution in nuclear fuels, supporting the development of next-generation nuclear reactors with improved efficiency and safety.

TALENT PIPELINE:

- Sasaank Bandi, student at Columbia University
- Zhengqian Cheng, postdoc at Columbia University

PAPER:

- S. Bandi, C. Jiang, and C. A. Marianetti, "Benchmarking machine learning interatomic potentials via phonon anharmonicity," Machine Learning: Science and Technology 5 (2024) 030502.



Machine learning-assisted discovery of three-dimensional to two-dimensional transformation for interstitial clusters in thorium mononitride containing three thorium interstitials (yellow spheres) and n nitrogen interstitials (blue spheres). Pink and gray spheres represent thorium vacancies and nitrogen vacancies, respectively.

Angle-Resolved Photoemission Spectroscopy of Uranium-based Systems Using Synchrotron Radiation

PROJECT NUMBER:
24P1087-022FP

TOTAL APPROVED AMOUNT:
$140,000 over 1 year

PRINCIPAL INVESTIGATOR:
Sabin Regmi

CO-INVESTIGATORS:
Krzysztof Gofryk, INL
Alexei Fedorov, Lawrence Berkeley National Laboratory

Angle-resolved photoemission spectroscopy enables direct measurement of uranium-based nuclear fuel electronic structure.

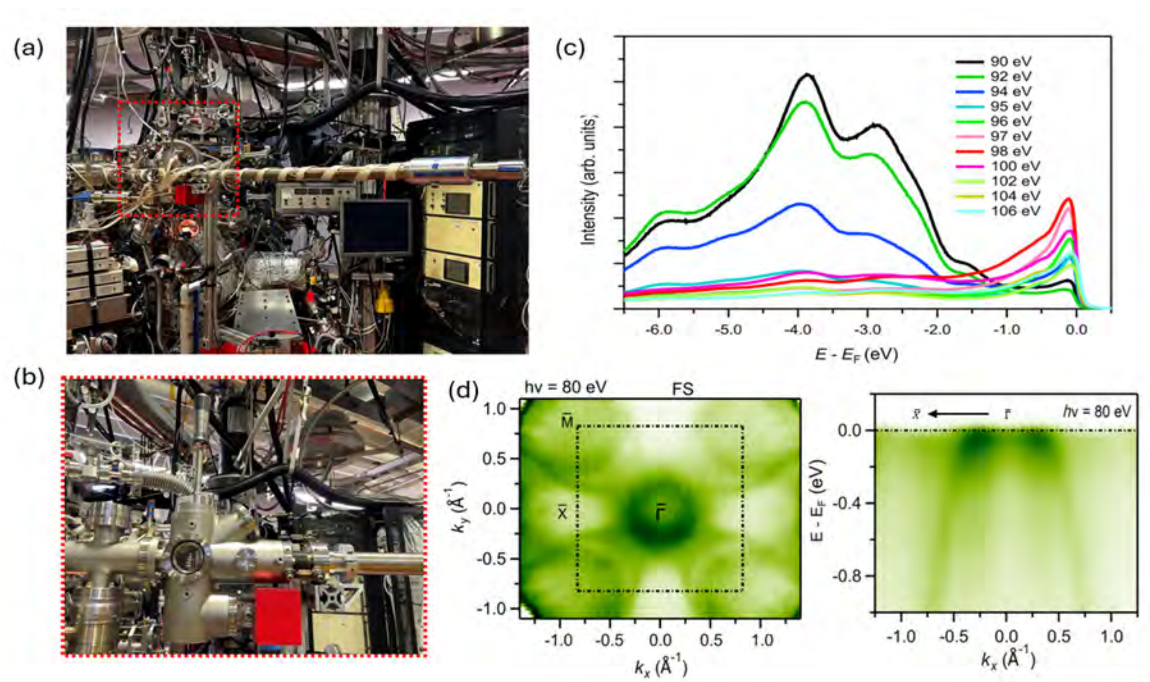
This project led to the development of capabilities for the angle-resolved photoemission spectroscopy (ARPES) measurements of uranium-based materials at Advanced Light Source, Lawrence Berkeley National Laboratory. By using the customized Ferrovac ultra-high vacuum suitcase, the team successfully carried out an ARPES study of a uranium-based ferromagnet [(uranium)(phosphorous)(sulfur)], revealing the nature of the uranium 5***f*** states and their hybridization with conduction states. The results of this study open exciting avenues to extend the work to 5***f*** electron systems to explore the existence of topological states. The next step in the measurements of 5***f*** electron systems is to build a dedicated endstation for ARPES measurements of uranium-based materials. The project also facilitated a strong interlab collaboration between INL and Lawrence Berkeley National Laboratory.

TALENT PIPELINE:

- Sabin Regmi, postdoc at INL

PAPER:

- B. Elius, J. F. Casey, S. Regmi, V. Buturlim, A. P. Sakhya, M. Sprague, M. I. Mondal, N. Valadez, A. K. Kumay, J. Scrivens, Y. Venkateswara, S. Dan, T. Romanova, A. K. Pathak, K. Gofryk, A. Ptok, D. Kaczorowski, M. Neupane, "Electronic structure of a nodal line semimetal candidate TbSbTe." Physical Review Materials 9, 064202 (2025).



(a) ARPES system with vacuum suitcase. (b) Zoomed in view of the vacuum suitcase connected to the ARPES system. (c) Valence band spectra measured with different photon energies across the 5d ⟶ 5f resonance of 98 eV. Sharp peak appearing when the photon energy approaches this resonance indicated strong 5f contribution just below the Fermi level. (d) Fermi surface (left) and energy versus momentum band dispersion along the high-symmetry direction $\bar{X} - \bar{\Gamma} - \bar{X}$.

Investigation of Spectrally Resolved Carrier Interactions Within Defect Configurations of Tungsten-based Refractory High-Entropy Alloys

PROJECT NUMBER:
24P1089-014FP

TOTAL APPROVED AMOUNT:
$150,000 over 1 year

PRINCIPAL INVESTIGATOR:
Himani Mishra

CO-INVESTIGATORS:
Shuxiang Zhou, INL
Pierre-Clément Simon, INL
Michael Moorehead, INL

A first principles computational model quantifies carrier scattering mechanisms that govern thermal conductivity in tungsten-based high-entropy alloys.

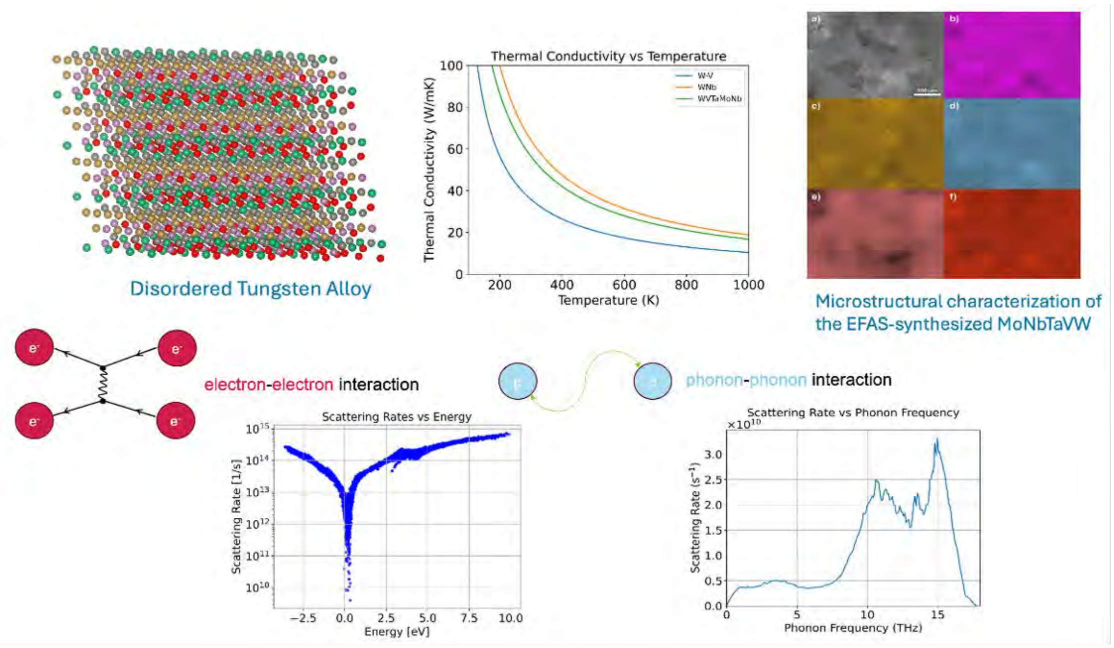
Refractory high-entropy alloys based on tungsten exhibit exceptional thermal stability and corrosion resistance, making them ideal for next-generation high-temperature applications. Using a fully ab initio methodology, we examine the effects of different heat carriers in tungsten-based refractory high-entropy alloys. Ground state energies are calculated via density functional theory, electron-electron scattering rates through Green's function and Coulomb interaction (GW) many-body perturbation theory, and phonon-phonon scattering rates via the finite displacement method. Our density functional theory analysis of tungsten-niobium, tungsten-molybdenum, tungsten-tantalum, tungsten-vanadium, and MoNbTaVW alloys shows major d-orbital contributions near the Fermi level, resulting in enhanced scattering and metallic bonding. GW analysis reveals renormalized band structures compared to density functional theory, indicating significant electron-electron correlation effects. Comparing electron-electron scattering rates, molybdenum-niobium-tantalum-vanadium-tungsten (MoNbTaVW) alloy shows higher scattering and lower thermal conductivity than tungsten-niobium. This trend is reflected in phonon-phonon scattering rates, with tungsten-niobium having the highest thermal conductivity, tungsten-vanadium the lowest, and MoNbTaVW in the middle. These findings align with the standard deviation of their atomic masses, highlighting the balance between structural composition and thermal transport properties. Experimental characterization of the MoNbTaVW alloy shows it to be fully densified with minimal intergranular porosity and an average grain size of around 50 μm. Thermal diffusivity measurements from room temperature to 1000°C show a significant increase with temperature, though lower than pure tungsten. Additionally, the coefficient of thermal expansion and density measurements as a function of temperature support the computational predictions, demonstrating the practical implications for these alloys in high-temperature environments. In conclusion, the balance between electron-electron and phonon-phonon scattering rates, along with experimental validations, underscores the potential of tungsten-based refractory high-entropy alloys for high-temperature applications.

TALENT PIPELINE:

- Himani Mishra, postdoc at INL, converted to staff

PRESENTATION:

- H. Mishra, M. Moorehead, P.C. Simon, S. Zhou, Conference talk in the MS&T conference, Columbus, Ohio, Sep 28–Oct 1, 2025.



Schematic of a disordered random MoNbTaVW alloy generated using the Special Quasirandom Structure method. This schematic is used to calculate electron-electron and phonon scattering rates, as well as the resulting thermal conductivity. The experimental findings from the microstructural characterization of the electric field sintered MoNbTaVW alloy are also included.

Epitaxial Synthesis of New Manganese-Based Magnetic Materials

PROJECT NUMBER:
25A1092-008FP

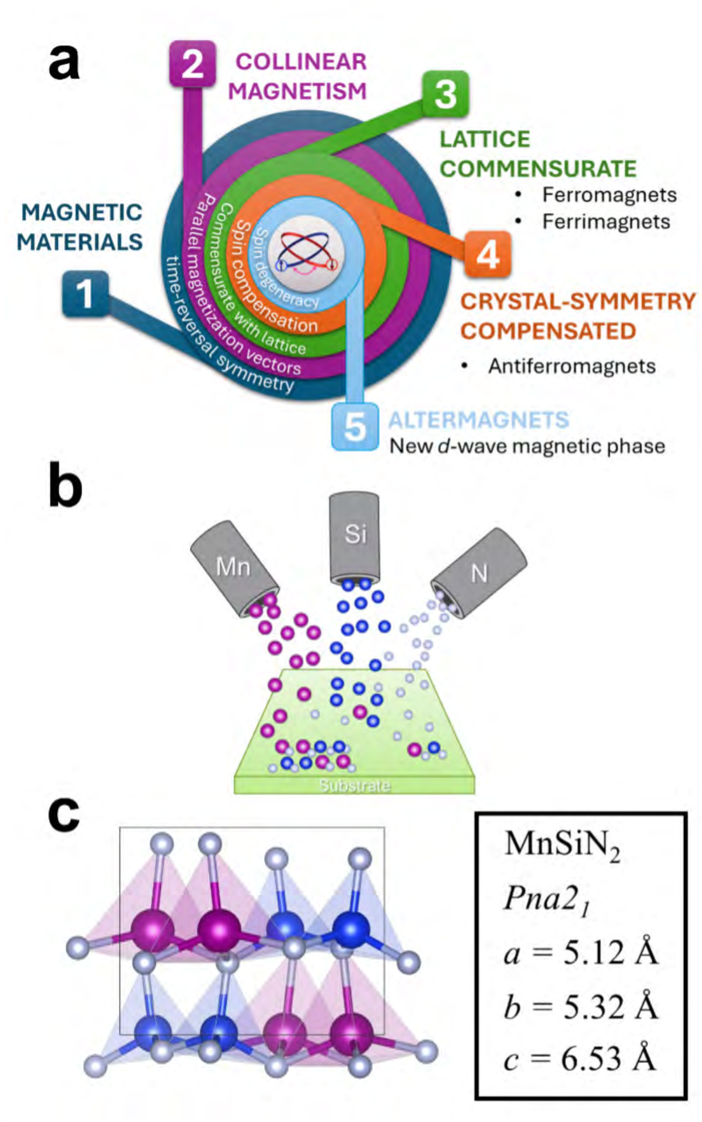
TOTAL APPROVED AMOUNT:
$217,000 over 1 year

PRINCIPAL INVESTIGATOR:
Kevin Vallejo

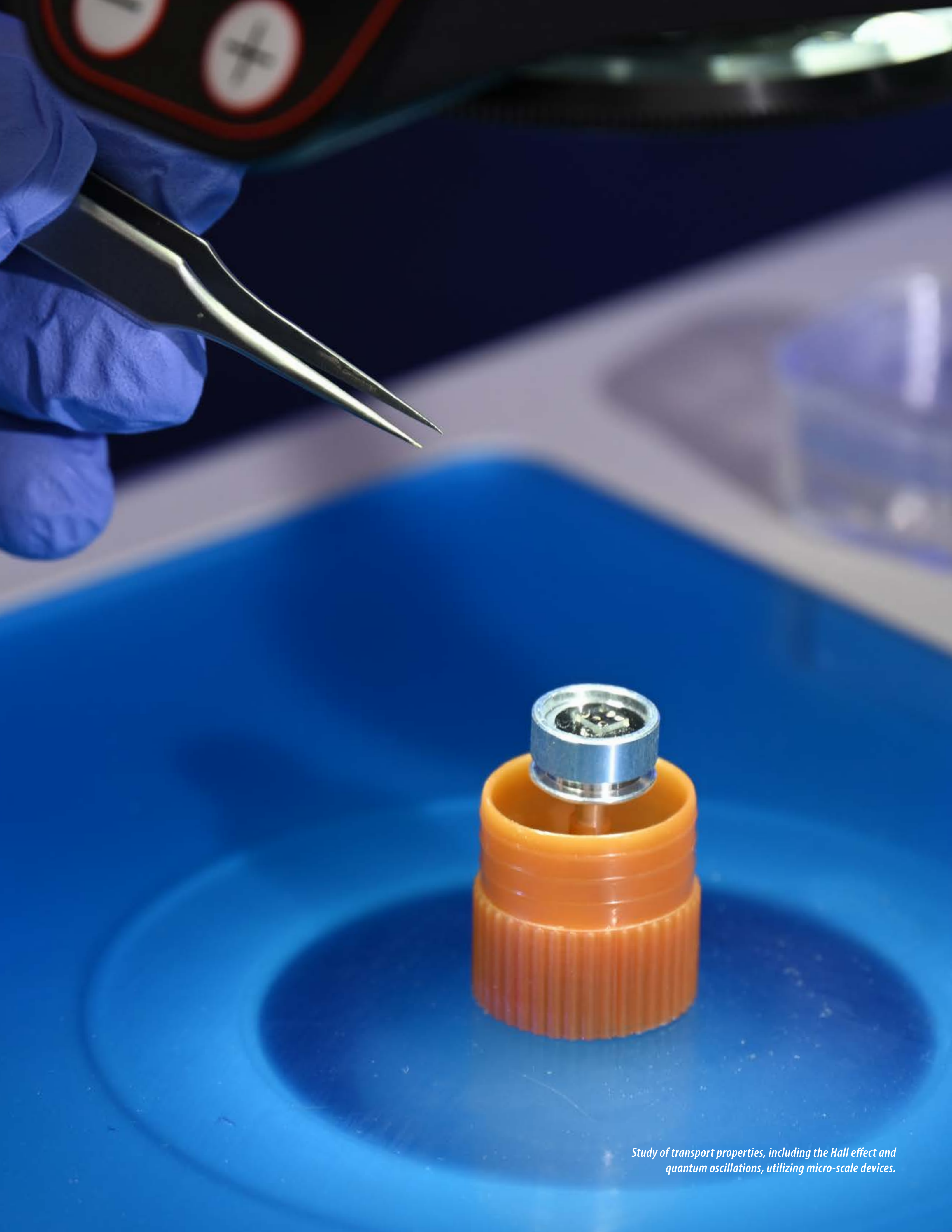
COLLABORATOR:
University of California, Santa Barbara

Newly predicted magnetic behaviors confirmed in manganese-based thin films.

Over the last couple of years, a new magnetic phase has been identified. Altermagnets, also known as non-collinear antiferromagnets, are magnetic materials with collinear, commensurate, and crystal-compensated magnetism that nonetheless share several characteristics with ferromagnets (not crystal-compensated), such as anomalous Hall effect, nonrelativistic spin-polarized current, giant magneto resistance, tunneling magneto resistance, and the inability to support singlet superconductivity. These physical properties give altermagnets materials applications in spintronics, non-volatile memories, spin caloritronics, and multiple-spin channel devices—all highly discussed topics in condensed matter physics. This proposal established the foundations to experimentally demonstrate the spin alignment of the altermagnet candidate manganese silicon dinitride. Through extensive epitaxial synthesis, strain and doping studies, computation, and characterization, this study set the initial steps for the synthesis of altermagnetism as a platform for spin-based physics and devices by realizing the optimal growth conditions of single-crystal thin films of this material. Through the study of polar and non-polar surfaces as substrates, as well as atomic flux ratios and temperatures, we established a path forward to the study of this new altermagnetic materials from synthesis to full characterization.



(a) Magnetic materials chart indicating the physical properties that define the known magnetic phases and the new altermagnetic one. (b) Schematic of a molecular beam epitaxy growth process, where atoms are evaporated from ultra-high purity sources onto substrate. (c) Structure and crystallographic parameters of altermagnet candidate manganese silicon dinitride.



Study of transport properties, including the Hall effect and quantum oscillations, utilizing micro-scale devices.

"Science, my boy, is made up of mistakes, but they are mistakes which it is useful to make, because they lead little by little to the truth."

– Jules Verne, Journey to the Centre of the Earth (1864), translated by William Butcher

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