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2025 LDRD Annual Report

Laboratory Directed Research and Development
Program Activities

Laboratory Directed Research and Development

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2025 LDRD Annual Report

Laboratory Directed Research and Development
Program Activities

By

Vivian S. Sullivan, LDRD Program Manager, Office of Strategy, Performance and Risk
Office of the Director, Argonne National Laboratory

LDRD Program Overview

Argonne National Laboratory's Laboratory Directed Research and Development (LDRD) program encourages the development of novel technical concepts, enhances the Laboratory's research and development (R&D) capabilities, and enables pursuit of strategic laboratory goals.

Argonne's LDRD projects are proposal based and peer reviewed, supporting ideas that require advanced exploration so they can be sufficiently developed to pursue support through normal programmatic channels. Among the aims of the projects supported by the LDRD program are the establishment of engineering proofs of principle, assessment of design feasibility for prospective facilities, development of instrumentation or computational methods or systems, and discoveries in fundamental science and exploratory development.

All LDRD projects have demonstrable ties to one or more of the science, energy, environment, and national security missions of the U.S. Department of Energy (DOE) and its National Nuclear Security Administration (NNSA), and many are also relevant to the missions of other federal agencies that sponsor work at Argonne. A natural consequence of the more "applied" type projects is their concurrent relevance to industry.

The LDRD program is managed in overarching portfolios, each containing multiple projects each fiscal year. The LDRD Prime portfolio is further divided into strategic focus areas aligned with Argonne's strategic plan.

FY 2025 LDRD Program Components

LDRD Prime

The largest component of Argonne's program is LDRD Prime, which emphasizes R&D explicitly aligned with Laboratory major initiatives in support of Argonne's strategic plan. Funded projects reflect the Laboratory major initiatives; the state of development of relevant technical fields; the potential value of advancing those fields to DOE/NNSA and the nation; and the compatibility of the fields with existing facilities, capabilities, and staff expertise at Argonne.

Director's Collaborations

The Director's Collaborations LDRD projects support research that is paired with coordinating research efforts at a partner institution. These are generally small projects selected through a collaborative process.

Named Fellows

Argonne's LDRD Named Fellows program aims to support the scientific or engineering research of exceptional early career scientists and engineers. Working with an Argonne sponsor (a senior member of research staff), LDRD Named Fellows carry out work that is either at the forefront of new research areas or is synergistic with current research efforts.

Innovate

The Innovate component of the LDRD program invests in a full spectrum of investigator-initiated proposals across the Laboratory in DOE-mission-related science and engineering areas. This provides an avenue for R&D staff to propose highly innovative projects in research areas outside the purview of the Prime Focus Areas. Within the Innovate LDRD portfolio is the Seed program, open to postdoctoral appointees and early career researchers to apply for a small project to perform independent research and explore their own ideas.

Swift

The LDRD Swift component provides an avenue for R&D staff to conduct short-term research with a targeted funding opportunity in mind, as well as a means for researchers to explore ideas before developing a full proposal. Projects funded through this component area have a maximum one-year duration. As with the Innovate component, the Swift component invests in a full spectrum of proposals across all mission-related science and engineering areas.

FY 2025 LDRD Summary Report

This summary report provides an overview of all LDRD projects at Argonne that concluded in Fiscal Year 2024. Many projects are funded for multiple years, the initial fiscal year for each project is indicated by the first four digits of the LDRD project number.

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LDRD 2022-0235	Intelligent Analysis of Scattering and Spectroscopic Signatures of Quantum Materials
Investigators	Nina Andrejevic

Thanks to recent advances in source brilliance and coherence, coupled with cutting-edge detectors and novel experimental setups, modern synchrotron facilities have enabled access to materials dynamics at unprecedented levels of detail and across time scales spanning several orders of magnitude. This new and vast data stream has necessitated complementary computational tools to efficiently extract physical insights and expedite scientific understanding. To address this, we developed a data-driven framework based on neural differential equations (NDEs) to uncover mechanistic models directly from time-resolved coherent X-ray scattering measurements. Importantly, this approach enabled the discovery of dynamics without solving the phase retrieval problem frame-by-frame, which can be prohibitively expensive. This opened up the possibility of visualizing otherwise inaccessible, real-space dynamics using existing experimental techniques and extrapolating well beyond the maximum observation time to critically inform experimental design and planning.

We demonstrated this framework in the context of several computational model systems, including domain synchronization, particle clustering, and source fluctuation, showcasing a range of possible problem types and network architectures supported by the framework. We further presented a proof-of-concept experiment using the framework to recover the probe trajectory from a ptychographic scan. Notably, our work established a versatile platform for data-driven discovery of dynamics, which is widely applicable across characterization modalities.

LDRD 2023-0004	Artificial Intelligence-Driven, Real-Time Optics Control System to Achieve Aberration-Free Coherent Wavefronts at 4th Generation Synchrotron Radiation Beamlines
Investigators	Luca Rebuffi Xianbo Shi

The research activities conducted under this project, which benefited from the collaboration of optics specialists, computational scientists, and beamline scientists, provided proof-of-principle results for the automatic control of beam properties—specifically in optics alignment and wavefront control. The goal of automatic X-ray beam control was not only to reduce alignment time and enhance beam stability but also to enable more advanced capabilities, such as the autonomous management of mirror-based zoom optics systems. These systems deliver variable focal spot sizes across a wide range at the sample location while maintaining a high-quality wavefront—an essential feature for modern coherent nanoprobe beamlines.

We completed and successfully tested AI/ML-driven software designed to address complex optical system challenges: an ML-driven controller for a bimorph adaptive mirror to refine the X-ray beam wavefront, and an auto-alignment system for nanofocusing Kirkpatrick-Baez (KB) mirror systems based on Bayesian optimization and informed by ultra-realistic digital twins of the Advanced Photon Source beamlines.

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Early demonstrations at the 28-ID-B beamline using real KB mirrors, followed by a full experimental campaign at the 3-ID beamline, underscored our ability to automatically produce a stable, aberration-free wavefront. Over the course of this project, initial prototypes evolved into fully functional systems engineered to operate real Advanced Photon Source Upgrade (APS-U) beamlines. In particular, a multi-stage, multi-fidelity auto-alignment and autofocusing system with a graphical user interface was deployed at several APS-U beamlines for testing and future development.

Throughout the three years of this project, we completed and delivered to the APS-U beamlines a comprehensive and easily configurable system capable of achieving sub-second, picometer-level wavefront control with exceptional beam stability and repeatability. While both systems demonstrated outstanding independent performance, their combination proved particularly powerful. Specifically, the machine learning-driven controller's effectiveness was enhanced by the rapid adaptability of the auto-alignment system, which ensured consistent beam conditions which was crucial for training the machine learning model and optimizing the neural network controller's performance.

These innovative developments represent a major step toward fully autonomous operation and optimization of beamlines, unlocking new scientific opportunities that were previously unattainable.

LDRD 2023-0007	Multiline Free Electron Laser Superconducting Undulators
Investigators	Yury Ivanyushenkov Joel Fuerst

The project expanded the application of superconducting undulator (SCU) technology, developed at the Advanced Photon Source, to free electron lasers (FELs). The goal of this study was to demonstrate the unique possibility of creating multiline free electron lasers using SCUs. As a result of the project, a prototype for a two-line free electron laser superconducting undulator was developed, fabricated, and tested.

LDRD 2023-0024	Development of Force Neutral Adjustable Phase Undulator Array for Synchrotrons and Free Electron Lasers
Investigators	Joseph Zhongde Xu Maofei Qian

Modern synchrotron and free electron laser (FEL) facilities require longer and more precise undulators than current designs, which rely on bulky supports to manage high magnetic forces while maintaining a challenging 10-micron gap profile tolerance over a multi-meter length. To address this, the Force Neutral Adjustable Phase Undulator (FNAPU) device was proposed, using compensation magnets to neutralize the magnetic forces acting on the support structures. This innovation resulted in a more precise, compact, less expensive, and simpler high-precision long undulator design that maintained the required gap tolerance, as reduced mechanical stress

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allowed for less bulky supports. Furthermore, FNAPU technology is crucial for implementing undulator arrays—a concept of stacking multiple undulators—to multiply the efficiency of FEL facilities by providing multiple simultaneous X-ray beamlines through electron beam switching, which conventional adjustable-gap undulators cannot achieve compactly.

The project successfully developed and tested two FNAPU prototypes with different period lengths, demonstrating their ability to form an array without field cross-talk and their potential to be rotated for polarization changes. The magnetic and mechanical design and analysis for both prototypes were completed, and the assembly and tuning of the first FNAPU (27 mm period) were accomplished. The second FNAPU (17.2 mm period) was designed, all components were ordered and received, and assembly was in progress at the time of reporting. FNAPU technology is now being considered for major synchrotron and future compact multilayer FEL facilities. Once fully verified, FNAPU could represent a paradigm shift in undulator technology, with high payoffs expected.

LDRD 2023-0038	APS-U PtychoProbe First Science: Decarbonizing Cement Manufacturing
Investigators	Volker Rose Junjing Deng, Yi Jiang, Barry Lai, Dileep Singh

This work enabled a pathway for initial science experiments at the featured APS-U PtychoProbe beamline following the upgrade, targeting decarbonization in cement manufacturing. We explored advanced visualization techniques and analysis algorithms to develop optimized materials and new technologies for reducing carbon dioxide emissions during the manufacturing process. For the first time, the binder structure was studied in an x-ray microscope at a sub-10 nm level.

LDRD 2023-0075	Developing Point-Focus High-Energy Diffraction Microscopy to Reveal Battery Material Degradation
Investigators	John S. Okasinski Daniel Abraham, Hemant Sharma

The long-term performance of lithium-ion batteries is limited by the chemo-mechanical degradation of the active materials in their electrodes. We developed operando methodologies and specialized electrochemical cells to examine the stresses and strains in battery materials using point-focus High-Energy Diffraction Microscopy (pf-HEDM). For this purpose, we leveraged high-energy X-ray instrumentation at the 1-ID and the forthcoming High-Energy X-ray Microscope 20-ID beamlines, the evolving MIDAS program for high-energy diffraction microscopy data, and lithium battery expertise in the Chemical Science and Engineering division. The novel X-ray analysis techniques and computational methodologies we developed have broader impact and applicability beyond battery materials.

We completed analysis of several sets of pf-HEDM data taken before and after the Advanced Photon Source Upgrade using updated software and computer hardware tools. We prepared

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samples for three pf-HEDM beamtimes at 1-ID and characterized the samples with complementary techniques. Additionally, we developed a forward simulation model and software to take electron backscatter diffraction (EBSD) grain mapping results and simulate pf-HEDM data. Performance of in situ battery cells was characterized with multiple techniques to demonstrate their capabilities with different types of battery materials.

LDRD 2023-0104	Artificial Intelligence/Machine Learning Accelerated High-Performance Image Analysis using Supercomputers
Investigators	Tekin Bicer Junjing Deng, Viktor Nikitin

The Advanced Photon Source upgrade (APS-U) provided two to three orders of magnitude higher brilliance compared to the current Advanced Photon Source. While this high brilliance enabled advanced experimentation, it also increased the amount of experimental data, reaching hundreds of terabytes to petabyte-scale in some cases. Ground-breaking scientific discoveries from these experiments were only possible with the timely analysis of these large datasets. This project conducted research on high-performance parallel and distributed computing and networking techniques to solve extremely large X-ray imaging problems on supercomputers, including, but not limited to, the Aurora and Polaris systems at the Argonne Leadership Computing Facility. We further accelerated and enhanced data-intensive image analysis pipelines by incorporating artificial intelligence and machine learning methods. The overarching goal of the project was to enable scientific breakthroughs by reducing analysis tasks that previously took months or years to minutes or hours using advanced computing techniques on supercomputers.

LDRD 2023-0108	Integrated Laminography Instruments for Three-Dimensional Characterization of Extended and Planar Samples
Investigators	Olga A. Antipova Francesco D. Carlo, Fabricio S. Marin, Viktor Nikitin, Sarah Wieghold

Micro- and nano-Computed Tomography are well-established techniques that offer fast, high-resolution visualization of internal structures. X-ray Fluorescence microscopy provides parts-per-million element sensitivity with resolution ranging from 100 to 2,000 nanometers. We developed laminography instruments and software enabling hyperspectral (spatio-spectral) scanning of extended planar samples with fluorescence and full-field imaging at beamlines 2-ID-E (Microscopy group), 2-BM, and 32-ID (Imaging group). Micro-CL capability was established at 2-BM in 2023, and several data sets were collected. The XRF-CL setup was tested at 2-ID-E and provided data sets for hyperspectral reconstructions. Laminography reconstruction algorithms were deployed in TomocuPy (Micro-CL) and XRFtomo (both XRF-CL and Micro-CL) software packages. In addition, we developed a tool for correlation of 2-BM Micro-CL and 2-ID-E XRF-CL reconstructed volumes for improved characterization of multimodal data sets. This tool enables users to easily navigate within low-resolution XRF-CL data using higher-resolution

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Micro-CL data for proper selection of regions for high-resolution XRF-CL data collection, significantly improving XRF-CL efficiency.

We also developed sample-specific phantoms to simulate self-absorption for XRF-CL applications. This approach assists users with selecting optimum samples and data collection workflows, as well as informing users of possible image artifacts.

These new capabilities unveil 3D structure-compositional information and elucidate dynamic processes inside samples. This development sets the stage for initial science experiments in solar cells, battery, and brain research, facilitating efficient utilization of resources by integrating beamlines and modalities.

LDRD 2023-0109	Three-Dimensional Multiscale Diffraction Imaging of Nano-Scale Defect Kinetics During Corrosion and Mechanical Deformation
Investigators	Ross J. Harder

The mechanical properties and longevity of structural materials in high-value industries, such as power generation and transportation, are governed by micro- and nanoscale defect evolution within the crystalline grain structure. This project employed a multi-scale approach to untangle the complex interplay between defect structure and mechanical properties. We developed experimental methods using electron and x-ray diffraction microscopy, combined with an in-situ nano-indentation device, to image plastic deformation of materials in both two and three dimensions at the nanoscale.

Advances were made in both data acquisition and analysis methods to enable these experiments. Significant investments in modeling and simulations were made to support a machine learning initiative aimed at understanding how plastic deformations are reflected in electron and x-ray diffraction microscopy data. As materials deform beyond elastic limits, Laue diffraction patterns become increasingly difficult to analyze, and electron microscopy provides only two-dimensional, surface information. We began leveraging machine learning, trained on high-fidelity materials simulations of defect dynamics, to extract important multiscale structural characteristics from both x-ray Laue diffraction and, eventually, electron microscopy. No other methods provide the required multiscale information to understand materials failure.

LDRD 2023-0119	Engineering Extreme Pressure Sample Environments for the Upgraded Advanced Photon Source
Investigators	Gilberto Fabbris Rostislav Hrubyak

The investigation of materials at high pressure is key in a wide range of topics, including condensed matter physics and geosciences. Diamond anvil cells have been employed to generate high static pressures, but the diamond shape has remained a key limitation, constraining experiments to approximately 300 GPa. These devices also require the use of

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small samples (dimensions greater than 50 microns), which imposes a substantial constraint on electrical transport techniques. In this project, we targeted the development of novel high-pressure research techniques by employing nanofabrication tools with diamond anvil cells. Our initial goal was to use focused ion beam (FIB) to fabricate a toroidal shape on the tip of the diamond, aiming to generate ultra-high pressures (greater than 400 GPa). We succeeded in producing such anvils at the Center for Nanoscale Materials, and the maximum pressure generated was in excess of 300 gigapascal (GPa). We optimized the fabrication of diamonds and developed novel methods to prepare pressure cells using these anvils. We are therefore ready to use this technology in the upgraded Advanced Photon Source.

LDRD 2023-0136	The Development of Combining Ptychography and Small-Angle X-ray Scattering for Nanomaterial Characterization
Investigators	Junjing Deng Byeongdu Lee, Joseph McCourt, Soenke Seifert, Gregg A. Wildenberg

This project developed a unified experimental platform that integrated X-ray ptychography and small-angle X-ray scattering (SAXS) to enable multi-length-scale structural characterization while minimizing radiation damage. Although ptychography (an imaging technique) and SAXS (a scattering technique) are traditionally performed at separate beamlines, both rely on small-angle diffraction, creating a unique opportunity to combine them within a single setup. Our team advanced beamline instrumentation by implementing a laser-interferometer-based scanning probe for high-precision positioning and successfully collected combined ptychography–SAXS datasets using both dual-detector and single-detector configurations. We also developed new data-analysis methods that leveraged synergies between the two techniques, including convolutional-neural-network–enabled deconvolution of SAXS diffraction patterns using the probe reconstructed from ptychography. These accomplishments significantly strengthened our ability to characterize materials across multiple length scales with higher accuracy and efficiency, advanced structural analysis capabilities for a broad range of samples, and have already attracted users interested in applying these developed techniques to their scientific studies.

LDRD 2023-0148	Novel Two-Dimensional Metal Carbides and Nitrides (MXenes) for Energy Storage and Decarbonization
Investigators	Sixbert P. Muhoza

This project focused on advancing transition metal carbides, oxy-carbides, nitrides, and carbonitrides (MXenes) by leveraging their unique properties to enhance energy storage and carbon management technologies. Specifically, the work implemented application-directed MXene functionalization techniques to tailor and optimize MXenes for carbon management (carbon dioxide capture and conversion) and energy storage (battery technologies and clean chemical storage) applications. Numerous MXene functionalizations were explored. Metal decoration where MXenes were decorated with copper and its alloys for use as carbon dioxide

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reduction electrocatalysts. Surface terminations customization where MXenes were uniformly terminated by: phosphorus for use as durable, high-capacity phosphide-type electrodes for next-generation batteries, and amines for use as energy-efficient carbon dioxide sorbents. Hybridization with self-healable polymers producing electrochemically active binders that enhanced the durability of high-capacity conversion-type battery electrodes, which typically experience volumetric changes during cycling. These changes lead to electrode cracking, capacity fade, and eventual battery failure. The novel MXene-based binders extended battery lifetime by reconnecting cracked electrodes, while also contributing to the battery's electrochemical performance—unlike other binders, which add “dead weight.” Metal-site substitution enabling the preparation of high-entropy MXenes, integrating metals with specific, targeted properties. The inherent disorder in high-entropy MXenes offered a novel strategy to control dimensional changes in battery electrodes during charge/discharge cycling. These materials will help minimize the content of noble metals in catalysts for hydrogen generation and other applications. Finally, nitride MXenes were synthesized and exhibited favorable catalytic properties, making them suitable for metal-air battery technologies.

LDRD 2023-0150	Nuclear Aspects of Neutrino Interactions
Investigators	Afroditi Papadopoulou

The project provided a quantitative understanding of neutrino–argon interactions, supporting the precision goals of the Deep Underground Neutrino Experiment (DUNE) and the Short Baseline Neutrino (SBN) program. Argonne-based analyses of data from the MicroBooNE liquid argon time projection chamber delivered the first high-statistics measurement of neutrino-induced quasielastic-like muon plus proton events, establishing an unprecedented benchmark for angular resolution and kinematic imbalance observables used in DUNE atmospheric neutrino oscillation studies. This effort also produced the inaugural dark sector electron-positron search in MicroBooNE, setting new limits on models invoked to explain the MiniBooNE anomaly. Within the DUNE collaboration, Argonne scientists contributed critical simulation, reconstruction, and photon detection performance studies that informed the design of the far detector modules and refined the neutrino interaction models incorporated in the experiment's oscillation analyses.

LDRD 2023-0151	Controlling the Efficiency, Phase, and Polarization of High-harmonic Conversion of Light: A Path to Compact, Tabletop, Femtosecond X-ray Sources
Investigators	Soham Saha

High harmonic generation is a process by which table-top pulsed laser outputs from visible wavelengths are converted to ultraviolet and even X-ray wavelengths. High harmonic generation offers applications in attosecond X-ray absorption spectroscopy, photoelectron measurements, nanoscale photolithography, and biomedical science. The goal of this project was to overcome the current limitations of low efficiencies (10^{-6}) of high harmonic generation using gas-filled

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capillaries by utilizing robust, refractory metals and dielectrics capable of withstanding remarkably high laser intensities (10^{14} W/cm²). I designed dielectric and plasmonic nanostructures to boost high harmonic generation efficiency, and to shape the polarization, phase, and amplitude of the high harmonics by designing tunable metasurfaces. I completed a study of the damage thresholds of prospective materials for high harmonic metasurface fabrication, including titanium nitride, single crystal and polycrystalline zinc oxide, aluminum-doped zinc oxide, and ultrananocrystalline diamond (grown at the Center of Nanoscale Materials). I demonstrated large optical nonlinearities in ultrananocrystalline diamond (UNCD), and prepared to measure high harmonic generation from them. 3. I conducted measurements of optical properties and relaxation dynamics of oxide films. Finally, I simulated nanoresonators utilizing niobium nitride, and performed optical and transient spectroscopic characterizations on them. These metals can be used for high harmonic generation metasurface applications.

LDRD 2023-0156	Enabling Compact X-ray Free-Electron Lasers with Ultra-Bright Electron Sources
Investigators	Philippe R. G. Piot Gongxiaohui Chen, John Power

Producing bright electron beams was critical to enabling compact X-ray free-electron lasers (XFELs). This project explored the design and testing of a bright-electron source based on a two-beam acceleration scheme. In this approach, the electron beam was emitted from a photocathode located in a high electric field region (sub-GV/m) within a radiofrequency resonant cavity. The project focused on both experimental aspects (testing the proposed electron sources and characterizing the produced electron bunches) and numerical design aimed at developing a concept for compact X-ray free-electron lasers. Our project expanded Argonne's research portfolio into the physics of ultra-bright electron sources while capitalizing on unique Argonne infrastructure, such as the generation of high-power short RF pulses at AWA. In the short term, this prototype photoinjector provided an experimental platform to develop compact X-ray sources, for example, based on inverse Compton scattering. Its potential extension to produce 100's MeV beams (pending extramural funding) could support a proof-of-principle compact FEL demonstration in the vacuum ultraviolet (VUV) or extreme ultraviolet (EUV) regimes—a spectral region of interest to the semiconductor industry.

LDRD 2023-0178	Novel Methods of Operando Imaging of Battery Cathodes
Investigators	Jordi Cabana-Jimenez

This research augmented our ability to spatially track storage reactions in battery electrodes using operando X-ray imaging and laid the foundation for new and unique synchrotron methods, through the design of setups with high electrochemical fidelity. Proof of concept was established by quantifying the inherent rates of charge of individual particles of leading lithium-ion cathodes. First, we initiated the design of the second generation of an operando tomography cell and secured access to the necessary beamlines. A series of imaging measurements of single

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battery particles, both ex situ and operando, were conducted, providing a wealth of data. Next, we conducted the first set of measurements at the upgraded APS, successfully acquiring operando diffraction imaging at three different rates of reaction of a Li-ion battery cathode. We then moved to the development of a data analysis workflow capable of handling the encoded complexity, scaling the extraction of insight from the multiple datasets collected in this project. By the end of our work, the workflow successfully handled data processing and produced the first results on the evolution of single particles as a function of electrochemical state.

LDRD 2023-0234	A Self-Aware Condition Monitoring Framework for Multiphysics Systems
Investigators	Yeni Li

In complex systems such as nuclear power plants, condition monitoring of components is crucial to ensure safety and optimal performance. Traditionally, condition monitoring has relied on conservatively scheduled inspections, resulting in significant costs. In the nuclear industry, operation and maintenance (O&M) expenditures accounted for approximately 66% of overall production costs. This project aimed to reduce O&M costs through predictive maintenance. Specifically, we applied this approach to feedwater heaters, predicting when and where maintenance interventions were necessary. High-fidelity modeling of degradation based on operating histories was used to infer the health condition and the remaining useful life of the feedwater heaters. To achieve these objectives, we conducted literature reviews, developed multiphysics models, evaluated model fidelity, analyzed plant inspection data, prototyped remaining useful life models, and validated estimated remaining useful life against maintenance records. Building upon these foundational efforts, a condition monitoring framework was formalized, adaptable across various designs and operating conditions, and capable of pinpointing degraded locations. These efforts paved the way for full implementation and validation of the proposed condition monitoring framework, which also provides a methodology to infer the health conditions of other key components.

LDRD 2023-0237	Advancing Topological and Quantum Materials Discovery
Investigators	Mercouri G. Kanatzidis Duck Young Chung

The project elevated our capability in tailored material design and advance predictive synthesis, transforming the concept of “materials by design” into a true science of “synthesis by design” for inorganic energy materials. The project delivered major achievements in the discovery and synthesis of new topological, superconducting, and correlated quantum materials. Using innovative flux-based and reaction-path-controlled approaches, we discovered a new homologous series that provides a molecular-level design framework for extended solids and introduces a transferable design rule based on anion electron-affinity differences. Through the mixed flux routes we developed, we synthesized twenty-three new silver chalcogenides with tunable structural motifs and electronic properties. We realized new tunable subsulfide

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compounds that host coexisting Dirac cones and flat bands, an uncommon combination in a single system, and synthesized a new lanthanum copper tellurium compound, a flat-band candidate for correlated electronic behavior and superconductivity. Additional exploratory efforts revealed superconducting, polar, magnetic, and charge-density-wave behaviors across multiple chemical systems. Collectively, these findings established new chemical design principles and synthetic pathways that accelerate the discovery of next-generation quantum materials.

LDRD 2024-0011	Force-Neutral Fast Polarization Switching X-Undulator for the POLAR Beamline
Investigators	Maofei Qian Daniel Haskel, Joseph Zhongde Xu

The Force-Neutral Fast Polarization Switching X-Undulator project successfully developed and tested a 1-meter prototype insertion device designed to generate X-rays with fully tunable polarization states (linear, circular, and elliptical) across a 2.8-27 keV energy range for next-generation synchrotron beamlines. The X-undulator employed innovative force compensation technology using secondary magnet arrays to neutralize magnetic forces between opposing magnetic jaws, enabling mechanical designs optimized for fast polarization switching. Key achievements included successful prototype fabrication and assembly, validation of magnetic field profiles and field integrals across all polarization modes, and demonstration of force neutralization effectiveness with precise mechanical tolerances required for micron-level jaw displacements. This breakthrough technology addressed critical limitations of conventional phase-retarding optics by enabling direct polarization control at the source with projected 5-30x flux gains, particularly at energies above 14 keV where traditional optics are impractical. The compact, scalable design established a foundation for implementation at the APS-U POLAR beamline to advance quantum materials research for next-generation technologies including spintronics, twistrionics, and quantum computing, while also enabling future compact free electron laser facilities with multiple beamlines and polarization control capabilities.

LDRD 2024-0089	Developing a Rapid, High-Fidelity, Multi-Infrastructure Energy System Simulation Framework to Address Global Energy Challenges for Enhanced Resiliency and Security of Global Energy Systems and Critical Infrastructure
Investigators	Jonghwan Kwon Bruce P. Hamilton, William N. Mann, David Sehloff

This project aimed to develop a robust energy system simulation framework by integrating the global TIMES/TIAM-WORLD energy model with sector-specific simulation tools created at Argonne National Laboratory. The primary focus was on the electric energy sector, where TIMES/TIAM-WORLD was linked with the Argonne Low-Carbon Electricity Analysis Framework (A-LEAF). A-LEAF enabled high-granularity power system analysis across diverse timescales and applications.

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A major accomplishment of this work was the successful linkage between the TIMES/TIAM-WORLD energy systems model and A-LEAF. The team developed a bridge model that translated outputs from TIMES into inputs suitable for A-LEAF power system simulations.

LDRD 2024-0091	Flexible Thermal Energy Storage System (FTESS) with Dual Electrical and Thermal Charging Options for Industrial Process Heat
Investigators	Dileep Singh Amgad Elgowainy, Robert A. Erck, Krista L. Hawthorne, Tianchen Hu, Wenhua Yu

Using modeling and simulations, we demonstrated the feasibility of using induction heating to charge thermal energy storage systems. A patent application was filed. To validate the concept, we built a test system and successfully demonstrated induction heating with both phase change and sensible heat storage media. Heat storage up to 1000 degrees centigrade and recovery of heat using air were achieved. Experimental results closely matched the modeling efforts. As part of the project, this technology will be beneficial for using electricity to generate and store heat when electricity prices are low, and recovering it as process heat, which will support efficient energy use in various manufacturing processes.

LDRD 2024-0094	Decarbonizing Industrial Burners using Hydrogen Combustion
Investigators	Joohan Kim Muhsin Mohammed Ameen, Chandrachur Bhattacharya, Ashwini Karmarkar, Sharanjeet Kaur, Robert S. Tranter

This project developed a predictive simulation framework for investigating hydrogen combustion in industrial burners and to enhance measurement techniques for burner flame characterization. The work was accomplished through (1) extensive validation of submodels used in engineering computational fluid dynamics (CFD) simulations by leveraging high-fidelity experimental data and gold-standard direct numerical simulations (DNS), and (2) enhancement of measurement techniques for flame characterization by utilizing DNS to supplement data that are difficult to measure. First, a CFD model of an in-house burner was developed using the commercial package CONVERGE. Simulations with methane and hydrogen were conducted to determine operating conditions and to evaluate turbulence, species transport, and nitrogen oxides formation models. From this work, best practices were established for grid configuration, ignition strategy, and time-step control, and then applied to simulations of an industrial burner. Second, CFD models of a McKenna diffusion burner and the in-house burner were developed using NekRS, yielding best practices for mesh generation, boundary conditions, ignition, and numerical stabilization to ensure computational robustness. Third, the in-house burner was designed, reviewed by safety and quality assurance teams, fabricated, and delivered.

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LDRD 2024-0096	Modeling Nuclear Supply Chain Needs and Constraints for Advanced Reactor Deployments
Investigators	Scott Richards Matthew E. Riddle, Jia Zhou

This research developed a framework for modeling nuclear supply chains to support the robust deployment of advanced reactors. This modeling framework combined supply chain market modeling, nuclear fuel cycle simulation, and power system simulation tools to perform in-depth analysis of critical supply chains, potential disruptions and constraints, and mitigating strategies for minimizing disruptions. The initial version of the framework, developed in the first year, demonstrated that in scenarios of rapid and aggressive decarbonization, the price of uranium could significantly impact the amount of nuclear power deployed—differing from projections from conventional methods by as much as 50%. In the second year, this capability was expanded to include non-fuel supply chains (e.g., graphite). The capability developed is becoming increasingly important as interest in advanced nuclear applications grows and the US continues to take steps to secure its critical supply chains.

LDRD 2024-0099	Bridging Data Gaps in Critical Material Industry Cost Curve Analysis
Investigators	Braeton J. Smith Matthew E. Riddle

This project estimated industry cost curves for critical material producers. These cost curves relied on data from material producers and processors, which was not always available. The project improved the estimation of industry cost curves where data was limited by leveraging both frequentist and Bayesian statistical techniques to develop a model for estimating unreported costs associated with specific raw materials producers. The costs generated from these statistical models were used to produce more rigorous industry cost curves that compared the ability of materials producers to be competitive in different market environments. The project developed a statistical model for rare earth element (REE) mining and processing costs, which was used to calculate a set of predicted values for out-of-sample REE projects (i.e., those with unreported costs) with known characteristics. This improved upon previous work in developing industry cost curves for global REE producers. The project then used the model to develop an industry cost curve for vanadium, a market that displays similar characteristics (i.e., small sample size, poor quality data, and co-production).

LDRD 2024-0118	Decarbonization of Iron and Steel Production: Near Room Temperature Leaching and Electrowinning of Iron Ore
Investigators	Michael J. Dziekan Justin G. Connell, Matthew R. Earlam, Zachary D. Hood, Jarod C. Kelly

This project established a novel, closed-loop method for iron production via near room temperature electrowinning of iron chloride, generating iron metal and oxygen gas. The electrowinning cells tolerated intermittent energy supplies, as modular electrolysis cells could be

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easily throttled. The method eliminated process carbon, such as metallurgical coke used in carbothermic reduction.

Additionally, this work presented a novel technology to produce metallic iron from magnetite through electrowinning in concentrated sodium hydroxide, as a carbon-free and energy-efficient alternative for iron production. While traditional pyrometallurgical routes require multiple processing steps at extremely high temperatures (~1500°C), this caustic iron electrowinning approach enabled solid-to-solid reduction that directly converted magnetite to metallic iron in a single step at a low temperature (80°C). The technology featured a novel electrolytic cell design with an unconventional stacked electrode configuration, where the cathode acted as a receptacle at the bottom of the cell and the anode was placed above the cathode. The process was further enabled with a magnet to help capture iron particles and polytetrafluoroethylene (PTFE) skived tape to prevent shorting and define the cathode active surface area. Experiments were conducted under constant current conditions and achieved high metallization as well as improved current efficiencies at lower current densities. Combustion oxygen analysis (LECO) confirmed significantly reduced oxygen content in the product, highlighting the potential for producing pure metallic iron for industrial scale-up.

LDRD 2024-0126	Development of Predictive Tools to Enable Low-emission Ammonia Combustion in Gas Turbine Engines
Investigators	S. Scott Goldsborough Pinaki Pal, Raghu Sivaramakrishnan, Chao Xu

This project comprised three technical components: (a) generation of novel experimental datasets; (b) enhancement of a state-of-the-art detailed kinetic model for ammonia and ammonia/hydrogen blends; and (c) development of a reduced kinetic model to enable high-throughput design simulations. First, we upgraded the laboratory infrastructure to handle the gas blends, which are toxic, corrosive, and contain highly flammable constituents. The detailed kinetic model was substantially updated, incorporating recent theoretical works and published data to improve predictive capability for flame speed calculations. An initial reduced model was derived from the detailed version, and initial parametric tests were performed.

LDRD 2024-0127	Supply Chain Resilience and Decarbonization of Critical Metal Production: Near Room Temperature Leaching and Electrowinning of Critical Metal Oxides
Investigators	Michael J. Dziekan Matthew R. Earlam, Timothy T. Lichtenstein, Daniel C. O'Hanlon

This project established a framework for closed-loop decarbonization of critical metal production via room-temperature electrowinning of critical metal oxides. Critical materials are non-fuel minerals, elements, substances, or materials that have a high risk of supply chain disruption or serve essential functions in energy technologies. Many critical metals are currently produced by carbothermic reduction of their oxides, which involves process carbon, such as metallurgical

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coke, and generates significant amounts of slag. In the first year, zinc metal was electrowon to provide proof-of-concept for the framework to decarbonize critical metal production. Tin was also electrowon in the first year, and in the second year, proof-of-concept decarbonization was demonstrated for other critical metals, including cobalt, bismuth, nickel, and manganese. The cell was also able to electrowin gallium metal.

LDRD 2024-0132	Fast AI-based Aerodynamics Characterization of Novel Wing Shapes for Electrified or Hydrogen Aircraft
Investigators	Katherine Asztalos Nirmit Prabhakar, Francesco Salucci

This project contributed to Argonne’s capabilities in next-generation aircraft design by developing an AI-driven tool that emulates computational fluid dynamics (CFD) to deliver near real-time predictions of aerodynamic performance for novel wing and airfoil configurations. The effort addressed structural and integration challenges posed by emerging propulsion technologies (electric, hybrid, and hydrogen) by enabling the design of wings capable of housing energy storage systems while maintaining aerodynamic efficiency. CFD-trained surrogate models for lift, drag, and moment coefficients were created and integrated into Argonne’s Aeronomie framework, establishing a robust CFD-to-AI workflow that leveraged hybrid computing resources. The successful completion of the project produced unique capabilities, streamlined aircraft design-to-mission simulation.

LDRD 2024-0136	Artificial Intelligence-Powered Data-Driven Rare Events Prediction and Uncertainty Modeling for Interdependent Transportation and Power Systems in Decarbonization
Investigators	Zhi Zhou Vishwas Rao, Jonghwan Kwon, Ismail O. Verbas, Natalia Zunig Garcia

The goal of this project was to develop a computational workflow with a suite of AI and machine learning-based methods to predict rare events and assess their impact on the interdependent electrified transportation and decarbonized power grid. The team conducted case studies to demonstrate the importance of modeling rare-event risks on the interdependencies of transportation and power systems in a decarbonized future, and provided pathways for the Department of Energy and industry to address system risk under potential future extreme events.

The team set up a case study based on northern Illinois transportation, power grid, and weather data. The study illustrated how the workflow identified extreme weather impacts on the interdependence between the grid and transportation infrastructure in both base case and future potential scenarios. The project also explored a set of AI and machine learning methods for representation, extreme event identification, and uncertainty modeling, particularly addressing challenges of multivariate, spatial, and temporal correlation preservation.

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LDRD 2024-0138	Development Towards Artificial Intelligence Enabled Autonomous Coating Manufacturing
Investigators	Yuepeng Zhang Santanu Chaudhuri, Noah H. Paulson, Jie Xu

This project developed a deep machine learning framework to demonstrate artificial intelligence-driven autonomous coating process, which supports United States domestic manufacturing in renewable energy industry. Deliverables included an ensemble of convolutional neural network (CNN) models for automatic coating defect detection and classification, and a machine learning framework that served as the foundation for future multi-parameter, multi-objective decision making in smart coating manufacturing. We also developed a strategic analysis of in-line metrology tools required for autonomous coating manufacturing and a machine learning model to guide ink design and formulation. The models developed in this project can be used for future LLM development for autonomous coating.

LDRD 2024-0149	Electromagnetically Enhanced Atomic Layer Deposition for Use-Inspired Materials for Microelectronics
Investigators	Jessica C. Jones Zachary D. Hood

Use of electrical fields and biasing during atomic layer deposition (ALD) represented a novel approach to directing material properties. Previous work had not distinguished between static biasing of substrates and the presence of electric fields in the reactor. For the first time, this project combined experimental methods with computational modeling to explain the mechanism by which substrate biasing alters the thermodynamics of surfaces. Advanced electron microscopy was used to probe films deposited by ALD and to observe material alteration from electron bombardment in situ in a STEM instrument. New capabilities were developed to apply bias to a sample in situ in an ALD chamber, where in situ conductivity was leveraged as an analytical tool.

LDRD 2024-0151	Exascale Framework for Artificial Intelligence-Enabled Coupled Electro-Thermal Modeling of Three-Dimensional Integrated Devices
Investigators	Pierre T. Darancet Maria K. Chan, Alvaro Vazquez Mayagoitia, Subramanian Sankaranarayanan, Huihuo Zheng

The goal of this project was to leverage state-of-the-art Department of Energy computing facilities to guide the design of specialized Compute-in-Memory (CIM) components capable of complementing current silicon-based technologies for data-intensive applications. Compute-in-Memory components operate based on a distinct set of physical principles from their silicon

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counterparts, making current optimization approaches unable to suggest improved thermal management and compositional strategies.

In this project, we developed and successfully deployed on Aurora (a newly commissioned DOE exascale computational facility) a model of a Compute-in-Memory component based on perovskite nickelates—a promising yet previously unmodeled-at-component-scale materials platform for emerging CIM technologies. Our approach leveraged and thoroughly validated a new neural network force field fully compatible with exascale computer hardware. We demonstrated near-ideal scaling up to 1,000 GPUs, enabling million-atom simulations necessary for CIM component modeling.

LDRD 2024-0155	Developing Self-Driving Laboratory System for Pathway Engineering by Adaptive Lab Evolution
Investigators	Christopher S. Henry Nidhi Gupta, Filipe Wan Liu

The goal of this project was to integrate AI foundational models, mechanistic modeling, and experimental evolution to enable the rational design and optimization of enzymatic reactions and metabolic pathways in microbial systems. We developed a novel framework that coupled AI-guided metabolic modeling with Argonne’s automated adaptive laboratory evolution (ALE) platform, enabling rapid, iterative testing of computational hypotheses. Using this platform, we established a fully automated ALE workflow and demonstrated successful transformation and selection of *Acinetobacter baylyi* ADP1 strains, including enhanced pathways for conversion of phenolic compounds derived from lignin degradation. We further fine-tuned and applied a protein-language AI model to predict beneficial mutations in enzymes involved in methoxylated-aromatic compound processing. In parallel, we constructed a metabolic model of ADP1 that integrated with AI tools to support strain design and automated experiment planning. Together, these advances represent a powerful synthesis of AI and evolutionary principles, establishing a foundation for accelerated enzyme discovery, metabolic pathway engineering, and autonomous experimental design.

LDRD 2024-0156	Climate Action Through Large Language Models (CALLM): A Tool for Analyzing Climate Risk and Building Resilience
Investigators	Tanwi Mallick Joshua D. Bergerson, John K. Hutchison

The goal of this project was to harness advanced large language models to interpret intricate climate data and scientific texts, translating complex information from these sources into straightforward, actionable insights. To expedite the overall Climate Action through Large Language Models (CALLM) methodology development in this project, the team selected a single hazard to pilot CALLM’s development. After reviewing the climate variables delineated in ClimRR and the climate hazards outlined in Community and Infrastructure Adaptation to Climate Change (CIACC), the team selected wildfire as the initial hazard of focus. Initially, the project

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team successfully developed WildfireGPT, establishing the majority of the overall CALLM methodology through this pilot development. This innovative tool leveraged a large language model to interpret complex wildfire projections from ClimRR, scientific literature from CIACC, and additional historical climate event data such as wildfire incidents. By translating these data and information sources into comprehensible narratives, WildfireGPT facilitated informed decision-making for wildfire management and adaptive strategies across various sectors. Then, the project team primarily focused on expanding the developed methodology from a single large language model agent to an optimized multi-agent framework addressing additional climate variables, as well as further methodology development focused on performance evaluation and uncertainty quantification of CALLM performance.

LDRD 2024-0181	The Role of Global and Pacific Ocean Warming on Atmospheric Rivers in the Western United States
Investigators	Brandi L. Gamelin Mustafa Siddik Altinakar, Dimitrios Fytanidis, Vishwas Rao,

This project developed and applied a GPU-accelerated, variable-resolution global climate modeling framework to simulate extreme atmospheric events with high regional fidelity across the Pacific Ocean and U.S. island territories. Using the Simple Cloud-Resolving E3SM Atmosphere Model: SCREAMv1 (currently EAMxx), we implemented a dual-multiple regionally refined mesh (RRM) configuration consisting of a 25 km background grid, approximately 12 km refinement over the Pacific Ocean, and nested ~3 km refinements over the Western US, Hawaii, American Samoa, Guam, and the Northern Mariana Islands.

The RRM SCREAM modeling system was evaluated using multiple extreme-event case studies from 2017, including Hurricane Irma in the Atlantic Ocean and atmospheric rivers in the Pacific Ocean. All model configurations were initialized with 0.25-degree ERA5 reanalysis. Results for Hurricane Irma demonstrated that while low-resolution uniform meshes captured large-scale storm tracks, high-resolution RRM configurations were essential for accurately representing storm intensity, structure, landfall location, and fine-scale radiative and dynamical features, as validated against satellite observations (GOES and MODIS) and HURDAT2 hurricane data. Comparisons between uniform and refined meshes showed substantial improvements in localized wind, pressure, and cloud-radiative signatures when kilometer-scale resolution was applied.

A key outcome of this work was the development of a novel multiple RRM strategy that dramatically reduced computational and storage costs relative to globally uniform high-resolution simulations without sacrificing accuracy. By targeting refinement only where physically necessary, the approach enabled efficient use of leadership-class GPU systems while overcoming practical constraints related to node counts, machine availability, and data movement across heterogeneous HPC environments. This capability supports scalable, high-resolution climate simulations, which can be further accelerated by new AI/ML-based emulators and foundation modeling capabilities introduced in the E3SM modeling system. Overall, this project demonstrated a computationally efficient pathway for next-generation regional climate simulation, advancing the ability to study Pacific-origin extreme events and their impacts on U.S. Island communities.

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LDRD 2024-0197	Advancing Sustainable Bioplastic Packaging Films from Agricultural and Food Waste: Integrating Machine Learning, High-Throughput Experimentation, and Dynamic Chemistry
Investigators	Wei Chen Chaoyi Ba, Jie Xu

This project advanced novel food-packaging materials by converting agri-food waste, primarily pectin-rich streams, into high-performance bioplastic films. By integrating pectin with complementary biopolymers such as starch and chitosan, and applying both chemical and physical modification strategies, we developed biodegradable films with improved mechanical integrity, flexibility, and barrier performance. Our approach leveraged dynamic covalent chemistry, careful selection of reinforcing agents, and multilayer lamination to enhance durability and enable tunable functionality tailored to food-packaging requirements. This project was critical for establishing proof-of-concept bioplastics synthesized directly from food-waste-derived components. These early results demonstrated the feasibility of replacing petroleum-based plastics with reprocessible materials.

Beyond material performance, this work contributed to broader circular-bioeconomy goals by valorizing waste streams into functional materials.

LDRD 2024-0200	Synthesis of Single Crystal Precursors for Sodium-Cathodes Using Novel Segmented Continuous Flow Reactor
Investigators	Ozgenur Kahvecioglu Isik Su Buyuker, Jihyeon Gim, Eungje Lee, Carrie Siu

The project introduced a novel method to synthesize single crystal precursors for lithium-ion and sodium-ion battery cathode active materials using a semi-autonomous segmented continuous-flow reactor (S-CFR) as the technology platform. The S-CFR design enabled isolated micro-mixing reaction media, which eliminated further nucleation and induced the formation of single crystals. Additionally, the segmented flow reactors could be scaled up or down by adjusting the number of reactors connected in series or the flow rates. During the project, the team developed scalable reaction mechanisms for uninterrupted continuous operations and established cost-effective synthetic strategies that eliminated hazardous chemical use.

LDRD 2024-0207	Continuous Quadruple Synthesis Platform for Simultaneous Single-crystal Formation, Lithiation, Doping, and Surface Coating
Investigators	Youngho Shin Seoung-Bum Son

This project developed a continuous quadruple synthesis platform for cobalt-free single-crystal cathode materials, enabling the simultaneous completion of single-crystal formation, lithiation, doping, and surface coating in one step within 10 minutes. During the second portion of our

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project, the focus was on improving the performance of lithium iron phosphate through doping. Additionally, a 30-liter co-precipitation system was successfully installed and operated to evaluate and compare the properties of sodium-ion cathode materials. Reactive spray drying technology was also applied as a process approach to address the low-density problem of sodium-ion cathode materials.

LDRD 2024-0231	Identifying and Characterizing Bioterrorism Agents in Complex Samples
Investigators	Justin C. Podowski James J. Davis, Daniel S. Schabacker

Bacterial pathogens posed serious risks to national security, but identification of pathogens in complex samples is challenging. Traditional laboratory methods for identifying pathogens and determining their source involved generation of cultures, which posed a risk of accidental exposure and required work in high-security Biosafety Level-3 facilities. Advances in DNA sequencing quality and decreasing costs opened up complex DNA sample sequencing as a promising avenue for pathogen identification and characterization. We developed a bioinformatic pipeline to ingest complex DNA sequence samples and determine if select agent pathogens were present, and, if so, performed analyses to enable source tracking of those select agent pathogens. This pipeline was tested using field samples containing *Bacillus anthracis* and validated using mock samples containing *Yersinia pestis* and *Francisella tularensis*.

LDRD 2024-0239	Cooperative Nitrogen Reduction by Heterobimetallic Active Sites on Electron Reservoir Supports
Investigators	David Kaphan Massimiliano Delferro

We received organometallic precursors and chemisorbed them onto lithium titanate. These materials were characterized, and their reactivity toward nitrogen was investigated. However, the persistent Ta-hydrides observed on SiO₂ in literature precedents were not persistent on titania-based materials. We attempted catalytic nitrogen reduction with these materials and also investigated silicon nitride as an alternative approach.

LDRD 2024-0241	Identifying and Characterizing Fluorinated Compounds Relevant to Nuclear Forensics Using Synchrotron Produced X-rays
Investigators	Anthony J. Krzysko John J. Arnish, Jeremy Lantis, Derek R. McLain, Jennifer L. Steeb

Fluorine and fluorinated compounds are an integral part of the nuclear fuel cycle. Collecting and characterizing fluorinated compounds may yield known chemical, physical, and isotopic

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signatures that provide information important to the nuclear forensic community. The purpose of this research was to identify and/or discover key signatures in fluorinated compounds relevant to nuclear forensics using X-ray experiments at the Advanced Photon Source (APS). In the first year, we conducted a foundational scoping study to identify key fluorinated compounds, signatures, and X-ray experiments with the potential to measure and discover novel signatures. The second year focused on resolving all safety concerns at the newly upgraded APS and carrying out EXAFS experiments at the facility. Raman experiments were attempted to provide confirmatory analysis but, due to difficulties with sample containment, were unsuccessful.

LDRD 2024-0243	A Novel Flux-Coupled Cryotronic Switch and Amplifier
Investigators	Tomas Polakovic Juliang Li

The project aimed to develop a superconducting switching device that couples to signal input through magnetic flux via a superconducting pickup loop, enabling new concepts in superconducting classical digital logic and signal processing. We successfully designed and demonstrated magnetic field operation of a three-terminal superconducting switching device, which serves as the building block of the proposed device. The device exhibited timing, stability, and noise characteristics that make it feasible to integrate with other superconducting sensors and microelectronics. We developed and fabricated early prototypes of these switches, achieving the final goal of the project.

LDRD 2024-0246	Develop and Validate an ALARM Platform for Radiation Hardness Characterization of Wide Bandgap Power Electronics
Investigators	Moinuddin Ahmed Patrick M. D. Lurgio, Daniel Santiago-Gonzalez

In this project we developed and validated a platform for in-situ radiation hardness testing of power electronic devices and created a machine learning-based prediction model with 90% accuracy. The outcome of this project will facilitate accelerated measurement of radiation reliability of electronic devices and detectors with increased precision and will enable scaling-up to reduce time of testing, and created machine-learning based modeling to predict systems reliability efficiently for enhancing national security.

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LDRD 2024-0247	Ultra-sensitive Low-stress TES Detectors for Light Dark Matter Searches
Investigators	Gensheng Wang Marharyta Lisovenko

This project aimed to develop an ultra-sensitive, low-stress superconducting Transition-Edge Sensor (TES) detector to address opportunities in light dark matter detection. We successfully fabricated and measured Iridium/Platinum (Ir/Pt) bilayer TES detectors with low transition temperatures and low stress. The detector transition temperature was tuned down to a few tens of milli-Kelvin by adjusting the relative thicknesses of Iridium and Platinum films. The detector's stress was independently tuned to be low by controlling the deposition pressure of the films. We extensively studied the transition temperatures, resistive transition profiles, and thermal conductance of Ir/Pt TESs for fabrication optimization. The Ir/Pt TES developed exhibited a measured energy resolution as low as 60 milli-electron-volts, and its intrinsic background rate due to film stress was reduced by a factor of 50. We also fabricated two types of large-area Athermal Phonon Detectors (APDs), which measure low-energy particles and light that generate phonons in a silicon substrate. One consisted of sensitive Ir/Pt TES sensors and large-area superconducting Aluminum phonon collection fins. The other used Iridium quasiparticle reservoirs connecting Ir/Pt TES sensors and large-area Aluminum phonon collection fins. Experimental data indicated that the latter had controlled thermal conductance, improved sensitivity, and a fast event counting rate. The athermal phonon detector using Ir/Pt TES sensors and Iridium quasiparticle reservoirs represents a technological advancement in TES detector development. These Ir/Pt TES detectors have applications in rare event experiments, including dark matter direct detection, neutrino-less double beta decay searches, and coherent elastic neutrino-nucleus scattering measurements.

LDRD 2024-0254	Imaging Magnonic Signatures for Magnon-Mediated Hybrid Quantum Architectures
Investigators	Joseph P. Heremans Yi Li, Haidan Wen

This project provided rapid demonstrations of new science in the field of hybrid systems and materials science, by building on our strengths in innovative instrumentation, hybrid quantum architectures, fundamental exploration of phonon and magnon coupled systems, and the underlying materials science for developing next-generation heterostructures. This multimodal platform enabled novel and unique capabilities for directly probing magnon transport, as well as for exploring quantum hybrid systems based on magnons and quantum defects. The latter is of particular interest for developing on-chip quantum interconnects. Initial proof-of-concept demonstrations explored magnetic order within solid-state materials.

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LDRD 2024-0260	Operando Nuclear Magnetic Resonance to Realize Silicon Anodes for Sodium-Ion Batteries
Investigators	Baris Key Jordi Cabana-Jimenez

The energy density of lithium-ion batteries has been greatly improved by incorporating silicon into the anode; however, little to no success has been achieved in replicating this phenomenon in sodium-ion batteries (SIBs). This is largely due to the challenges in forming the only possible sodium silicide Zintl phase through electrochemical methods, as well as the slower kinetics of the larger sodium ion. Previous studies have claimed sodiation of amorphous silicon, but the exact mechanisms have not been extensively studied. Nuclear magnetic resonance (NMR) spectroscopy can probe local atomic structure regardless of crystallinity, making it an ideal technique to examine the stages of electrochemical (de)sodiation, if any, in sodium silicides.

We investigated the feasibility of silicon as an anode material for SIBs in two ways: (1) starting from a chemically synthesized model compound to examine the desodiation mechanism and reactivity of the Zintl phase, and (2) conducting electrochemical sodiation tests using a variety of silicon-type materials. The model compound was successfully desodiated electrochemically for the first time, resulting in an amorphous silicate product. However, sodiation of different Si materials and subsequent resodiation of the desodiated model compound were not observed. This is attributed to the barriers in inserting sodium ions into the specific tetrahedral clusters that make up the Zintl phase through solely electrochemical methods. The project identified the main challenges of realizing silicon as an anode material for Na-ion batteries and developed an in-situ NMR methodology for Na-ion batteries at Argonne.

LDRD 2024-0261	Scalable Scientific Machine Learning to Accelerate High-Fidelity Simulations of Extreme Events in Energy Conversion Systems
Investigators	Shivam Barwey

This research developed novel in-situ, physics-informed scientific machine learning frameworks based on scalable geometric deep learning, with a focus on fluid dynamics prediction for power and propulsion applications. Key research successes in the second year included the application of developed methods and continued method development in other areas, such as foundation modeling, to address complex problems relevant to energy systems and scientific foundation modeling. For example, scalable artificial intelligence/machine learning methods developed in the first year were used to model realistic turbulent flow and detonation physics dynamics using variations of the NekRS and Nek5000 solvers, with which the artificial intelligence/machine learning methods were made compatible.

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LDRD 2025-0007	Integrated Analysis Modeling for Electrocatalytic Carbon Conversion to Chemicals
Investigators	Taemin Kim Zachary D. Hood, Haoran Wu

This project developed an integrated analysis model capable of accommodating various electrocatalytic carbon conversion pathways that produce chemicals with more than two carbon atoms, such as ethylene and ethanol. The pathways evaluated with the model included copper-based electrocatalytic carbon dioxide reduction, MXene-based electrocatalytic carbon dioxide reduction, molten carbonate carbon dioxide reduction, and microbial electrosynthesis. The model assessed greenhouse gas emissions, capital expenditure, and operating expenses for envisioned electrocatalytic carbon reduction pathways, using assumed Faradaic efficiency and full cell voltage. This enabled the estimation of anticipated environmental impacts and economic feasibility for experimentalists at different Faradaic efficiencies and cell voltages. The model was built as a Python-based script, leveraging environmental impact datasets from Argonne's R&D GREET model. It incorporated options for different electricity grids and captured carbon dioxide sources to estimate gas emissions for electrocatalytic conversion pathways under varying conditions. For techno-economic modeling, Argonne's CER model served as the basis for capital and operating expenditure calculations. The results showed that gas emissions and capital expenditure for electrocatalytic carbon dioxide reduction pathways decreased with improved Faradaic and energy efficiency.

LDRD 2025-0038	Methods Development for Production of Core Melt Compositions for Reactors Utilizing Accident Tolerant Fuel to Support Safety Testing
Investigators	Mitchell T. Farmer Jeremy R. Licht

This project developed methods for producing molten simulants of a new type of nuclear reactor fuel called accident tolerant fuel (ATF). ATFs are designed with higher melting points and greater oxidation resistance to enhance reactor safety in the event of a loss of coolant accident. Near-term ATF concepts include iron-chromium-aluminum (Fe-Cr-Al) cladding, zirconium alloy cladding coated with chromium, and chromium oxide dopants in uranium oxide fuels. These new ATFs require testing under severe accident conditions involving melting of reactor core materials, such as uranium oxide, zirconium, and chromium. Previously, our research group conducted such testing for conventional fuel types but not for ATF. This project successfully developed several thermite formulations to produce molten ATF simulants, extending Argonne's reactor safety research capabilities and ability to offer testing relevant to current requirements.

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LDRD 2025-0039	Machine Learning-Assisted Imaging of Nuclear Spins
Investigators	Benjamin Pingault Maria K. Chan

Increasing the spatial resolution of nuclear magnetic resonance spectroscopy down to the atomic scale has the potential to significantly impact materials investigation and quantum technologies. Optically active atomic defects can be used to locally probe microscopic environments and build three-dimensional maps of spins in their vicinity. However, extracting such maps from measurement data is tedious and time-consuming, limiting the use of this approach. This project focused on developing machine learning models to automate and accelerate the extraction of relevant information from experimental data to help reconstruct three-dimensional maps of local spin environments, using silicon carbide as a test material. We first developed simulations of interacting spins in silicon carbide to generate spectra for model training and testing. We then designed a machine learning model to identify nuclear spin signatures in spectra and determine their nature and number. After multiple rounds of training and refinement, the model was expanded to extract coupling parameters between spins, which form the basis for building maps and designing control sequences of individual nuclear spins for quantum protocols.

LDRD 2025-0065	Millimeter-wave and Sub-terahertz Sensors for Signature Detection and Observation of Electron Beams
Investigators	Clarence L. Chang Thomas W. Cecil, Philippe R. G. Piot

This project explored the application of technologies developed for cosmological studies at millimeter wavelengths to the characterization of electron beams at accelerators. It developed new superconducting materials that can be further advanced for a broad range of applications and fostered connections between scientists in experimental cosmology and accelerator science. An interesting outcome was the emergence of interest in new concepts for millimeter wave spectrometers, which could have potential uses in both experimental cosmology and accelerator science.

LDRD 2025-0076	Integrating Artificial Intelligence Features into the Assessment of Capabilities in Energy Security Tool in a Secure Laboratory Environment
Investigators	Ashton L. Raffety Darren Chen, Zachary W. Pleasant, Duane R. Verner

This project focused on providing externally facing, large language model-powered tools to stakeholders within a CUI environment. Through collaboration with experts across Argonne, the project team successfully developed a method for integrating AI capabilities into tools and applications in a secure environment. The project also established core practices for developing

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AI back- and front-ends at Argonne, prototyped a knowledge base and API layer, and validated rapid UI workflows using natural language coding.

LDRD 2025-0100	A Multiscale Modeling Framework for Deployment of Negative Emission Technology
Investigators	Beth A. Drewniak Yan Feng, Troy R. Hawkins, Saurajyoti Kar, Doris Oke

Bioenergy has been identified as a critical component of America's energy portfolio to maintain energy independence, security, and resilience. Biomass-based energy technologies are competitive options alongside others such as geothermal and hydro energy. However, modeling frameworks have lacked the capability to analyze the full impact of bioenergy solutions because separate models exist for the life cycle of bioenergy production (Life Cycle Analysis (LCA) Models), socioeconomic scenarios of energy supply and demand, land cover and land use change, and emissions (Socioeconomic Models), and land-atmosphere interactions (Earth System Models). When these models are separated, functional and conceptual mismatches arise between human and environmental models. By coupling these models, we extended the current modeling framework to incorporate feedbacks from and to the LCA models, thereby capturing dynamics between bioenergy and land-atmosphere interactions to identify holistic effects on energy technologies, estimate the effectiveness of bioenergy, reduce uncertainty, and optimize deployment and production.

LDRD 2025-0167	Holistic Machine Learning Autotuning for Massive-Scale Artificial Intelligence for Science
Investigators	Michael Wilkins

To reduce the training cost of massive-scale Artificial Intelligence models for science, we created a novel holistic online auto-tuning approach in this project. The auto-tuner optimized both application parameters (hyperparameters) and system parameters to improve system efficiency while the training workload was running. By tuning application and system configurations together online, we achieved a new state of the art for AI training efficiency and enabled massive-scale AI models for science. ACCLAiM used active learning to intelligently train a machine learning (ML) model to predict performance with various parameter values. We validated our strategy for large-scale autotuning by developing a full prototype of the ACCLAiM design and studied its usefulness on Aurora. We also developed a novel parallel data collection strategy that generalizes to all modern high-performance computing (HPC) systems.

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LDRD 2025-0174	Model Evaluation and Future Projections of Argonne’s Dynamically Downscaled Data Archive version 2 (ADDA2): North Atlantic Tropical Cyclones
Investigators	Chunyong Jung Lara N. Tobias-Tarsh

Tropical cyclones (TCs) are among the most destructive weather systems globally, yet accurately simulating them has remained a major challenge in climate modeling due to limitations in traditional convection parameterization schemes. This project advanced the state of the science by applying convection-permitting (CP) regional climate modeling, which explicitly resolved deep convective processes rather than parameterizing them, to improve the representation of TCs and their underlying physical mechanisms. Building on the Argonne Downscaled Data Archive Version 2 (ADDA V2)—a 4 km resolution dataset spanning North America and the North Atlantic basin—our team conducted a 20-year CP simulation forced by ERA5 reanalysis to evaluate TC climatology, structure, and variability.

Our analyses showed that ADDA V2’s simulation of TC frequency and intensity distributions exhibited significantly stronger statistical agreement with observations than the ERA5 reanalysis. Over the 20-year period from 2001 to 2020, the model reproduced annual TC counts closely matching observed values and successfully resolved Category 3 and higher storms that were absent in ERA5. These results challenge the conventional reliance on ERA5 as a high-resolution reference for TC climatology. In addition, ADDA V2 demonstrated strong skill in capturing realistic inner-core structures and small-scale convective processes, as shown through composite analyses and a detailed case study of Hurricane Isabel (2003). Together, these findings highlight the added value of CP modeling for representing TC dynamics, particularly in data-sparse regions such as the Caribbean and Central America, and for identifying physically consistent predictors of TC intensity such as minimum sea level pressure.

The scientific outcomes of this project provide a foundation for enhanced regional climate risk assessments and support resilience planning for coastal infrastructure systems vulnerable to TCs. The resulting datasets and methodologies have already supported follow-on analyses of future TC changes and serve as an important resource for the broader research community. In particular, ADDA V2 provides a robust dataset for training and validating artificial intelligence and machine learning models designed to detect, classify, and predict TC behavior.

LDRD 2025-0175	Efficient High-Resolution Emulator for the Energy Exascale Earth System Model
Investigators	Veerabhadra R. Kotamarthi

This project supported the porting and operation of DOE high-resolution climate models to DOE leadership computing facilities. We developed model simulations for creating an emulator, with a focus on aerosols in the model and capturing their thermodynamics. The results from the project are useful for fine-tuning the AERIS AI Foundation Model for seasonal-to-subseasonal forecasts.

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LDRD 2025-0176	Scaling Regional Climate Models to Aurora
Investigators	Veerabhadra R. Kotamarthi Akash Awasthi, Anshu Dubey

Frontier research questions in climate science and weather forecasting require high-fidelity spatial models that resolve most known physics and minimize sub-grid scale parameterizations. A critical parameterization in these models is the representation of clouds. Models that have spatial resolution 1 kilometer or less have been shown to be capable of resolve clouds without the need for a sub grid scale cloud model. However, performing simulations at these resolutions are not feasible in the existing central processing unit (CPU) based models. We produced a version of the regional climate model that could scale to Aurora and its accelerated GPU architecture. This enabled us to perform large-scale (North American continental) simulations at cloud-resolving resolutions. We developed an LLM-based workflow for making legacy Fortran software compatible with and operable alongside C/C++ code designed for GPU infrastructure.

LDRD 2025-0177	Developing Analytical Methods to Combine Statistically and Dynamically Downscaled Climate Datasets for use in Decision Science and Resilience Applications
Investigators	Jordan R. Branham Chunyong Jung

This project developed improved methodologies for accounting for regional patterns in the development of downscaled 4km historical and future weather data. These methods were used to create more reliable and actionable outputs for a wide range of constituents, including utilities and power system operators, emergency managers, planners, and other decision-makers. This was a critical step not only in the development of the 4km models, but also in refining key metrics for evaluating model performance and developing methodologies for better creating ensembles of model outputs.

LDRD 2025-0189	Enabling Climate Resilience with Advanced Computational Methods
Investigators	Carmella A. Burdi Vijay P. Ramalingam

This project successfully delivered a minimum viable product (MVP) that demonstrated a scalable, high-performance computational pipeline capable of querying Argonne's ADDA v1 and v2 climate model datasets. The project proved, for the first time at Argonne, that large multidimensional NetCDF climate datasets could be queried, processed, and returned to users at scale using high-performance computing resources. The MVP allowed users to request customized climate variables, automatically extract and calculate relevant data, and return results through automated charts and tables, validating the feasibility of on-demand climate-impact generation. Throughout development, the team identified key insights regarding dataset

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organization, storage constraints, and integration workflows, which will guide future climate model archiving and pipeline design. This project established the core architecture needed to support on-demand climate impact computation, enable users to explore more specialized variables, and significantly expand ClimRR's future capabilities.

LDRD 2025-0192	Fully Coherent X-rays Using Photoinjected Electron Bunches at Argonne Photon Source
Investigators	Philippe R. G. Piot Ryan R. Lindberg, Kent P. Wootton

This project successfully advanced two complementary fronts toward fully coherent X-ray generation at the Advanced Photon Source (APS).

On the source side, it leveraged a new high-reliability laser system to produce brighter, photoinjected electron bunches for the APS complex and the Linux Extension Area. Beam-dynamics modeling was completed and demonstrated that the required beam brightness was attainable; these results directly informed the design of the laser-shaping crystals. In parallel, a single-shot longitudinal phase-space diagnostic in the APS linac was upgraded, with initial experimental results reported at a conference.

On the X-ray side, the project developed a high-fidelity, cavity-based storage-ring free-electron laser (FEL) model tailored to APS, coupling ELEGANT beam dynamics with FEL simulation tools and revisiting earlier concepts proposed for other storage rings in the specific context of APS. This integrated modeling capability provided a critical foundation for assessing cavity-based FEL options at APS and for future experimental demonstrations of longitudinally coherent X-ray generation.

LDRD 2025-0196	Redox-Mediated Electrodialysis for Efficient Enrichment and Purification of Germanium and Gallium Materials
Investigators	Chaoyi Ba Wei Chen

This project aimed to develop a cost-effective, energy-efficient, and modular redox-mediated electrodialysis method for the selective recovery of value-added compounds, such as germanium and gallium, from electronic waste and acid mine drainage. The approach involved three key steps: 1) designing size-exclusion nanofiltration membranes using natural polymers like alginate and carboxylated cellulose for the efficient separation of germanium and gallium from dilute feed streams; 2) developing durable, conductive polymeric anion exchange membranes for the selective removal of anions; and 3) integrating these membranes into a four-chamber redox-flow electrodialysis cell to perform separations under low electrical potential.

The team successfully fabricated ion-selective nanofiltration membranes by casting a sodium alginate solution onto a porous support membrane, followed by cross-linking. Three types of anion exchange membranes were developed, all demonstrating high anion conductivity.

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LDRD 2025-0197	Sustainable Aviation Fuels from Tandem Bio-Thermo Catalytic Upgrading of Waste Foods
Investigators	Magali S. Ferrandon Haoran Wu

Conversion of biomass into commodity fuels required highly efficient catalysts. In particular, the ketonization of fermented waste biomass to produce synthetic aviation fuels necessitated highly active catalysts. Preliminary catalyst screening of nine metal oxides supported on five high surface area oxides showed that transition-doped metals supported on MgO achieved high yields for the ketonization of heptanoic acid (used as a benchmark compound) into tridecanone, which falls within the carbon range of interest for producing Synthetic Aviation Fuels (SAFs). Fe/MgO and Mn/MgO demonstrated over 99% yield at a low temperature of 300 °C in batch mode (6 h), as confirmed by gas chromatography and NMR. Fe/MgO, Mn/MgO catalysts, and MgO support were subsequently tested for continuous ketonization using heptanoic acid (0.5 mL/hr for 200 mg catalyst). The ketonization of waste-derived medium-chain organic acids (from fermented cheese whey) was also conducted in the continuous flow reactor using Mn/MgO at temperatures between 250 °C and 400 °C, achieving full conversion at 250 °C. The catalysts were characterized by High-Resolution Transmission Electron Microscopy (HRTEM), X-ray Absorption Spectroscopy (XAFS), X-Ray Photoelectron Spectroscopy (XPS), X-Ray Diffraction (XRD), H₂-Temperature-Programmed Reduction (H₂-TPR), and Thermogravimetric Analyses (TGA). HRTEM revealed the presence of single Mn and Fe atoms on MgO after calcination at 300 °C and following the ketonization reaction.

LDRD 2025-0200	Electrochemical Adsorbent-Wafer Separation Technology for Removal of Short- and Long-Chain Per- and Polyfluoroalkyl Substances (PFAS) From Drinking and Groundwater with in-situ Adsorbent Regeneration
Investigators	YuPo Lin Pietro Papa Lopes

This project aimed to demonstrate the technical feasibility of the electrochemical adsorbent-wafer separation technology (EAST) for cost-effective removal and concentration of both long- and short-chain PFAS from drinking water and groundwater. The project benchmarked EAST performance at exploratory scale using surrogate PFAS compounds and developed analytical protocols capable of handling diverse aqueous chemical backgrounds. Building upon prior proof-of-concept results showing 99.75% removal of perfluorooctanoic acid (PFOA), EAST provided simultaneous electrochemical adsorption and desorption to selectively extract target ions and recover them in a small-volume concentrate stream. Compared with existing technologies such as granular activated carbon, ion exchange, and membrane filtration, EAST offered key advantages, including high removal efficiency for PFAS of varying chain lengths, in-situ adsorbent regeneration without waste-generating ex-situ treatment, and a minimal PFAS concentrate stream representing less than 1% of treated water. EAST has the potential to become a unique national-laboratory capability for PFAS separation, concentration, and eventual destruction technology development. The combination of emerging electrochemical

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treatment methods and validated ultra-trace PFAS analytical protocols enhances DOE's ability to address PFAS contamination challenges affecting industrial sectors and household drinking water.

LDRD 2025-0201	Electrically Modulated Selective Adsorption of Critical Minerals, Nickel and Cobalt
Investigators	Ashley R. Bielinski Jeffrey W. Elam

Nickel and cobalt have been identified as critical minerals for the United States, largely due to their growing use in batteries, electrolyzers, and fuel cells for applications such as electric vehicles, energy conversion, and energy storage. Recycling or reclaiming nickel and cobalt from waste streams is one approach to maintaining these minerals in the circular economy, but selective separation of metal ions remains challenging. Vapor-phase functionalization has proven effective in creating adsorbents capable of removing metal ions from dilute aqueous solutions. In this project, we developed high surface area conductive electrodes that were stable across a range of pH values and applied electrical potentials. We then functionalized the surfaces of these electrodes using atomic layer deposition and vapor phase grafting of thiol-functionalized silane. We hypothesized that applying a variable electrical potential to these surfaces would provide an additional means to tune the selective adsorption and desorption of nickel and cobalt ions at neutral pH by altering the local electrostatic environment, thereby promoting or inhibiting deprotonation of the thiol group. Our mechanistic investigation showed that previously reported pH-swing plus filtration methods remove certain elements, including cobalt, via precipitation rather than true surface adsorption. We quantified this effect and defined a narrower pH window needed to keep nickel and cobalt soluble, which is essential for mitigating fouling risk of high surface area porous electrodes and membranes and enabling the targeted electrochemical strategy. While applied potential was not found to have a significant impact on selective adsorption in the tested electrochemical systems, the synthesis procedures and mechanistic insights developed during this project provide a strong foundation for future development of electrically-modulated surface adsorption for critical mineral recovery.

LDRD 2025-0204	Insights into Electrochemical Methane Oxidation on Medium Entropy Oxides
Investigators	Gengnan Li Peter Zapol

The low-temperature electrochemical oxidation of methane using water offered an economically viable path for methane valorization under mild conditions, compared to conventional thermocatalytic processes that require high temperature and pressure. However, a lack of fundamental understanding of the active sites and reaction mechanisms has limited the rational design of new materials with improved activity and selectivity. This gap highlighted the need for a systematic investigation into how interface parameters influence performance, enabling the establishment of design principles for methane conversion. Elucidating the active site structure-

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performance relationship was critical to developing mechanistic insights that accelerate the discovery of materials with enhanced performance.

We evaluated a series of transition metal oxides and their mixtures through a combination of experimental studies and theoretical calculations. Compared to pristine oxides, medium entropy oxide with multiple metallic elements exhibited significantly enhanced performance for the electrochemical conversion of methane into valuable oxygenates, such as methanol and ethanol. Through comprehensive structural characterization, we identified the active site structures responsible for the conversion, which provided guidance for theoretical modeling of the active sites. Reactions were influenced by several factors, including methane adsorption and activation, surface intermediate formation, and oxygenate desorption. These factors collectively determined the competition among direct methane oxidation, oxygen evolution reaction, and overoxidation of the desired products. Density functional theory (DFT) calculations revealed how different transition metals contributed to the activation of the C-H bond in methane and the O-H bond in water, thereby modulating reaction pathways and governing both activity and selectivity.

These results provide a framework for optimizing electrochemical methane oxidation over transition metal oxides through controlled site distribution and composition. This approach could significantly accelerate the development of efficient electrocatalysts and energy-efficient systems for methane conversion.

LDRD 2025-0206	Design Principles for Porous Polymers as Fluoropolymer Alternatives
Investigators	Kevin Hickey Samuel B. Hunt

The purpose of this project was to develop design criteria for replacing fluoropolymers as electrical insulators with polymers of intrinsic microporosity (PIM). This was necessary because PFAS feedstocks associated with fluoropolymer manufacturing have become increasingly susceptible to litigation, presenting a significant risk to the continued production of electrical insulators. PIM materials are a new class of polymers that leverage void space within the polymer matrix to generate ideal dielectric properties, offering potential to replace fluoropolymers as insulators. Specifically, this work combined polymer synthesis and characterization with modeling efforts to develop guidelines for how these materials can be developed for this purpose.

LDRD 2025-0212	Recovery of Lithium from Wastewater of Battery Recycling Processes Using Solvent Extraction Method
Investigators	FNU Kurniawan Ana Belen Cuev Sola

This project investigated solvent extraction of lithium from complex battery-recycling wastewaters to advance recovery pathways and strengthen lithium supply chains. We

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performed lithium solvent extraction on various types of battery recycling wastewaters containing different chemistries, such as carbonate, hexafluorophosphate, sulfate, and nitrate. We found that lithium solvent extraction was highly affected by the chemistry of the battery recycling wastewaters; some wastewaters did not present any issues, but carbonate-rich wastewaters resulted in turbid raffinate after extraction, necessitating the addition of phase modifiers. Process variables, including extractant concentration, addition of phase modifiers, contact time, initial pH, and aqueous-to-organic phase ratio, were optimized. The potential for lithium enrichment was approached via optimization of lithium stripping. We confirmed the results using advanced methods such as nuclear magnetic resonance (NMR), Raman, and Fourier transform infrared (FTIR) spectroscopy. The selected extractants also showed high recyclability, reducing chemical consumption during the process. Additionally, we advanced the project by utilizing other recovery methods, including ion-exchange and electrodialysis, enabling direct comparison of the effectiveness of each method for lithium recovery from battery recycling wastewaters.

LDRD 2025-0219	High Throughput Screening via Additive Manufacturing of Tungsten-based Alloys for Fusion Applications
Investigators	Srinivas Aditya Mantri

Tungsten (W) and its alloys possess several advantageous properties, including an exceptionally high melting temperature, high thermal conductivity, and strong resistance to radiation damage, which make them prime candidates for demanding applications such as plasma-facing components in fusion reactors. However, these same properties also present substantial challenges for processing W using conventional and many advanced manufacturing techniques. This project evaluated the feasibility of fabricating tungsten components for fusion applications using laser-based additive manufacturing. The initial plan considered the use of directed energy deposition (DED) to tailor alloy compositions; however, theoretical calculations and energy-density estimates indicated that the laser power required to melt tungsten and its alloys far exceeded the capabilities of the BEAM DED system. Therefore, no experimental DED trials were conducted, and the effort was redirected toward laser powder bed fusion (LPBF) using a Renishaw system. To manage material consumption, the reduced build-volume mode was employed for all builds. Initial fabrication trials focused on pure tungsten, printed across a wide range of process parameters, including variations in laser power and scan speed. All builds were completed without major process interruptions such as delamination or warping, indicating good powder spreading and general process stability. However, post-build examination consistently revealed extensive cracking throughout the samples. The cracks typically propagated along grain boundaries and exhibited a network-like pattern, suggesting thermally driven solidification cracking. Importantly, the severity and density of cracking remained high across all tested parameter sets, indicating that process-parameter adjustments alone were insufficient to mitigate defect formation. To investigate whether alloying could reduce tungsten's cracking susceptibility, additional builds were performed with three alloy compositions: W-10Mo, W-10Fe, and W-10Cr (all compositions in wt.%). While each alloy produced fully built samples with surface quality similar to that of pure W, all three also exhibited pervasive internal cracking. Among the tested alloys, W-10Fe showed the highest crack density,

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whereas W-10Mo and W-10Cr displayed slightly reduced but still significant cracking. Microstructural observations suggested that the addition of these alloying elements did not sufficiently reduce thermal gradients or improve solidification behavior to prevent crack formation. Based on these experimental results and supporting evidence from existing literature, we conclude that successful fabrication of crack-free, high-density W and W-based alloys via LPBF will likely require substantially higher laser power (>600 W) to provide adequate energy input, along with a heated build platform capable of reaching temperatures above 800 °C to reduce thermal stresses during solidification. These capabilities exceed the limits of the current LPBF system and will be essential for future efforts aiming to process tungsten and tungsten alloys additively.

LDRD 2025-0235	Towards Multimodal Artificial Intelligence Foundation Modeling of Energy Systems
Investigators	Pinaki Pal Ibrahim Jarrah, Ashwini Karmarkar, Kiran Kumar Yalamanchi

We developed a unified transformer-based foundation modeling framework for spatiotemporal flow prediction in multimodal datasets. The models employed a hierarchical Vision Transformer (Swin-UNet) architecture that processed planar slices and integrated projections in a consistent manner. The architecture was conditioned on auxiliary tokens encoding the data modality and time increment, enabling two complementary tasks: (1) temporal rollout, where models autoregressively predicted the flow state at future times; and (2) feature transformation, where models inferred unobserved fields or viewpoints from the current state. We trained separate models sharing this common architecture on in-house 3D Computational Fluid Dynamics (CFD) simulations of an argon jet in nitrogen, covering multiple resolutions, turbulence models, and gas laws, to expose them to diverse physics and data types. The resulting multimodal models learned to generalize across resolutions and modalities, accurately forecasting the flow evolution and reconstructing missing field information from limited views. This work demonstrated how large transformer-based models can be adapted to advance predictive modeling in energy-relevant fluid systems.

LDRD 2025-0240	Characterizing Real-time Electric Vehicle Impacts: Integrated Transportation and Grid Modeling under Extreme Weather
Investigators	Yantao Huang Siyuan Wang

This project focused on integrating transportation and power distribution grid models to improve urban resilience under extreme weather conditions, particularly with the rise of electric vehicle (EV) adoption. Extreme weather strained both systems, requiring real-time coordination to optimize grid emergency operations and traffic flow. The dynamic features from model integrations helped minimize disruptions, improve recovery, and optimize EV resource use for a more resilient and sustainable infrastructure.

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An emergent operations model for the urban power grid was developed using the Austin-area synthetic test case. This model captured grid behavior under disruptive conditions, enabling detailed analysis of extreme weather impacts. The POLARIS model was enhanced to evaluate non-recurring delays, road closures, and congestion, while expanding EV charging behavior to reflect grid capabilities. A comprehensive integration of the Austin synthetic power grid test case with the POLARIS transportation network established a benchmark co-simulation dataset for the region.

Results showed that derating and disruption of power plants during extreme winter storms led to unmet load in local power stations. EV charging station availability was strongly affected by power outages across the grid network. As outages propagated through the city's power system, many stations operated at reduced capacity, with impacts varying by location. These spatial and temporal disruption patterns increased electric-vehicle miles traveled by up to 30%. Network congestion was moderately impacted by the re-routing of EV charging demand, compared to more delays from road work disruptions.

LDRD 2025-0241	Real-Time Power System Co-Simulation Platform with Power-Hardware-in-the-Loop (PHIL) for Grid Edge Algorithms Reliability and Performance Testing
Investigators	Siby J. Plathottam Sonam Rajendra Kharade

The project focused on developing a real-time co-simulation platform for testing electric power grid algorithms and grid-edge devices using Argonne's Opal-RT real-time simulator and Power Hardware-in-the-Loop (PHIL). In this project, we developed and integrated a real-time transmission system model, a real-time distribution system model, and an inverter-based distributed energy asset hardware to create a testbed. This work involved establishing a digital and electrical interface between the software simulation and the hardware connected to the simulation using the Ideal Transformer method. We also created a workflow that allowed researchers to deploy grid algorithms on edge computing nodes seamlessly and to evaluate the algorithms' performance and reliability on data streamed in real time from the testbed. Using the platform, we tested algorithms for applications including residential solar inverter characterization, harmonics analysis, cyber penetration testing, congestion management, and dynamic state estimation. The platform helped bridge the gap between simulation and the real world and provided a verification stage before in-field trials.

LDRD 2025-0243	Developing a Plasma-Electrified Continuous Flow Process to Rapidly and Scalable Manufacture Ultra-Small Metallic Nanoparticles
Investigators	Jie Li Qiang Dai, Jessica D. Macholz, Pengxi Zhu

This project investigated an efficient plasma-based process technology for scaling up the production of nanomaterials. Plasma-based synthesis took advantage of rapid heating and

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cooling within the plasma-liquid system for small nanoparticle synthesis, as well as ultrafast electron/thermal dual heating. These factors contributed to exponentially accelerated chemical kinetics and enhanced energy efficiency. The project accomplished the following: 1) Assembled and tested a novel continuous flow plasma reactor system by integrating a high-voltage pulsed plasma generator, a cylindrical gas source and liquid pumping system, and a new continuous circulating liquid-fluidized reactor; 2) Conducted various flow synthesis experiments in both aqueous and organic solutions to synthesize Pt and PtNi metal and alloy nanoparticles; 3) Characterized the synthesized nanoparticles using DLS, XRD, and SEM/TEM methods. The results showed that 45 nm PtNi nanoparticles were synthesized in aqueous solution, while 13 nm PtNi nanoparticles were synthesized in ethylene glycol solvent within an hour. It was concluded that the proposed plasma-assisted continuous flow reactor can be used to upscale the synthesis of high-quality PtNi nanoparticles.

LDRD 2025-0247	Resiliency of Transportation Supply Chains
Investigators	Christopher P. Kolodziej Erna L. Grelle

This project developed a framework for lifecycle resiliency assessment of transportation energies and technologies using Probabilistic Risk Assessment (PRA). The project conducted risk identification and established a framework for PRA through Dynamic Fault Tree Analysis (FTA) to quantify the resiliency of US shipbuilding.

LDRD 2025-0248	Thermal Plasma Processing Route for Recovery of Critical Materials from Industrial Wastes
Investigators	Rakesh R. Kamath Tianchen Hu

The goal of this project was to recover valuable metallic materials, such as nickel, copper, and iron, from industrial wasteforms using hydrogen plasma reduction. Hydrogen plasma reduction was chosen due to several key advantages over current practices: (i) thermal plasma is an electrified heat source, (ii) it is a reagent-free process, reducing chemical waste, and (iii) ionic species in the plasma state increase the reaction rate. During the project, a model iron oxide was successfully reduced to iron metal using hydrogen plasma. The reduced product was characterized using scanning electron microscopy and x-ray diffraction to understand the kinetics of the reduction reaction as a function of plasma residence time.

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LDRD 2025-0253	Estimating the Scale of Carbon Conversion in Physical Products
Investigators	Matthew E. Riddle Braeton J. Smith

This project conducted analysis to understand and quantify the use of carbon in physical products across the global economy. The analysis was completed, and we generated figures showing flows of materials under business-as-usual, reasonably achievable, and maximum possible scenarios based on current economic needs, as well as an analysis of other factors that could limit adoption, such as energy requirements.

LDRD 2025-0259	Advancing Methane Quantification: A High-Fidelity Simulation Framework for Modeling Methane Plumes Under Various Atmospheric Conditions
Investigators	Joohan Kim

Traditional methane monitoring techniques, which require flux inversion methods, are highly sensitive to weather conditions and can lead to errors when inaccurate inputs are used. In contrast, high-fidelity computational fluid dynamics (CFD) simulations generate detailed surrogate images of methane plumes to train machine-learning (ML) models, enhancing the accuracy of aerial data interpretation. This project developed a first-of-its-kind, high-fidelity CFD framework to model methane plumes under a range of atmospheric conditions. We used NekRS—Argonne’s GPU-accelerated CFD code—to run the simulations. We built a model that simulated methane leaked from a single point source in a horizontal wind, capturing the evolution of methane plume dispersion in the atmosphere. We identified and resolved critical numerical setup issues, including boundary and initial conditions, grid configuration, source characterization, and numerical schemes.

LDRD 2025-0304	Towards Portable Laser Desorption Postionization Mass Spectrometry Utilizing Microchip Laser Pulses
Investigators	Jason M. Gross David J. Bettinardi, Nicholas J. Condon

A 355 nanometer, 1.5 nanosecond, up to 1 kilohertz microchip laser system was tested to produce ablation spots and post-ionize material within a plasma plume. A 30 microjoule pulse energy microchip laser successfully ablated all samples: 6601 aluminum, 316 and 304 stainless steel, and molybdenum metal. Visible ablation craters were observed on all samples, and the stainless-steel samples exhibited color changes in the resolidified iron, indicating ionization with the 355 nanometer pulses during ablation. Additionally, when used to intercept a plasma plume of cesium carbonate generated with a separate laser system, the microchip laser pulses produced a cesium ion emission signal that was otherwise not observed. With these experiments completed, the microchip laser was successfully verified for readiness to be integrated into the front end of a mass spectrometer system as the ion source.

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LDRD 2025-0305	Investigating Benefits of Tight Integration of Nuclear and Datacenters
Investigators	Nicolas E. Stauff Benjamin A. Lindley

This project resulted in the development of a unique modeling framework to assess the efficiency of nuclear-powered datacenters, with a particular focus on various types of absorption chillers. Preliminary results indicated potentially significant efficiency gains—ranging from 5% to 15% higher IT load, depending on nuclear reactor technologies—and identified several novel coupled configurations.

LDRD 2025-0307	Completing a Forensic Examination of the Chicago Pile
Investigators	Michael A. Brown John J. Arnish, Derek R. McLain, Shayan Shahbazi

The CP-1 experiment, conducted in 1942, marked the conception of controlled nuclear criticality and the dawn of the nuclear age. The original pile had an immeasurable impact on global nuclear sciences, leading to CP-2, CP-3, CP-5, other seminal research reactors, Argonne National Laboratory, plutonium production, naval reactors, and ultimately commercial nuclear power plants. The commemorative piece of CP-1 studied here was examined using radiochemical methods and fuel depletion models to determine more information about the development and operations of CP-1 and CP-2. The results corroborated and expanded historical knowledge of Fermi's CP-1 experiment within the Manhattan Project. Finally, the experimental results led to a computational reconstruction of the Chicago Pile using Argonne supercomputers. This simulated reactor allowed us to determine that this particular fuel assembly was located on the outskirts of CP-2 in the 'removable stringer' sections.

LDRD 2025-0308	Leveraging Large Language Model-Based Agents for Automated Information Gathering in Nonproliferation Research
Investigators	Michael A. Jaynes Benjamin A. Blakely

This project determined whether agent-based Large Language Models (LLMs) could successfully accomplish complex data collection tasks, primarily focused on web scraping. We built on our experience writing applications to scrape multiple online marketplaces for nonproliferation data, which required custom code to parse the content of each specific website. We successfully created a group chat of LLM agents, including one to build a scraping plan, another to validate the settings of the plan, and another to scrape each website generated by the planning agent. An important outcome of our project was that while these models are capable of effectively generating a list of websites to scrape in response to a user's request, agent-based LLMs still struggle to interact with live websites and smoothly extract data from them. Our research provided valuable insights into interacting with both local and API-based

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LLMs and how they can be assigned roles as part of a group chat to break down a complex task for better completion, something with broad applicability to many potential sponsor tasks, even if web scraping continues to pose considerable difficulty.

LDRD 2025-0309	Artificial Intelligence/Machine Learning-based Pebble Power Reconstruction for Pebble-bed Reactor Analysis
Investigators	Seoyoon Jeon

This project aimed to develop an artificial intelligence (AI) and machine learning (ML) based framework to estimate individual pebble neutron fluxes and power distributions from porous-media solutions for pebble bed reactor analysis. A critical concern in core design was ensuring that the power of each pebble did not exceed a temperature limit, making accurate predictions of individual pebble power essential. The developed framework enabled such predictions without requiring computationally expensive and impractical high-fidelity calculations that explicitly model all individual pebbles.

To complement the conventional porous-media approach, pebble power reconstruction was explored, as detailed heterogeneous geometry calculations are computationally expensive. The random distribution of pebble fuels within the core challenged the application of conventional pin power reconstruction methods. To address this, we introduced a machine learning approach based on the Transformer model, comprising Encoder and Decoder layers, to predict flux and power form functions for reconstructing individual pebble neutron fluxes and powers. The homogeneous neutron flux distribution within each spectral zone was obtained from finite element solutions of global diffusion or transport calculations using the deterministic neutron transport code Griffin.

Verification tests demonstrated that the trained Transformer model accurately predicted power form functions over a range of conditions, including variations in pebble enrichment, location, type, spectral zone size, and burnup. In particular, verification using a three-dimensional pebble bed reactor benchmark with burned pebbles showed good agreement in heterogeneous pebble power distributions with reference solutions produced by the Serpent Monte Carlo code employing an explicit heterogeneous model. These results highlighted the potential of applying conventional pin power reconstruction approaches, combined with AI/ML techniques, to pebble bed reactor cores with randomly distributed pebbles.

LDRD 2025-0310	Streamlining Artificial Intelligence Integration: A Rapid Deployment Template for Sponsor-Driven Decision Support Tools
Investigators	Michael R. Alexander Parfait Ugizinshuti Gasana, John K. Hutchison

The Streamlining Artificial Intelligence Integration project developed a complete, operational pipeline that enabled Decision Infrastructure Sciences teams to rapidly deploy artificial intelligence-enabled decision support tools for sponsors. The team built a modular end-to-end

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system with five integrated components: automated data ingestion, multi-database backend architecture, artificial intelligence model integration across multiple platforms, Retrieval Augmented Generation for custom knowledge bases, and automated research reporting capabilities. This framework reduced artificial intelligence tool development time from months to weeks, allowing researchers without artificial intelligence expertise to deploy sophisticated applications. The pipeline became operational and supported document analysis, interactive research tools for infrastructure and climate planning, and multi-model artificial intelligence comparisons. This work positioned the division with a competitive advantage in artificial intelligence-enabled projects and enabled early sponsor engagement in solution co-development.

LDRD 2025-0311	Liquid-Liquid Extraction in Molten Liquids for Critical Element Recycling
Investigators	Timothy T. Lichtenstein Anna Servis

The differential distribution of metals between immiscible high-temperature molten salt phases was used to recover critical elements from secondary resources such as mining waste or used nuclear fuel. In this project, we measured fundamental distribution coefficients for rare earth elements and battery cathode materials in the immiscible lithium chloride-potassium chloroaluminate and lithium chloride-potassium iron chloride systems. We found that these salt systems chemically chlorinated oxide materials such as neodymium oxide, and that the resultant chlorides partitioned between phases, enabling efficient recovery by electrolysis. These results suggest that novel processes incorporating chemical digestion, liquid-liquid extraction, and electrolysis can be developed to recover critical materials.

LDRD 2025-0313	Lithium Compound Background Research
Investigators	Derek R. McLain

Project final report is complete.

LDRD 2025-0314	Leveraging Large Language Models for Enhancing Nuclear Safeguards Knowledge Transfer
Investigators	Scott F. Parent Benjamin A. Blakely, Marianne N. Fisher, Douglas E. Johnson, Heather A. Seger

A multidisciplinary team successfully leveraged advanced AI technologies to address critical knowledge transfer challenges in the nuclear safeguards domain. By integrating secure large language models (LLMs) with instructional design principles, the project automated the creation

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of modular e-learning courses from curated document sets within the Safeguards Knowledge Repository (SKR). This innovative approach enabled the rapid generation of learning objectives and instructional content, significantly reduced manual effort, and maintained high-quality educational outcomes. The initiative established a foundation for preserving institutional memory during workforce transitions and enhancing training efficiency for the U.S. National Nuclear Security Administration (NNSA). Through a structured workflow that combined AI acceleration with expert oversight, the team demonstrated the potential of AI-assisted course generation to strengthen the safeguards workforce and advance national security priorities.

LDRD 2025-0320	Exploiting Graphics Processing Units for Agent-based Simulation
Investigators	Jonathan Ozik Nicholson T. Collier, Charles M. Macal, Eric R. Tatara

Supercomputing resources have achieved new levels of computing power by exploiting the concurrency of GPUs and other accelerators, and this trend shows no sign of slowing. In this work, we advanced the ability of large-scale agent-based modeling (ABM) to exploit the massive concurrency made available through current and next-generation high-performance computing resources. Leveraging our group's extensive experience in developing the Repast toolkit and applying it across domains, we developed broadly applicable, GPU-enabled ABM capabilities, enabling faster and more detailed simulations. This enhancement will benefit current and future ABM projects at Argonne and expand Argonne's reputation in ABM innovation.

We demonstrated a 70x throughput per node improvement on a schedule-based, city-scale ABM, and achieved performance parity or improvement over existing state-of-the-art GPU ABM frameworks for single GPU performance on a 3D continuous space benchmark model. We have begun incorporating these GPU performance improvements into our Repast4Py User Guide as use cases and are developing streamlined methods for enabling GPU acceleration for our broad user base.

LDRD 2025-0328	Mapping Occupations and Skills Across Industries and Counties (Project MOSAIC)
Investigators	Iain R. Hyde Parfait Ugizinshuti Gasana, Gregory Guibert, Alison Peoples, Braeton J. Smith

The Mapping Occupations and Skills Across Industries and Counties (MOSAIC) model addressed a critical data gap by providing localized insights into the composition of the workforce. MOSAIC used a statistically rigorous Bayesian hierarchical multinomial-logit methodology to generate employment-by-occupation estimates for approximately 850 different occupations for every county in the United States. In parallel, the model mapped North American Industry Classification Codes (NAICS) to Standard Occupation Codes (SOC) to predict the relationship between industries and their required occupations.

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MOSAIC leveraged employment, occupational, and industry data from the U.S. Census, Bureau of Labor Statistics, and other sources. The insights generated by MOSAIC helped to better understand local and regional talent pools, identify workforce gaps and risks, and prioritize industry-specific workforce development solutions.

LDRD 2025-0330	High-Energy and High-Temperature Proton Irradiation Effects on Long-Term Hydrogen Permeation in Multilayer Barriers for Evaluating their Potential as Tritium Barriers
Investigators	Sumit Bhattacharya Wei-Ying Chen

The project developed a Chromium-Alumina-Yttrium oxide multilayer-based tritium permeation barrier that demonstrated strong, fusion-relevant performance across thermal, mechanical, and radiation environments, establishing a viable pathway toward DEMO-class blanket coatings. Using a scalable metal–ceramic multilayer architecture fabricated through combined atomic layer deposition and physical vapor deposition processing, the coating exhibited excellent microstructural stability, maintaining crack-free interfaces, fully intact amorphous aluminum oxide layers, and phase-stable body-centered crystalline structures of chromium. Static gas permeation testing revealed substantial permeation suppression, significantly exceeding the permeation reduction factor ≥ 100 requirement for future fusion blankets. Mechanical assessments showed controlled layer deformation with effective crack arrest at chromium-aluminum layers, confirming strong resistance to fracture and delamination. The coating demonstrated compatibility with HT-9 steel and survived combined thermal and radiation loading, positioning it as a promising, scalable tritium permeation barrier solution for lithium-lead and water-cooled lead-lithium blanket environments.

LDRD 2025-0331	Geospatial Post-Processing of Large Language Model-Extracted Events
Investigators	Scott F. Parent Joseph J. Adduci, Benjamin A. Blakely, Marianne N. Fisher, Julie L. Muzzarelli

A multidisciplinary team evaluated the ability of large language models (LLMs) to identify geographic locations from open-source text and assessed post-processing measures to strengthen the reliability of those extractions in support of international nuclear safeguards. The study addressed challenges such as toponym ambiguity, imprecise descriptions, and misinformation, which can undermine the accuracy of LLM-derived geospatial assessments. By integrating authoritative geospatial datasets and employing rigorous validation techniques, the project enhanced the precision, transparency, and reproducibility of geospatial localization workflows. The findings demonstrated that while LLMs exhibited significant potential for accelerating geospatial analysis, their outputs required systematic grounding and verification to ensure reliability in high-stakes applications.

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LDRD 2025-0345	Enabling Air-Storage and Aqueous Processing of Air- and Moisture-Sensitive Layered Sodium-Ion Battery Cathode Materials for Sodium-Ion Battery Supply Chain
Investigators	Runming Tao

This project focused on the development of protective coatings for ambient-sensitive (moisture and carbon dioxide) sodium battery layered cathode materials, aiming to reduce cost and energy input for sodium battery manufacturing at the supply chain level by enabling air storage and cathode aqueous processing. In this project, a facile incipient impregnation coating strategy was proposed and tested for the stabilization of ambient-sensitive sodium battery layered cathode materials in air and water. Several coating materials and solvents were tested for compatibility with the layered cathode materials. It was determined that titanium dioxide coating was the only candidate that exhibited some effectiveness in stabilizing the cathode material in air. However, its protective effectiveness was insufficient and could not enable final aqueous electrode processing due to the extreme sensitivity to water, indicating that this project was not successful. These results suggest that further efforts may potentially realize the proposed air storage and aqueous electrode processing of these ambient-sensitive (moisture and carbon dioxide) layered cathode materials for sodium batteries.

LDRD 2025-0353	Transforming Molecular Design with Literature-Aware Language Models and Property-Driven Foundational Models
Investigators	Hossam Mostafa Abdelhamid Mostafa Farag Hassan Harb

This project delivered an AI-guided workflow to accelerate molecular discovery. We combined large-language-model (LLM) literature mining and controllable text-to-molecule generation with differentiable, property-guided sampling to propose chemically valid candidates aligned with electrochemical performance targets. The end-to-end pipeline automatically harvested domain knowledge, generated novel structures, and scored them with data-driven evaluators, enabling rapid iteration and learning from failures. Using this framework, we expanded the RedDB dataset of redox reactions by approximately 70%, to about 26,000 molecules, significantly increasing the chemical diversity available for screening and model training. Additionally, this project delivered a modular molecular generation-evaluation architecture that is adaptable to other chemical spaces, enabling application to different scopes of chemistry. This substantially enriched the public dataset for the community and provided a reusable codebase that supports follow-on proposals and collaborations focused on generative AI-accelerated materials design.

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LDRD 2025-0356	A Global Benchmark Climatology of Boundary Layer Cloud-Top Winds
Investigators	Arka Mitra

The accurate characterization of the planetary boundary layer (PBL)-free troposphere interface is crucial for improving weather forecasts and climate simulations, testing and validating AI-based models, and energy studies. This project provided a global climatology of cloud top-height (CTH) winds for clouds lower than 3 km, based on 22 years of Multi-angle Imaging SpectroRadiometer (MISR) multi-angular satellite retrievals. Since CTH for low clouds coincides with PBL heights, this also served as a global climatology of PBL-top winds. The resulting benchmark dataset supports advanced model validation. To demonstrate the importance of the benchmark dataset, we utilized our funding to conduct a novel satellite retrieval of cloud-top entrainment velocities and mesoscale vertical velocities from the MISR benchmark Cloud Motion Vector (CMV) record. To our knowledge, this is the first purely satellite-derived retrieval of these crucial PBL variables.

LDRD 2025-0358	Portable Machine-Perception Sensor Calibration Kit
Investigators	Yihe Chen

The Portable Machine-Perception Sensor Calibration Kit project aimed to develop a field-deployable, multi-modal sensor calibration capability that enabled reliable, repeatable, and user-friendly calibration across camera, LiDAR, and inertial sensing systems. Accurate cross-sensor calibration is essential for machine perception and high-fidelity navigation, yet existing toolchains were fragmented, often required expert knowledge, and were not easily usable in field environments. To address this gap, the project developed an integrated toolkit consisting of a unified software stack, graphical user interface, sensor I/O framework, and associated portable hardware. The toolkit supported monocular and stereo camera intrinsic and extrinsic calibration, camera-to-LiDAR and multi-Light Detection and Ranging (LiDAR) extrinsic registration, and Inertial Measurement Unit (IMU) bias and noise characterization using both static bias and Allan-variance methods. It operated in both offline (dataset-based) and online (live sensor) modes, providing intuitive workflows that required no prior expertise. The system included built-in demonstration datasets, a mathematics-aware user manual, and auxiliary hardware such as lighting and photometric tools for controlled or in-field recalibration. This project established a new capability for end-to-end machine-perception sensor calibration, forming a critical foundation for ongoing and future research in high-accuracy perception and navigation within our group.

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LDRD 2025-0359	Evaluating Protein Structure Prediction Programs Through Long Timescale Molecular Dynamics
Investigators	Christian G. Seitz

Since the advent of AlphaFold2 and RoseTTAFold in 2021, protein structure prediction became accurate and generalizable enough to be regularly considered for use in structural biology projects. Since then, a variety of machine learning-based protein structure prediction programs have been developed, such as Chai, Boltz, and OpenFold. However, community standards and benchmarking across different structure prediction programs have lagged behind; without proper benchmarking, prospective researchers cannot determine which program is most accurate for specific structure prediction tasks. We created a dataset containing one member from each of the 44 protein architectures defined by the Class, Architecture, Topology/fold, and Homologous superfamily (CATH) database. This dataset serves as a baseline to compare the performance of each structure prediction program, and all members of the dataset have been prepared for molecular dynamics simulation. We developed structure prediction modules for free public use in the Bacterial and Viral Bioinformatics Resource Center (BV-BRC) and the Disease X Knowledge Base (DXKB). These modules run AlphaFold2, Chai-2, and Boltz-2. We predicted structures through these modules and compared them with reference PDB structures.

LDRD 2025-0364	Novel MBene Materials for Advanced Tribological and Lubricant Applications
Investigators	Shiba Adhikari Dongjea Seo

This project successfully established the foundation for developing a new class of transition metal boride-based two-dimensional materials, known as MBenes, for advanced tribological and lubricant applications. Unlike traditional lubricants such as graphite or MoS₂, MBenes exhibited exceptional hardness, oxidation resistance, and self-lubricating characteristics, making them ideal for use in high-temperature and high-load environments. The team synthesized and characterized Mo-, Cr-, and Ti-based MBenes and demonstrated their potential to significantly reduce friction and wear compared to state-of-the-art 2D materials.

LDRD 2025-0370	Atomic Layer Deposition of Extrinsic P-Type Molybdenum Disulfide for Advanced Low-Power Microelectronics
Investigators	Sungjoon Kim

Atomic layer deposition (ALD) is a vacuum thin film deposition technique capable of depositing a wide variety of materials with atomic precision, excellent uniformity, and conformality. Molybdenum disulfide (MoS₂) is a semiconductor material with a two-dimensional structure and many useful properties and applications, including optoelectronics, spintronics, and electrochemical catalysis. ALD of molybdenum disulfide enables the mass production of high-

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quality MoS₂; however, the lack of thermal ALD methods to synthesize and deposit p-type MoS₂ has limited the usefulness this method, especially for semiconductor applications. The primary objective of this project was to study and develop a suitable thermal ALD process that yields p-type, extrinsically doped semiconductor films with easily tunable charge carrier concentrations. As a result of this project, a new thermal ALD process for MoS₂ was developed, with the capability to vary the material's charge carrier concentration and conductivity over a wide range. This makes the process attractive for many applications, including p-n junctions, transistors, and photovoltaics. This advancement will accelerate the incorporation of 2D semiconductors into microelectronics and help develop faster and more compact devices that extend the projections of Moore's law.

LDRD 2025-0380	Domain-Specific Foundation Models to Connect Observations and Simulations in Cosmology and Astrophysics
Investigators	Azton Wells

This project developed a multi-modal foundation model for astrophysical galaxy data, designed to map between simulation- and observation-based galactic features. Our encoder-only transformer flexibly ingested scalar quantities (e.g., redshifts, galaxy masses) and vectors (e.g., star formation histories, spectra), supporting multi-task training that included within-modality reconstruction and cross-modality prediction. Using a dynamic masking strategy, the model queried arbitrary galaxy properties from partial inputs—including predicting spectra from redshift and mass, or estimating photometric redshifts from broadband magnitudes—while also recovering missing segments within a modality. We trained the model on 185,000 simulated galaxies from a gigaparsec-scale cosmology simulation, enabling effective use of cross-modal information to create more robust predictions. The model demonstrated strong generalization across multi-modal tasks and laid the groundwork for future integration of higher-dimensional and structured data such as images, merger trees, and 3D fields. This approach provides a unified framework for connecting simulations and observations.

LDRD 2025-0388	Sustainable Solutions for Critical Metals: Acid-Free Rare Earth Recovery from Magnet Swarf
Investigators	Ana Belen Cueva Sola

This project developed a leaching method for recovering neodymium (Nd) from magnet swarf using an acid-free lixiviant, ammonium oxalate. The lixiviant was designed to selectively dissolve iron, leaving Nd as Nd-oxalate for further use. The project began with initial characterization of the magnet swarf sample using ICP-OES, SEM-EDS, and XRD, which showed Fe as the main component (~50.0 wt%), Nd (38.2 wt%), and B (0.6 wt%). XRD analysis confirmed the presence of metallic iron and Nd as NdOH. Leaching experiments investigated the effects of ammonium oxalate concentration and temperature. Increasing ammonium oxalate concentration enhanced iron leaching, reaching ~50% at the highest concentration and

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minimized Nd co-leaching. However, increasing the temperature decreased iron leaching, likely due to decomposition of ammonium oxalate.

LDRD 2025-0394	Development of Event-Based Vision Technologies for High-Speed X-ray Imaging
Investigators	Songyuan Tang

This project focused on developing event-based sensing capabilities for the high-speed imaging user program at the 32-ID beamline of APS. The event camera, a new generation detector featuring low latency, high dynamic range, and high data efficiency, has been actively researched across various sectors, but its potential in the scientific domain has been largely unexplored. In this project, we developed AI/ML methods to investigate several data fusion strategies and common detector configurations to integrate event data streams into routine high-speed x-ray experiments, using past experimental data and theoretical models of the event camera. We conducted real experiments with both the event camera and a frame-based high-speed camera at the beamline to study the technical feasibility and potential benefits of deploying an event camera during high-speed experiments. Our preliminary results showed that: 1) it is possible to train a deep learning model to fuse event data with noisy x-ray images and improve image quality, and 2) it is feasible to operate the event camera and the frame-based camera simultaneously during a high-speed experiment to monitor the same process. Future studies are needed to characterize the service utility of the event camera in specific user experiments.

LDRD 2025-0399	Beyond the Extremes: Integrating Generative Models and Theoretical Bounds for Predicting Rare Disaster Events
Investigators	Arkaprabha Ganguli Jeremy Feinstein, Anirban Samaddar

This project advanced a new generation of extreme-aware generative models to improve the prediction of rare and high-impact events in scientific and climate data. We developed a methodological and computational framework for deep generative models, focusing on the Variational Autoencoder (VAE) architecture, to better capture the heavy-tailed and non-stationary data distributions that characterize extreme weather and natural hazards. The team created and evaluated an “extreme-aware VAE” that preserved the occurrence of rare events in both simulated heavy-tailed datasets and the real-world High-Resolution Rapid Refresh (HRRR) dataset. We also investigated this approach for a lumped rainfall-runoff modeling problem, where catchment-average meteorological forcing (e.g., precipitation, temperature, evapotranspiration) was mapped to basin-scale outlet streamflows. Comparisons with recently proposed heavy-tailed diffusion and VAE models showed comparable or improved performance in modeling extremes. Ongoing work integrates the strong reconstruction capabilities of our extreme-aware VAE with the generative strengths of diffusion and flow-based models. This

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project established foundational tools for more reliable modeling of rare events, with potential applications in climate risk assessment and disaster resilience.

LDRD 2025-0411	Correspondence Learning in Retrieval-Augment Generation for Enhancing Transparency and Domain-Aware Large Language Model in Power System Context.
Investigators	Sang-il Yim

The project was designed to address critical challenges such as contextual misalignment, hallucination, and lack of data source transparency in applying large language models (LLMs) to the power systems dataset domain. By leveraging retrieval-augmented generation (RAG) frameworks and developing novel correspondence learning algorithms, the project successfully bridged the gap between text-based and structured power system datasets. Key innovations included: a) transforming heterogeneous power system data into homogeneous knowledge graph embeddings with integration of power system physics models, and b) creating a context-aware retrieval mechanism that interconnects vectors from heterogeneous data. These advancements resulted in the development of a prototype software system, a comprehensive capability development document, and strategic presentations to foster collaboration with related research. The outcomes from this project enhanced the transparency, domain-awareness, and decision-support capabilities of AI systems in power systems datasets.

LDRD 2025-0420	Enhancing Message Passing Neural Network Efficiency with Argonne Artificial Intelligence Hardware Accelerators for Foundation Model Development
Investigators	Kasidet Trerayapiwat

This project advanced the efficient training of equivariant message-passing neural networks for machine learning interatomic potentials by identifying data-loading and data-packing bottlenecks that limited performance at scale and dominated training costs for foundation-model-scale workloads on artificial intelligence accelerators such as Argonne's Graphcore intelligent processing units. Through investigation of large atomic structure datasets, the project demonstrated that datasets with significant size heterogeneity required fine-tuned packing strategies to load efficiently, yielding practical heuristics for implementing optimized data pipelines compatible with Graphcore's execution and memory model. The project also developed visualization capabilities to display information and chemical structure of training databases, improving diagnostics for foundation model development. These outcomes support strategic investment in artificial intelligence accelerators like Graphcore and established best practices for training machine learning interatomic potentials.

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LDRD 2025-0428	Reactive Separation for Methanol Dehydration with Crosslinked Poly(vinyl alcohol)
Investigators	Samuel B. Hunt

This project focused on the initial demonstration of reactive separation in gel-like media for thermodynamically limiting catalysis, where current efforts for value-added transformations of carbon waste have been restricted due to critical thermodynamic limitations. Specifically, methane as a carbon synthon has had zero value beyond flaring, resulting in a loss of over \$10 billion per year. Far-from-equilibrium catalysis represents the next frontier of catalyst research, given the limitations of current thermally driven systems for robust kinetic sequestration of products. The work successfully incorporated surface-supported catalysts within polymer gel membranes and validated their catalytic activity. More than six catalysts and catalyst/membrane composite systems were synthesized, characterized, and validated catalytically as a baseline for initial studies. Methane-to-methanol conversion was successfully demonstrated in preliminary experiments by incorporating copper catalysts on surfaces through surface organometallic chemistry within polyvinyl alcohol membrane systems. Turnover numbers of 2.51 and turnover frequencies of 0.313 per hour were achieved, with methanol selectivity at 200 °C of 33.8% with PVA compared to 16.4% without PVA.

LDRD 2025-0429	Research and Development of Time-of-Flight Mass Spectrometry for Nuclear Physics
Investigators	Andrew Jacobs

This project focused on improving a key performance metric of a multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS): its mass resolving power. During the project, a novel operation scheme was developed to shift the time focus of an ion bunch to the location where the ions would be either detected or separated. The necessary hardware was ordered, received, and tested to ensure stable operation. Simulations were completed, and optimal values for MR-TOF-MS operation were determined. Initial simulation results indicated a gain in resolving power of approximately 100%. Implementation at the MR-TOF-MS was limited due to ion beam availability and incomplete downstream beam diagnostics. Once these are in place, the system is ready to implement the upgrades.

LDRD 2025-0445	Artificial Intelligence Driven Framework for Enhancing High-Resolution Climate Modeling in Energy Exascale Earth System Model
Investigators	Dimitrios Fytanidis Akash Vijaykumar Dhruv

We successfully extended CodeScribe (<https://github.com/akashdhruv/CodeScribe>) to support AI-assisted code generation and updates driven by structured specifications embedded directly within chat-completion templates. This enhancement enabled a consistent, model-agnostic

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workflow for translating, generating, and maintaining scientific codebases across languages and frameworks. The framework was validated on multiple example use cases, demonstrating reproducibility and consistency across diverse software systems such as ERF and Noah-MP, and is now mature enough to generalize to broader HPC applications. We also extended CodeScribe's code generation and translation capabilities into an agentic workflow, where bindings for coupling and translation between two codebases can be automatically generated and tested using initial build and testing configurations provided by the developer.

LDRD 2025-0447	Steering Vision-Language Models for X-ray Science Applications
Investigators	Xiangyu Yin

Vision-Language Models (VLMs) have recently emerged as powerful tools for multi-modal data analysis, but adapting them to the specific requirements of X-ray data analysis tasks has been challenging. We utilized a novel “activation steering” method for VLM adaptation. Rather than retraining model weights, we injected physics-informed “steering vectors” that guided the model’s internal activations toward key features and constraints, preserving its broad reasoning capabilities. We successfully demonstrated this “activation steering” approach on an open-source VLM, the miniGPT-4 model, using a published X-ray diffraction image library. By performing contrastive calculations, we derived specific activation vectors associated with various X-ray diffraction image artifacts. We then conducted steering experiments by injecting these vectors at inference time with adjustable coefficients and investigated tuning the steering coefficients to overcome inherent model bias and improve artifact detection accuracy. Overall, this lightweight approach has the potential to make VLMs practical tools at APS, enabling automated human-level data analysis workflows and potentially reducing reliance on expert oversight.

LDRD 2025-0455	Modeling a Novel Induction Pre-Chamber to Mitigate Misfire and Preignition for High Efficiency-Operation of Fuel-Flexible Internal Combustion Engines
Investigators	Shawn A. Reggeti

Prechamber-equipped internal combustion engines are fuel-flexible and highly efficient, but engine performance was limited by the pre-chamber’s ability to 1) purge residual exhaust gases, 2) induct air/fuel, and 3) reject heat. This project investigated a novel pre-chamber configuration, known as an Induction Pre-Chamber, to overcome the limitations of current pre-chamber designs. A 1-D model was developed, validated against experimental and multi-physics computational data, and then utilized to quantify performance improvements. The results showed that the Induction Pre-Chamber reduced residual exhaust gases by 50%, increased fuel enrichment by 7%, and enhanced heat rejection. Literature suggests that such improvements to mixture formation in the pre-chamber would improve ignitability, and therefore engine efficiency

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and emissions. Overall, it was demonstrated that the Argonne-invented Induction Pre-Chamber is a robust, low-cost solution for improving engine performance.

LDRD 2025-0458	Foundation Models for Analyzing Cyclic-Voltammetry Profiles
Investigators	Yunkai Sun Fakhrul Hasan Bhuiyan

In this project, due to the recent and rapid development of vision-language models (VLMs) over the past year, we extended our work from VLM fine-tuning to foundation model pipeline design and knowledge extraction for electrochemistry discussions and cyclic voltammetry (CV) figure annotation from literature. Our processing steps mirrored how real experts analyze CV figures across electrochemistry literature. In total, 120 CVs from the literature were manually labeled by domain experts and made available to validate the responses from current-stage VLMs. We successfully prototyped a pipeline for knowledge extraction and annotation across multiple layers of information (e.g., article-structure layer, scientific-domain layer, fundamental-category layer, technique layer, and CV-parameters layer). Furthermore, we prototyped figure analysis and physics-aware fitting tools to improve the quality of automatic figure annotation of CV data points, which can be further integrated into the LLM/VLM pipeline for higher-quality CV figure annotations.

LDRD 2025-0464	Locally Hosted Large Language Models for Scientific Documentation Management
Investigators	Simon Corrodi

This project successfully developed a framework for locally hosted Large Language Models (LLMs) to improve knowledge retrieval for the Mu2e experiment. By leveraging semantic embeddings and local inference services, the team demonstrated that open-weight models were sufficient for retrieval tasks involving scientific documentation. A key research outcome identified that synthetic Q&A generation modes significantly impacted performance metrics, establishing that "real-life" data was essential for accurate system evaluation. This work led to refined strategies for implementing a knowledge base for Mu2e and collaboration with Fermilab to deploy a Knowledge Base prototype that leverages existing infrastructure such as PostgreSQL and local inference services.

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LDRD 2025-0467	Enhancing Ionic Conductivity in Solid-State Electrolytes through Morphology Control Using Poly(Ionic Liquid)s
Investigators	Ting-Wei Hsu Pei-Tzu Lee, Qian Liu

This project successfully established a comprehensive platform for the development of solid-polymer electrolytes (SPEs) with improved ionic conductivity through morphology control for all-solid-state lithium metal batteries (ASSLMBs), delivering impactful advancements across molecular design, synthesis, membrane fabrication, and electrochemical evaluation. We designed and synthesized a family of ionic-liquid-based polymers (PILs) with strong potential for improving ionic conductivity and electrochemical stability, providing a solid foundation for next-generation SPEs. The optimized synthetic routes yielded high-purity PIL materials via ring-closing radical polymerization and established reproducible workflows that will streamline future material production. PIL membranes were fabricated with excellent uniformity, as confirmed by scanning electron microscopy (SEM), demonstrating precise microstructure control. Electrochemical impedance spectroscopy (EIS) revealed that pairing the polymer with LiFSI achieved significantly enhanced conductivity compared to LiTFSI systems. Symmetric-cell testing further validated the robust thermal and electrochemical stability of the SPEs across a wide temperature range, and ongoing full-cell evaluations build on these strong early results.

LDRD 2025-0480	AI Infrastructure and Grid Security Platform
Investigators	Duane R. Verner Joshua D. Bergerson, Carmella A. Burdi, James A. Kuiper, Todd Levin, David Sehloff, Prakash R. Thimmapuram

This project established a practical, extensible framework for an AI-enabled decision-support capability to guide secure and resilient siting and growth scenarios for hyperscale AI data centers and other energy-intensive industries across the United States. We delivered an end-to-end concept architecture that integrated Argonne’s Geospatial Energy Mapper (GEM) with Google’s Geospatial Reasoning Framework (GRF) for rapid geospatial screening, and orchestrated multi-utility and resilience modeling—including MCDA scoring and optimization, A-LEAF power expansion and dispatch, NGfast gas constraints, EPfast cascading outage risk, EPHazard weather stressors, and water–power nexus analysis—through a scenario API and site-comparison workbench. Key outcomes included a repeatable workflow that reduced the time and iteration burden of multi-model studies, produced defensible suitability maps, comparative site reports, and risk and resilience dashboards, and provided a clear blueprint for sponsor-funded buildout to support grid operators, utilities, regulators, and industry partners in planning synchronized AI and energy infrastructure development aligned with DOE energy security priorities.

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LDRD 2025-0483	High-Throughput Membrane Fabrication and Characterization for Autonomous Workflows
Investigators	Ilya A. Shkrob

This project established a high-throughput materials fabrication capability, focusing on advancing membrane technology and combinatorial materials chemistry by creating automated, parallel-track fabrication, and addressing the current bottleneck between materials manufacturing and characterization.. A 24-membrane production rig was designed and demonstrated along with a farm of 72 permeation cells. A robotic workflow involving a 24-cell farm was developed, incorporating a robot, a rack hotel, a robotic arm on a rail, a high-throughput inductively coupled plasma atomic emission spectrometer with an autosampler, and three sensors. This workflow was used to measure ion permeation rates across thin membranes for Argonne's Materials for Energy and Water consortium, which aims to develop new clay-based ion-selective membranes. In the workflow, electrolyte solution compositions were varied and permeabilities measured to correlate them with ion concentrations. Machine learning methods were employed to rapidly and efficiently make these correlations and to track and eliminate measurement errors during unattended experiments lasting 12–48 hours. The campaigns were used to develop new materials and to understand the factors controlling ion separation efficacy. The project demonstrated Argonne's ability to focus institutional resources and facilities to resolve logistics bottlenecks for high-throughput autonomous discovery workflows.

LDRD 2025-0484	Integrating PETSc With External Solvers and Preconditioners
Investigators	Junchao Zhang

PETSc (the Portable, Extensible Toolkit for Scientific Computation) is a mathematical software library widely used in academia and industry. It provides scalable linear and nonlinear solvers for scientific applications governed by partial differential equations (PDEs). PETSc achieves this in part through interfaces with various third-party libraries, among which HPDDM and MUMPS are particularly significant. HPDDM offers a suite of robust domain decomposition preconditioners that interoperate with PETSc's Krylov solvers, while MUMPS is a sparse direct solver indispensable for certain challenging engineering problems. As modern supercomputers increasingly rely on GPUs (graphics processing units) to deliver their primary computational power, it was essential to exploit their massive parallelism and superior low-precision performance. This project aimed to define a batching interface between PETSc and HPDDM and to incorporate mixed-precision support in the PETSc–MUMPS interface. We made substantial progress in both areas: developing new code, enhancing the PETSc/HPDDM interface, and extending PETSc to enable MUMPS calls at precisions different from those used by PETSc itself. These new capabilities were released as part of the PETSc library, and early adopters have already reported promising results.

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LDRD 2025-0485	Fabrication and Characterization of Integrated Superconducting Quantum Circuits
Investigators	Xu Han Mohammad M. K. Alzgool

Superconducting quantum circuits have become a pivotal platform for Quantum Information Science (QIS). In this project, we developed on-chip superconducting quantum circuits that integrated key building blocks such as resonators and couplers for various quantum tasks at Argonne. Despite the short duration of this project, we accomplished several key developments in integrated superconducting circuits. Specifically, we (1) successfully fabricated high-quality (Q factor $>10^6$) superconducting resonators and (2) completed preliminary design and fabrication of tunable couplers for transmon qubits.

LDRD 2025-0486	A Foundational Model to Minimize Solvent Degradation in Carbon Management Applications (FM4CM)
Investigators	Chandrachur Bhattacharya Lorenzo Nocivelli, Sibendu Som

This project had two primary objectives: (1) to develop an agentic, AI-driven scientific assistant capable of supporting literature review, data analysis, and related scientific tasks, and (2) to apply this capability to analyze process data from the National Carbon Capture Center (NCCC) to study monoethanolamine (MEA) solvent degradation and propose mitigation strategies. Both objectives were achieved through the development of AISAC (AI Scientific Assistant Core), a reusable, multi-agent scientific foundation, and FM4R2P (Foundational Model for Resources to Products), which was aligned with emerging programmatic priorities. FM4R2P ingested and autonomously analyzed large NCCC datasets, with results shared with NCCC and validated by feedback confirming that the AI correctly identified key processes and parameters of interest. The AI scientist also generated novel research ideas to mitigate MEA degradation, which were reviewed by NCCC domain experts and found to closely align with approaches pursued by their scientific partners, leading to strong external validation.

LDRD 2025-0487	Energy-Efficient Foundation Model for Power Grid Resilience Analysis
Investigators	Feng Qiu Mihai Anitescu, Alinson Santo Xavier

The project developed a multi-modal diffusion foundation model for power outage forecasting and scenario generation, integrating diverse data sources such as historical outage records, weather patterns, and grid operational metrics. This model enabled the generation of realistic spatio-temporal scenarios for risk assessment, resilience planning, and operational decision-making within complex power systems. These efforts demonstrated the potential of leveraging next-generation AI to improve predictive capabilities, inform strategic planning, and strengthen the resilience of modern electrical grids.

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LDRD 2025-0488	Benchmarking and Design of Agentic Foundation Models for the Accelerated Materials Discovery of Selective Ion Absorbers for Water and Recovery Applications
Investigators	Angel Yanguas-Gil Jeffrey W. Elam, Murat Keceli, FNU Kurniawan

The design of sorbent materials that are selective towards specific ions is a critical need for water treatment, resource recovery, and chemical separations. The complexity of this challenge, involving surface and liquid phase chemistry of non-ideal materials whose properties are often influenced by their microstructure, makes them unsuitable for traditional AI approaches. In this project, we developed benchmarks to evaluate an agentic foundation model's ability to design new processes involving atomic layer deposition for selective ion absorbers and water recovery applications. We also conducted a brief experimental demonstration of autonomous materials synthesis driven by an AI agent in process discovery tasks.

LDRD 2025-0489	SAFER-AI: Strategic Assessment Framework for Evaluating Risks in Artificial Intelligence Innovation
Investigators	Duane R. Verner Benjamin A. Blakely, Kibaek Kim

This initiative managed risks linked to rapidly evolving AI, including threats to critical infrastructure (CI) sectors and the proliferation of Chemical, Biological, Radiological, Nuclear, and Explosive (CBRN/E) capabilities, while fostering innovation and maintaining US global AI leadership. The project leveraged Department of Energy and industry expertise to introduce a novel red-teaming approach for evaluating AI models, supported by the development of a flexible software framework. Using non-sensitive technology analogs, this framework enabled effective risk assessment across both CI and CBRN/E proliferation domains, ensuring robust defense mechanisms. The SAFER-AI initiative standardized an evaluative process to ensure the ethical development of AI and promote sustainable prosperity through technological advancement. By addressing both CI threats and CBRN/E proliferation, this partnership set a new benchmark in AI risk management, delivering significant benefits for US safety and economic strength.

LDRD 2025-0490	AI for Sensor Network Optimization for Advanced Reactor and Integrated Energy System Design
Investigators	Akshay J. Dave

This project addressed a costly problem in industrial safety: determining which sensors are truly necessary for comprehensive fault diagnostics. Sensor systems for nuclear reactors, chemical plants, and other critical infrastructure cost millions, yet engineers previously lacked tools to

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optimize placement. This project successfully developed an AI-powered web application that reduced sensor requirements by 40–60% while maintaining full diagnostic coverage, resulting in potential savings of millions per facility. The system leveraged Argonne's PRO-AID diagnostic algorithm, augmented with AI vision capabilities to automatically analyze engineering diagrams and genetic algorithms to identify optimal sensor configurations. When deployed, the tool would provide immediate value to nuclear and chemical industries, demonstrating how AI can augment complex engineering workflows to achieve measurable economic impact in safety-critical applications.

LDRD 2025-0491	Enhanced Viral Pathogen Surveillance: Leveraging Foundation Models for Wastewater Analysis
Investigators	Rosemarie Wilton Nicholas Lee-Ping Chia, Sarah Owens, Andreas Wilke

Wastewater surveillance has proven to be a powerful, scalable early warning system for population-level infectious disease monitoring. Since March 2021, our laboratory deployed high-throughput sequencing to track SARS-CoV-2 variants at 81 sampling sites in Chicago and across Illinois. Building on this foundation, we expanded our efforts to include a broader set of circulating and emerging viral pathogens and integrated AI-driven analytics to enhance wastewater data analysis. In this project, we integrated GenSLM, a genome-scale foundation model, into the data analysis pipeline. This accelerated and streamlined sequence analysis and visualization, automated detection of high-risk viral variants, and enabled forecasting of likely mutations. These efforts facilitated efficient, real-time surveillance that supported rapid public health action and helped safeguard national security.

LDRD 2025-0492	Nepho: Automating Data Searching for Atmospheric Data Users Using Large Language Models
Investigators	Robert C. Jackson Joseph O'Brien, Bhupendra Ashokrao Raut

This project evaluated the feasibility of applying multimodal large language models (mLLMs) for automated data interpretation and search within atmospheric science. To support this analysis, we constructed a benchmark dataset comprising 144 prompt–answer–plot triplets designed to test an mLLM's ability to interpret atmospheric data visualizations. For example, given a weather radar reflectivity plot, a representative question was: "What type of weather conditions are shown in this plot?" All questions were formatted as multiple-choice to enable objective, quantitative evaluation. To facilitate reproducible benchmarking, we developed Nepho, an open-source codebase for evaluating mLLM performance on atmospheric data plots. Using this framework, OpenAI's mLLMs achieved an average accuracy of 67%, compared to 33% for leading open-source alternatives. These findings indicate that OpenAI's mLLMs currently offer a more practical pathway toward automated atmospheric data analysis. Future work will extend this framework to Department of Energy Atmospheric Radiation Measurement (ARM) Facility

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datasets, focusing on deploying mLLMs for automated data quality control in support of the ARM Data Quality Office.

LDRD 2025-0493	Use of Generative Artificial Intelligence and Large Language Models for Accelerator Design and Optimization
Investigators	Brahim Mustapha Rajkumar Kettimuthu

The main purpose of the project was to investigate the feasibility of using Generative AI (Gen-AI) and Large Language Models (LLMs) for accelerator design. By developing specialized AI tools utilizing Retrieval-Augmented Generation (RAG) and the Model Context Protocol (MCP), we demonstrated the feasibility and usefulness of Gen-AI and LLMs for accelerator design. We also developed specific applications covering both accelerator component and full accelerator lattice designs.

LDRD 2025-0494	Artificial Intelligence-Accelerated Electrochemical Simulation for Advanced Nuclear Energy Systems
Investigators	Jicheng Guo Nesar Soorve Ramachandra

Electrochemical methods have been widely applied in nuclear energy research and development, particularly in molten salt reactor development and pyroprocessing technology. Accurate experimental characterization of electrochemical processes increasingly depended on numerical simulation, as classical models such as Randles–Sevcik and Berzins–Delahay relied on simplifying assumptions that were often not satisfied under realistic experimental conditions.

Existing electrochemical simulation tools were generally not designed for molten salt systems and were typically proprietary. To address this gap, we developed a researcher-led, AI-assisted simulation software toolkit. This toolkit was applied to model electrochemical processes such as cyclic voltammetry, linear sweep voltammetry, and square wave voltammetry for both soluble-soluble and soluble-insoluble systems. We were also able to incorporate different kinetics (e.g., Nernstian, Butler-Volmer) and compensating effects like uncompensated resistance. The simulation toolkit included the use of various partial differential equation (PDE) solvers, including FiPy, PETSc, and customized implicit solvers.

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LDRD 2025-0495	Incentivizing the Reasoning Capabilities of Vision-Language Models for X-ray Imaging
Investigators	Yi Jiang Neil J. Getty, Xiangyu Yin

X-ray ptychography is a powerful computational imaging technique that has been used in a wide range of applications. However, images reconstructed by ptychography depend on many parameters and often required complex manual tuning. This project aimed to develop domain-aware vision-language models (VLMs) to facilitate more automated ptychography data analysis at the Advanced Photon Source (APS). To achieve this goal, we first curated a large benchmarking dataset with diverse ptychography reconstructions produced at the APS over the last five years. We then fine-tuned open-weights models using several state-of-the-art techniques. The models demonstrated better performance than vanilla models trained on natural images, showing capabilities in recognizing typical image artifacts and providing strategies for improvement through scientific reasoning. This project successfully established an end-to-end workflow—linking data curation at the APS to model training at the Argonne Leadership Computing Facility—which yielded critical insights into the development of foundation models for scientific discovery.

LDRD 2025-0496	Agentic Artificial Intelligence Workflow for Automated Feature Tracking and Instrument Tuning in Energy-Resolved X-ray Microscopy Experiments
Investigators	Ming Du Srutarshi Banerjee, Yanqi Luo

This project developed a workflow-regulated vision–language model (VLM) agentic system, termed Experiment Automation Agents (EAA), to advance autonomous experimentation at synchrotron beamlines. EAA integrated multimodal large models with standardized tool interfaces to enable natural-language and vision-driven control of scientific instruments. The system combined conversational intelligence with deterministic Python-based workflows, allowing reliable execution of complex, multi-step beamline tasks such as microscope focusing and feature-based imaging. A modern tool framework was implemented, supporting both internal tools and Model Context Protocol (MCP) interoperability, which ensured cross-platform compatibility. In June 2025, the team successfully tested EAA’s feature-search capability at the Advanced Photon Source 2-ID-D beamline, demonstrating vision-guided recognition of user-described sample features and automated scan refinement. This work established a foundation for intelligent, human-in-the-loop automation that enhances efficiency, accessibility, and reproducibility of synchrotron experiments, aligning with the DOE’s vision for artificial intelligence-enabled scientific discovery.

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LDRD 2025-0497	Artificial Intelligence for Fundamental Physics: Quarks to Cosmos
Investigators	Timothy J. Hobbs Patrick Barry, Chiara Bissolotti, Azton Wells

This project delivered the first agentic AI framework for cross-frontier physics in just 3-4 months, expanding Argonne's leadership in AI for Science. The team designed, implemented, and publicly released ArgoLOOM (Linked Oracles for Observables and Models), an open, cross-divisional computational framework that leveraged a large-language model backbone and orchestrated cosmology, collider, and nuclear/QCD analyses by integrating physics tools with a curated knowledge base to plan, execute, and document multi-domain physics computations. Early case studies, spanning sterile-neutrino cosmology and collider/DIS kinematic mappings, demonstrated unified, reproducible pipelines for AI-enabled discovery workflows across quarks-to-cosmos science.

LDRD 2025-0498	Artificial Intelligence Driven Characterization of Galaxy Clusters for Cosmology
Investigators	Lindsey E. Bleem Nesar Soorve Ramachandra

Galaxy clusters, the largest gravitationally bound objects in the universe, have served as powerful probes of the physical laws governing the evolution of the universe. With the rapid expansion of survey capabilities in the U.S. Department of Energy (DOE) Cosmic Frontier, we entered a new era for cluster cosmology. Identifying cluster central galaxies (CCGs) was an important part of calibrating galaxy cluster observations for use in cosmology. We developed a multi-modal AI framework that integrated knowledge from cluster astrophysics with data-driven inference to robustly identify CCGs. This framework was applied to the cluster sample from the SPT-3G experiment and will be used in the future on data from the Vera Rubin Legacy Survey of Space and Time (LSST).

LDRD 2025-0499	Philosopher-Informed Large Language Model-based Electrolyte Design
Investigators	Yunkai Sun Nicholas Lee-Ping Chia, Hassan Harb, Brian J. Ingram

In this project, we completed and benchmarked Socratic-Method (SM) agents on standard datasets. We also developed a probabilistic content-refinement framework inspired by philosophy of science concepts, including dynamic system prompts, a terminology-mapped knowledge graph, and an induction–deduction–validation pipeline (AGB) based on Toulmin-style argument components for more structured scientific reasoning. We evaluated multiple optimization approaches for internal reasoning, collected tester feedback, and assessed the reasoning styles from these models for electrolyte-design tasks, which required structured and systematic reasoning across multiple domains.

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LDRD 2025-0500	Long-Term Memory-Enabled Artificial Intelligence-Assistant for Materials Chemistry Discovery
Investigators	Jordi Cabana-Jimenez Cailin Buchanan, Tanjin He, Rajeev Surendra Assary

Large language models (LLMs) have shown promise as experimental guides in self-driving laboratories, but their lack of long-term focus, memory, and continuity has limited their impact in this area. This project focused on developing a long-term memory-enabled artificial intelligence (AI) agent to create an immersive human-in-the-loop research environment for an automated electrochemical platform, FLOW-AIDE. Specifically, the experimental campaign investigated the effect of pH on a redox-active molecule's electrochemical behavior to inform mechanistic understanding of proton-coupled electron transfers. We developed an AI agent accessible through Slack, enabling multi-scientist collaboration and retaining project life-cycle memory for continuous engagement. An architecture incorporating data analysis, retrieval-augmented generation (RAG), and literature search was built to support human-AI interaction. Throughout the interaction, the agent automatically created and maintained a project-specific wiki to capture and organize conversation history into structured information buckets, promoting more informed and context-aware exchanges between scientists and the AI agent. As part of the investigation of indigo carmine, hundreds of electrochemical experiments and simulations were performed, and the resulting data were fed into the agent for analysis. The agent was trained to analyze the data and subsequently interpreted the findings to suggest future experiments and simulations, demonstrating its capability to direct experiments for self-driving laboratories. The memory-driven context engineering reduced the manual prompting required from scientists to guide experimental campaigns. This project resulted in a memory-informed AI infrastructure that can be applied to topics beyond electrochemistry and is therefore of high value to the broader research community, where self-driving laboratories and LLMs with specialized knowledge sets are increasingly prevalent.

LDRD 2025-0501	Closed-loop Fundamental Electrochemical Deposition of Critical Minerals
Investigators	Brian J. Ingram

This project established an innovative electrochemical concept to enhance the selectivity of electrochemical critical materials capture from solutions containing multiple metals. We validated the applicability of potential-selective absorption electrodes for selective capture of critical minerals and developed autonomous electrochemical data processing and analysis to accelerate experimentation, utilizing a modular electrochemical test station, automated data collection, and closed-loop feedback controls. Our approach coupled molecularly designed electrolytes developed in the Center for Steel Electrification by Electrosynthesis (C-STEEL) with high surface area electrodes functionalized with redox-active molecules. We demonstrated the generalizability of this approach using glassy carbon electrodes functionalized with quinone-based derivatives and cyclic voltammetry (CV), which provided a rapid tool to evaluate a wide range of electrolyte-electrode combinations. Our results laid the groundwork for future

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investigations into foundational mechanisms and molecular/electrolyte design principles. Additionally, the closed-loop feedback controls for CV data analysis developed and validated in this project are readily expandable to other chemical characterization tools across a wide range of applications.

LDRD 2025-0502	Designing Narrow-Band Terahertz Light Sources for Coherent Control of Quantum Processes
Investigators	Youngjun Ahn Branko K. Popovic

Terahertz (THz) radiation offers a uniquely powerful means to selectively drive low-energy collective excitations that govern functional behavior in quantum materials and photochemical systems. The ability to isolate and resonantly control specific collective excitations requires the development of tunable and narrowband THz radiation sources. Accelerator-based THz generation naturally achieves clean spectral lines and a wide range of accessible frequencies, making it ideal for resonant excitation of specific quasiparticle modes. This project developed computational and experimental platforms to predict and diagnose THz radiation sources, initiating efforts toward the development of accelerator-based THz radiation sources at Advanced Photon Sources. A key scientific accomplishment was the development of a new computational framework for simulating THz radiation emitted when relativistic electron beams interact with periodic grating structures. Using particle-in-cell and wakefield simulations, we established the ability to model frequency, efficiency, bandwidth, and spatial mode structure across a range of grating geometries. These simulations now quantitatively guide design choices for optimizing narrow-band THz emission and provide predictive capability that did not exist prior to this project.

LDRD 2025-0503	Foundation Model for Coherent X-ray Imaging
Investigators	Aileen Luo Yijiang Li

This project prototyped a foundation model for coherent X-ray imaging. While machine learning solutions existed for individual X-ray imaging techniques such as Bragg coherent diffractive imaging (BCDI) and ptychography, they remained specific to a single technique, instrument, and sample. Our approach integrated physics-based modeling into machine learning architectures to handle diverse imaging techniques and data formats. By combining BCDI and ptychography data in the training process, we aimed to create a generalizable model for coherent X-ray imaging that could be fine-tuned for specific tasks. We implemented a physics-aware vision transformer for phase retrieval that handled both two- and three-dimensional data and demonstrated scaling on high-performance computing.

LDRD Project Summary Report for FY 2025

LDRD 2025-0504	Rapid Crystallography Foundation Model Development via On-Premise Artificial Intelligence Training Platform
Investigators	Ming Du

Using 30 million powder x-ray diffraction (PXRD) patterns synthesized from multiple large crystallography databases, we trained an AI model capable of predicting crystallographic symmetries such as crystal system, space group, and structural information (lattice parameters) from the PXRD diffraction pattern of a material. Our model generalized excellently on experimentally collected data that was not used in training, outperforming current state-of-the-art methods with a crystal accuracy of 77%, a space group accuracy of 66%, and a lattice parameter mean absolute percentage error of 22%. This work lays the foundation for developing a larger, more generalizable, and more intensively trained model for crystallography.

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