

# LDRD

Laboratory Directed  
Research and  
Development at the  
National Laboratories

# HIGHLIGHTS

ADDRESSING TOMORROW'S BIGGEST CHALLENGES

FALL  
2021

**NNSA**  
National Nuclear Security Administration



U.S. DEPARTMENT OF  
**ENERGY**

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**LDRD**

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FALL 2021

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# Laboratory Directed Research and Development

*Enabling the national laboratories to address tomorrow's biggest challenges*

US Department of Energy (DOE) national laboratories have always pushed the boundaries of science, technology, and engineering. The Atomic Energy Act of 1954 provided the basis for these laboratories to engage the best minds in cutting-edge science and technology. To help reenergize this commitment, in 1991 the US Congress authorized the national laboratories to devote a relatively small percentage of their budget to creative and innovative work that serves to maintain their vitality in disciplines relevant to DOE missions. Known formally as the Laboratory Directed Research and Development (LDRD) Program, LDRD has been an essential mechanism to enable the laboratories to address DOE's current and future missions with leading-edge research. LDRD projects are proposed independently by laboratory technical staff, evaluated through expert peer review committees, and funded by the individual laboratories consistent with the authorizing legislation and DOE LDRD Order 413.2C.

Today, this work continues to meet critical challenges. The LDRD Program enables high-risk research and development (R&D) at DOE's laboratories in areas of potential value to national R&D programs. LDRD's flexibility allows the laboratories to assemble experts from different fields into teams whose collaboration uncovers vital synergies and multidisciplinary solutions that result from reaching across technical

boundaries. LDRD researchers are exploring new ideas in fundamental science that touch on energy, environmental, and nuclear security.

Accelerating the pace of scientific and technological innovation requires engaging the brightest researchers and creating necessary advanced computational

and experimental tools. The LDRD Program is helping the nation advance foundational sciences through development of next-generation experimental, characterization, and computational tools, as well as distinctive scientific instrumentation. These capabilities and tools, when fully developed, can also be made available to academia, industry, and other scientists nationally to help advance DOE's mission and accelerate technological innovations. LDRD investment in undergraduate and graduate students, postdoctoral researchers, and scientific

collaborations will help develop new scientific talent while paving the way for potentially high-payoff R&D projects.

This publication highlights some of the cutting-edge research projects facilitated by the LDRD Program that are key to addressing the DOE mission. The projects address our energy and environmental needs and nuclear security concerns and promote US leadership in scientific discovery and innovation. While each project is impressive in its own right, all are part of a much larger portfolio that helps keep the national laboratories ready to respond to tomorrow's important challenges.

## LDRD PROGRAM OBJECTIVES

- 1. Mission agility:** Enable agile responses to energy, environmental, and national security challenges
- 2. Scientific and technical vitality:** Advance the frontiers of science, technology, and engineering
- 3. Workforce development:** Attract, retain, and develop tomorrow's scientific and technical workforce



# Energy & Environmental Security

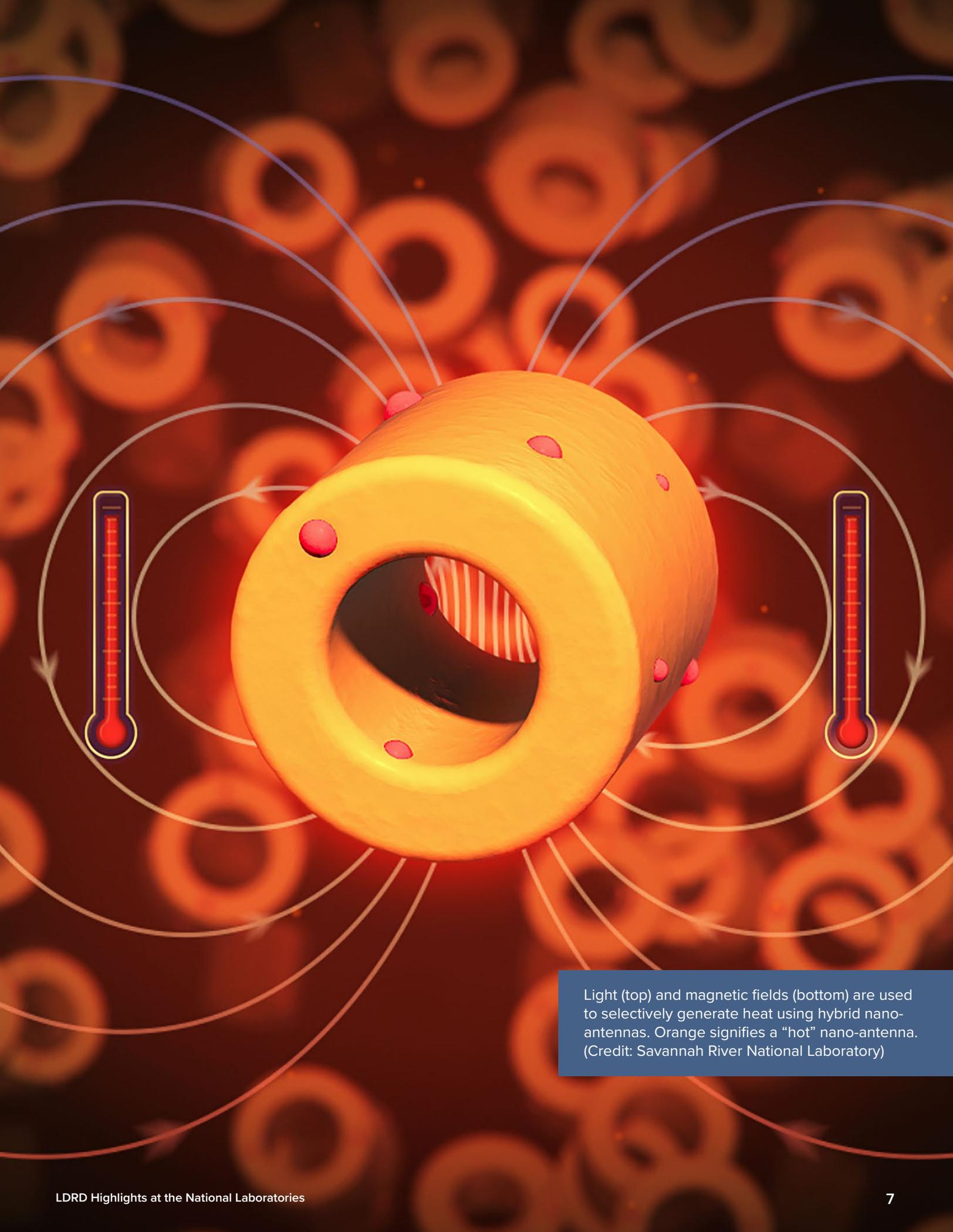
Innovative and transformative LDRD efforts are leading the way to almost exclusively clean energy, which will improve energy security, increase the nation's economic competitiveness, and cut greenhouse gases. The LDRD Program is working to ensure environmental security through remediation efforts and by detecting and responding to natural or human-caused biothreats.

LDRD projects are helping to achieve the nation's aggressive goal of net-zero greenhouse gas emissions by no later than 2050 and reaching 100% carbon pollution-free electricity by 2035. LDRD research is contributing to these goals by enabling improved clean energy technologies, smart-grid solutions for integrated energy sources, energy storage technologies and transportation and manufacturing capabilities, enhanced waste reduction technologies, and efficient water usage and recycling technologies.

Implicit in these challenges is the requirement to integrate modeling, simulation, and experimental capabilities for designing and developing novel, high-performance materials with applications in solar resources, energy storage, clean water production, environmental remediation, and molecular-to-systems-scale studies to address energy and climate challenges.

LDRD projects are helping to develop solutions leading to new electrochemical carbon dioxide reduction processes, waste heat conversion to electricity, and an integrated, efficient, and resilient electric grid. LDRD researchers are seeking ways to increase the accuracy of extreme weather and climate pattern identification through deep learning models, as well as enhancing the detection and extraction of contaminants using iron oxide-gold nanomaterials.

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Light (top) and magnetic fields (bottom) are used to selectively generate heat using hybrid nano-antennas. Orange signifies a “hot” nano-antenna. (Credit: Savannah River National Laboratory)

# Revealing Structures of Energy Materials Atom-by-Atom

AMES LABORATORY

*Scientists push solid-state NMR spectroscopy to new heights*

## OVERVIEW

LDRD investments at Ames Laboratory have expanded solid-state nuclear magnetic resonance (NMR) spectroscopy—and in particular dynamic nuclear polarization (DNP)—as the technique of choice for investigating materials surfaces and interfaces at the atomic level. The newly developed experiments have enabled 3D reconstruction of the

local and long-range structures of sites situated on the surfaces of amorphous materials, including the visualization of their dynamics, using nuclei that were previously inaccessible to solid-state NMR. In addition to providing superior capabilities, LDRD investments have led to new research projects and an Early Career Award for an Ames staff member.

## WHY IT MATTERS

Highly performing materials for catalysis, energy storage, upcycling of polymers, quantum information, separations, and other areas critical to our nation's energy future can be developed and improved only with detailed knowledge of their atomic structure. The most relevant structural features of these materials are situated on surfaces or within interfacial regions. "Understanding complex interfaces at the atomic level is critical to the discovery of new energy technologies," Ames Laboratory scientist and NMR expert Marek Pruski says. "NMR is the tool to gain that understanding." Progress in catalysis, which drives innovations in chemical industries by delivering new products, reducing energy costs, and upcycling waste materials

such as plastics, relies on fundamental understanding of chemical conversions facilitated by surface-bound active sites. Similarly, the efficiency of batteries, photovoltaic devices, and hydrogen storage materials depends on the atomic structures of electrode materials, electrolytes, complex hydrides, and semiconductor nanoparticles. Many of these challenges can be addressed by using solid-state NMR to study, element by element, the compositions, bond structures, and molecular motions of these materials. Although traditional solid-state NMR methods have lacked the sensitivity and resolution to deliver that knowledge, recently developed DNP and fast magic angle spinning methods have revolutionized surface and interface science.

## THE SCIENCE AND IMPACT

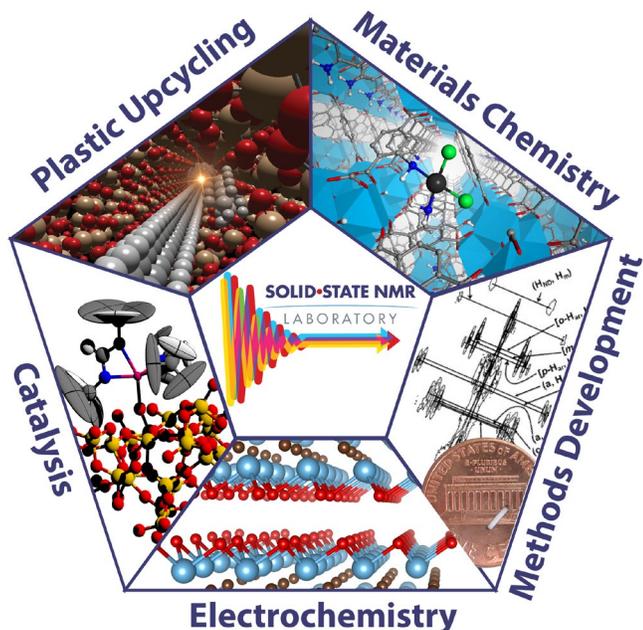
Parallel efforts are yielding a better understanding of DNP mechanisms, expanding the range of nuclei and materials that are accessible to NMR characterization, exploring the limits of DNP at very low temperatures, and probing

atomic-scale structure dynamics of molecules at interfaces.

- DNP is used to detect incredibly dilute  $^{17}\text{O}$  nuclei (natural abundance of 0.038%) from the surfaces of materials, as such experiments are beyond the capabilities



Researchers pause for discussion in front of the recently constructed Solid-State NMR Laboratory at Ames. The 400 MHz/263 GHz DNP-NMR instrument is visible in the background. (Credit: Ames Laboratory)



The scope of solid-state NMR research at the Ames Laboratory, facilitated through LDRD investments. (Credit: Ames Laboratory)

of conventional solid-state NMR. This enables scientists to characterize local structure and dynamics (e.g., hydrogen bonding, metal coordination) with unprecedented detail.

- Most NMR investigations focus on the detection of organic ligands coordinated to metal catalysts rather than detecting the metal itself. Advancements in DNP and  $^1\text{H}$  detection enable the direct detection of surface-supported platinum sites in metal–organic frameworks as

well as single-site catalysts.

- Obtaining detailed structures of the surfaces of amorphous catalysts is far from trivial. DNP has made this possible, in one case enabling the discovery of a novel catalyst deactivation mechanism and opening the door for the design of better biomass conversion catalysts. Recent work also demonstrates that structural motions from catalyst surfaces can be measured with atomistic detail.

## WHAT'S NEXT

The methodologies and tools developed through this LDRD project are being used to develop better-performing supercapacitors, plastic upcycling strategies, 2D and 3D semiconductor nanomaterials, and heterogeneous catalysts. LDRD investments are also being used to pave the way for next-generation DNP technology, which

will operate at a higher magnetic field and lower temperatures and use more advanced microwave sources. Preliminary results show that DNP can be enhanced more than a hundredfold through these efforts, further broadening the scope of solid-state NMR to the detection of sites on thin-film surfaces and the challenging characterization of internal interfaces.

***Understanding complex interfaces at the atomic level is critical to the discovery of new energy technologies.***

## Publications, Patents, and Videos

Camacho-Bunquin, J., et al., *J. Am. Chem. Soc.* **140**, 3940–3951 (2018).

Kobayashi, T., et al., *J. Phys. Chem. Lett.* **7**, 2322–2327 (2016).

Matsuki, Y., et al., *Phys. Chem. Chem. Phys.* **23**, 4919–4926 (2021).

Paterson, A.L., et al., *Inorg. Chem. Frontiers* (2021, in press).

Perras, F.A., et al., *J. Am. Chem. Soc.* **137**, 8336–8339 (2015).

Perras, F.A., et al., *J. Am. Chem. Soc.* **139**, 2702–2709 (2017).

Perras, F.A., et al., *J. Magn. Reson.* **276**, 95–102 (2017).

[Dynamic Nuclear Polarization \(video\)](#)

[What is NMR? \(video\)](#)

# Enabling Deep Learning Pattern Recognition for Extreme Weather and Climate

LAWRENCE BERKELEY NATIONAL LABORATORY

*ClimateNet increases the accuracy of weather and climate pattern identification*

## OVERVIEW

Extreme weather events, whether scorching temperatures that ruin crops or killer storms that drown coastal towns, are likely to be more frequent and more powerful with climate change. Quantifying the increase in these extreme events—and their economic and public health costs—requires combing through the massive amounts

of data that climate models generate every day. For decades, scientists have relied on heuristics—mathematical definitions of an object of interest—to pinpoint extreme weather events. However, heuristics often cannot capture the complexity and variability of weather. ClimateNet replaces heuristics with a new generation of deep learning algorithms.

## WHY IT MATTERS

Access to reliable, expert-labeled ground truth data remains the biggest challenge to improving the accuracy and performance of deep learning models, successfully deploying these models at scale, and building better models for all classes of weather and climate patterns.

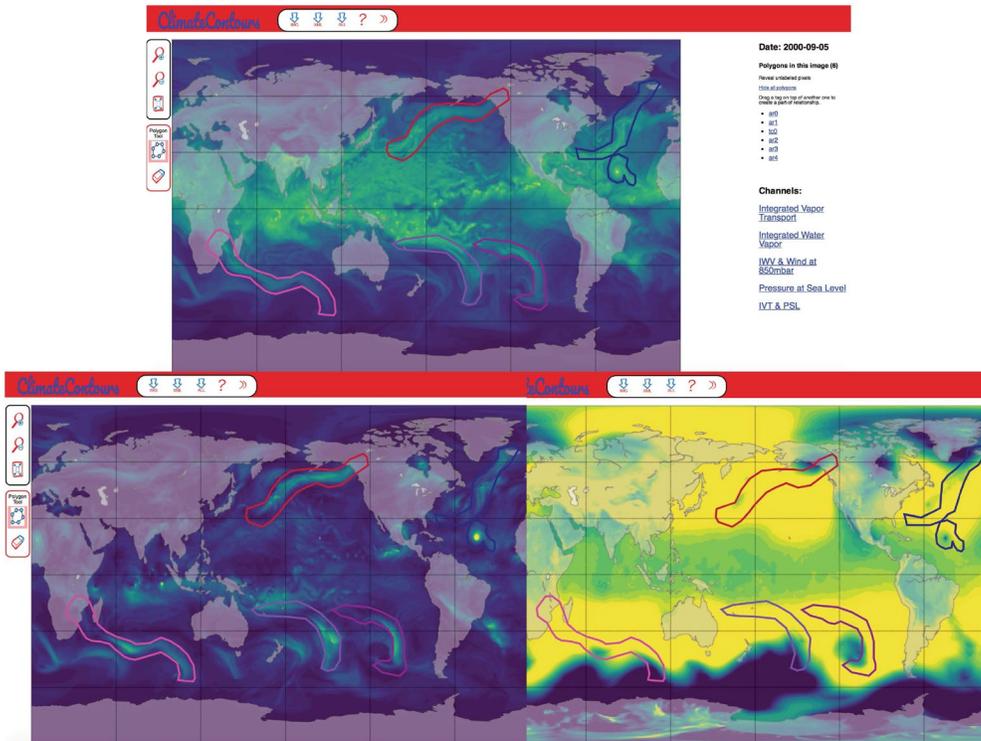
ClimateNet creates community-sourced open-access expert-labeled datasets and architectures for improved accuracy and performance of deep learning

models on a range of supervised learning problems: classification, detection, segmentation, and tracking. While there exist many heuristics and algorithms for detecting weather or climate patterns, including extreme events, the disparities between the output of these different methods within a single class of event are huge and often impossible to reconcile. This project circumvents this problem, drawing on success stories in the computer vision and deep learning communities.

## THE SCIENCE AND IMPACT

The primary goal of this project is to enable scientists to more accurately count how many extreme events a climate or weather model predicts will happen in the future and compare the results with present-day or historical

numbers. This, however, barely scratches the surface of what is possible using sophisticated deep learning systems. For example, researchers can look at underlying physical data for each event in the



ClimateContours, an online labeling tool adapted from MIT's LabelMe, allows scientists to annotate weather and climate data and create a database of carefully curated images. (Credit: Lawrence Berkeley National Laboratory)

datasets and extract information such as how much precipitation is expected to fall in a specific geographical area at a particular time.

This information can be used in many ways, including estimating insurance costs in high-risk areas and managing future drought. In places like California, which depend on rain delivered by atmospheric rivers—narrow corridors of concentrated moisture in the atmosphere—authorities could be alerted to activate contingency plans if those rivers are not going to make

landfall in California. “It’s not that you could have never answered these questions without resorting to deep learning,” Prabhat, LBNL Data and Analytics group leader, explains, “but the new approach will likely make it easier and faster and better than with heuristics.” The new methods enable highly precise analytics that yield very high-quality results, which Prabhat points out heightens the credibility of climate models’ results and the plans that rely on them for preparing for the extreme weather events of the future.

## WHAT’S NEXT

The ClimateNet team is pioneering efforts to expand the expert-labeled datasets to dozens of extreme weather and climate events in collaboration with national and international agencies. Furthermore, deep

learning models trained on ClimateNet are being deployed on a host of Intergovernmental Panel on Climate Change climate model output, reanalysis products, and observational datasets.

## Publications, Patents, and Videos

Barbuzano, J., *EOS* **101** (2020). <https://eos.org/articles/teaching-machines-to-detect-climate-extremes>.

Prabhat et al., *Geoscientific Model Dev.* **14**, 107–124 (2021). <https://doi.org/10.5194/gmd-14-107-2021>.

[Predicted Labels on UNHAPPI \(video\)](#)

[Powered by TensorFlow: Utilizing Deep Learning to Better Predict Extreme Weather \(video\)](#)

## Acknowledgments

External collaborators included scientists at UC Berkeley, ETH Zurich, and National Center for Atmospheric Research. The work was led by National Energy Research Scientific Computing Center (LBNL) scientists Karthik Kashinath and Prabhat.

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***ClimateNet overcomes the biggest barrier to making deep learning truly successful for climate science.***

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# Using Dark Fiber and Distributed Acoustic Sensing to Probe the Subsurface

LAWRENCE BERKELEY NATIONAL LABORATORY

*Unused  
fiber-optic  
cables can be  
used to image  
the ground  
beneath our  
feet*

## OVERVIEW

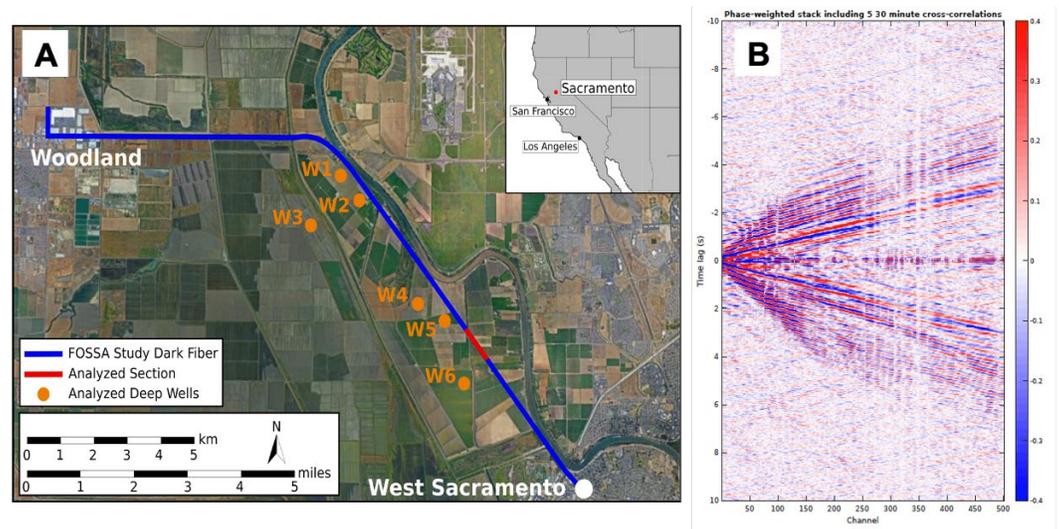
In traditional seismology, researchers rely on a small number of seismic sensors to detect earthquakes, monitor ground motion, and measure the properties of underground formations. LBNL researchers leveraged unlit fiber-optic cables, referred to as dark fiber, to perform seismic measurements at thousands of locations in California's Central Valley using a relatively new technique called distributed acoustic

sensing (DAS), which measures the "stretch" in fiber-optic cables by analyzing the scattering from rapid pulses of laser light. The team demonstrated that such cables could be used to generate images of soil properties, detect both local and distant earthquakes, and measure changes in the soil column due to rainfall. This is one of the first case studies to employ a large regional network as a seismic sensor.

## WHY IT MATTERS

The sparsity of existing seismic sensors presents challenges when attempting to accurately locate small earthquakes and characterize the complex network of faults present in tectonically active regions of the United States. Similar challenges

exist when attempting to characterize soil properties and aquifers; the limited spatial extent and resolution of existing sensor networks forces expensive and time-consuming local experiments. LBNL's research demonstrated an



(Panel A) The dark fiber section monitored as part of the LDRD experiments. (Panel B) Example of an ambient noise gather generated as part of the study. (Credit: Lawrence Berkeley National Laboratory)

alternative approach to large-scale seismic monitoring that uses existing fiber-optics, currently part of the telecom network, and DAS to measure local and distant

earthquakes and characterize near-surface soil properties. As the cost of DAS acquisition decreases, telecom networks across the United States could be exploited for seismic monitoring.

## THE SCIENCE AND IMPACT

During the dot-com boom, telecom companies installed vast networks of underground fiber-optic cable to meet the demands of a growing industry. As data transmission technologies improved, fewer cables were needed, causing a sizable portion to fall into disuse. LBNL scientists have been investigating a new use for this dark fiber: seismic sensing. Conventional seismic networks often employ only a few dozen sensors to cover a relatively large area. The team used DAS, a technology that measures seismic wavefields by shooting short laser pulses across the length of the fiber, along a 20-mile stretch of ESnet's Dark Fiber Testbed. ESnet, DOE's high-performance network for extreme-scale data, maintains the test bed for network research; using

the test bed for seismology is a novel idea that emerged from conversations at Berkeley Lab. Because the ESnet Testbed has regional coverage, the researchers were able to monitor seismic activity and environmental noise with finer detail than previous studies. The coverage of the test bed provided subsurface images at a higher resolution and larger scale than would have been possible with a traditional sensor network. In addition to being able to distinguish between a car and moving train versus an earthquake and to detect both local and distant earthquakes, the technology could also be used to characterize soil properties, provide information on aquifers, and be integrated into geotechnical studies.

## WHAT'S NEXT

After demonstrating the sensitivity and utility of dark fiber coupled to DAS, the team has worked to rapidly deploy the technology for a range of DOE-relevant applications. At present, they are recording data using this approach in California's Imperial Valley as part of a project funded by the DOE Office of Energy

Efficiency and Renewable Energy (EERE) Geothermal Technologies Office to locate, characterize, and monitor geothermal reservoirs as well as detect small earthquakes on major faults. The team is also working on using offshore fiber-optic cables to understand seafloor sediment properties.

***This is one of the first case studies employing a large regional fiber-optic network as a seismic sensor.***

## Publications, Patents, and Videos

Ajo-Franklin, J.B., et al., *Sci. Rep.* **9**(1), 1–14 (2019).

Lindsey, N.J., et al., *Science* **366**(6469), 1103–1107 (2019).

Rodríguez Tribaldos, V., and Ajo-Franklin, J.B., *J. Geophys. Res. Solid Earth* **126**(4), e2020JB021004 (2021).

Nayak, A., et al., *Seismol. Soc. Am.* **92**(4), 2441–2452 (2021).

## Acknowledgments

Collaborators include Nathaniel Lindsey (UC Berkeley, now FiberSense), Horst Rademacher (UC Berkeley), and T.C. Dawe (Monterey Bay Aquarium Research Institute).

The work was led by LBNL EESA/Rice researcher Jonathan Ajo-Franklin (now Rice University) with significant assistance from Shan Dou (EESA), Inder Monga (ESnet), Chris Tracy (ESnet), Barry Freifeld (EESA), Tom Daley (EESA), Veronica Rodriguez Tribaldos (EESA), Craig Ulrich (EESA), Avinash Nayak (EESA), and Sherry Li (CRD).

Telecom fiber access was provided by Century Link (Sacramento). DAS support was provided by Silixa LLC.

# Demonstrating the Scalability of Electrochemical CO<sub>2</sub> Reduction

NATIONAL RENEWABLE ENERGY LABORATORY

*A platform was developed to demonstrate scalability of electrochemical CO<sub>2</sub> reduction*

## OVERVIEW

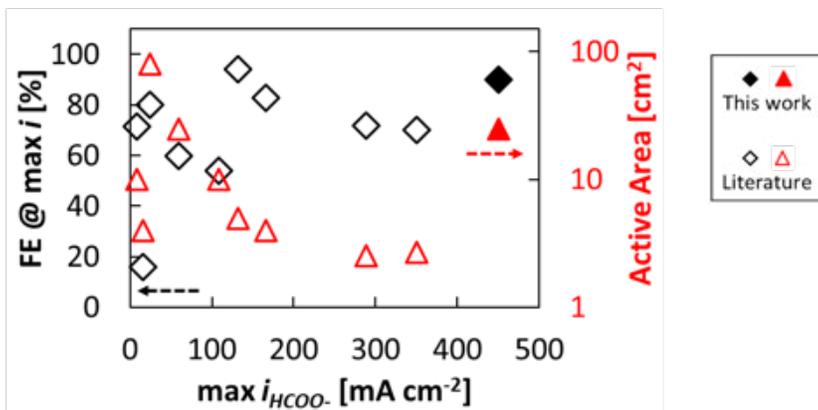
In recent years, electrochemical CO<sub>2</sub> reduction—the conversion of CO<sub>2</sub> to more reduced chemical species using electrical energy—has been used almost exclusively in small-scale experiments and materials development in environments likely different from those in a commercialized system. With no common subscale platform (i.e., 25–100 cm<sup>2</sup>) such as those that exist for other

electrochemical conversion technologies like fuel cells and electrolyzers, comparing meaningful improvements to performance, selectivity, and durability has remained challenging. The project clearly demonstrates the potential of gas-phase CO<sub>2</sub> reduction for scalable processes while also enabling the cross-comparison of materials and methods as society shifts towards an electrified and decarbonized manufacturing industry at scale.

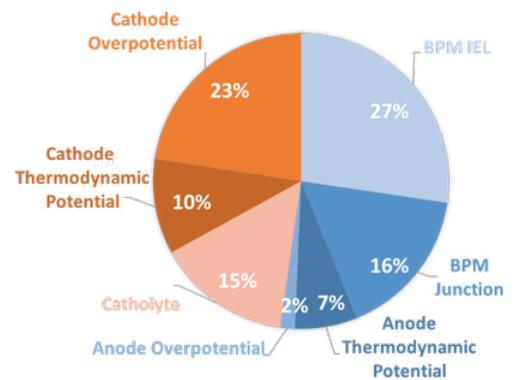
## WHY IT MATTERS

Formate and formic acid are interesting target molecules for CO<sub>2</sub> reduction as they require no C–C coupling, enabling high selectivity. Additionally, formic acid has agricultural and industrial uses and is a relevant biological intermediate for the subsequent production of fatty acid methyl esters that can lead to renewable jet fuel as well as an emerging liquid energy

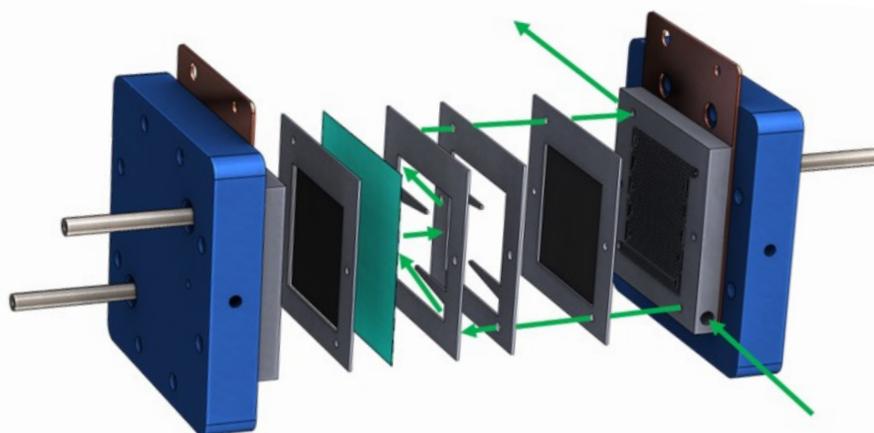
(hydrogen) carrier. The project bridged the gap between fundamental development and industrial application and leveraged NREL's unique capabilities and institutional knowledge of electrochemical conversion devices to uplift the field. Providing solutions to electrify and decarbonize the entire energy system has been a focus of NREL and the national lab system as a whole.



FE for CO<sub>2</sub> to formate achieved on an electrode nearly 10× that of prior efforts in the field. (Credit: National Renewable Energy Laboratory)



Voltage loss contributions at 0.5 A/cm<sup>2</sup>. (Credit: National Renewable Energy Laboratory)



The novel platform enables standardized testing, identification of future research needs, and tunable catholyte flow through gaskets for adjustable catholyte thickness. (Credit: National Renewable Energy Laboratory)

## THE SCIENCE AND IMPACT

This project enabled NREL to use small-scale laboratory demonstrations to show a pathway to commercialization by demonstrating feasibility in subscale cells that project to industrially relevant conversions of CO<sub>2</sub> to formate. This new capability provides a test bed for materials and processes and has already shown very high Faradaic efficiency (i.e., the efficiency with which

charge is transferred in a system, facilitating an electrochemical reaction) and current density necessary for moving electrochemical CO<sub>2</sub> reduction processes to commercialization. The innovative design of the electrolysis test bed device allows for the study of all parts of the process in isolation to identify kinetic and transport bottlenecks.

## WHAT'S NEXT

This work has validated NREL's contribution to electrochemical CO<sub>2</sub> reduction and has led to funding from the DOE Bioenergy Technologies Office on three separate proposals with industry and academic partners. It has also led to funding from the Office of Fossil Energy and Carbon Management (FECM) to work collaboratively with the National Energy Technology Laboratory on

the incorporation of novel materials into scalable CO<sub>2</sub> devices. The work has enabled NREL to lead a recently awarded ARPA-E (Advanced Research Projects Agency–Energy) project with industry and academic partners that focuses on CO<sub>2</sub> conversion to jet fuel. The project has enabled NREL to obtain funding from FECM to focus on the direct capture and conversion of waste CO<sub>2</sub>.

***This platform enables screening of CO<sub>2</sub> reduction systems at application-relevant scales.***

## Publications, Patents, and Videos

Chen, Y., et al., *ACS Energy Lett.* **5**, 1825–1833 (2020). <https://pubs.acs.org/doi/10.1021/acsenergylett.0c00860>

Klein, E., and Neyerlin, K.C., "Cell Hardware Configurations for Electrochemical Conversions," US patent application no. 62/988,207 (NREL PROV/19-152B).

## Acknowledgments

This work was led by NREL researcher K.C. Neyerlin with significant contributions from Yingying Chen and Ellis Klein.

# Untangling the Dynamics of Entangled Polymers

OAK RIDGE NATIONAL LABORATORY

*Researchers  
revise a  
fundamental  
polymer theory  
underlying  
processing of  
plastics and  
other products*

## OVERVIEW

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Scientists combined the laboratory's strengths in neutron scattering, materials science, and supercomputing to study a gap in our understanding of polymer dynamics. Materials developed from polymers—long chains of entangled molecules—are ubiquitous in consumer and industrial products, from plastics to electronics to jet fuel. The novelty and high performance of such materials depend in part on their polymer dynamics, which can determine properties such as elasticity

and stability across temperatures. The team studied topological constraints in entangled polymers, which are important for processing materials that undergo deformation. Much of the past research on polymers has focused on simple interactions due to the complexity of the scientific problem. However, many properties are determined by topological (i.e., compositional) constraints—a result of excluded volume interactions and chain connectivity—that span short-to-long spatial scales and can be difficult to predict and observe.

## WHY IT MATTERS

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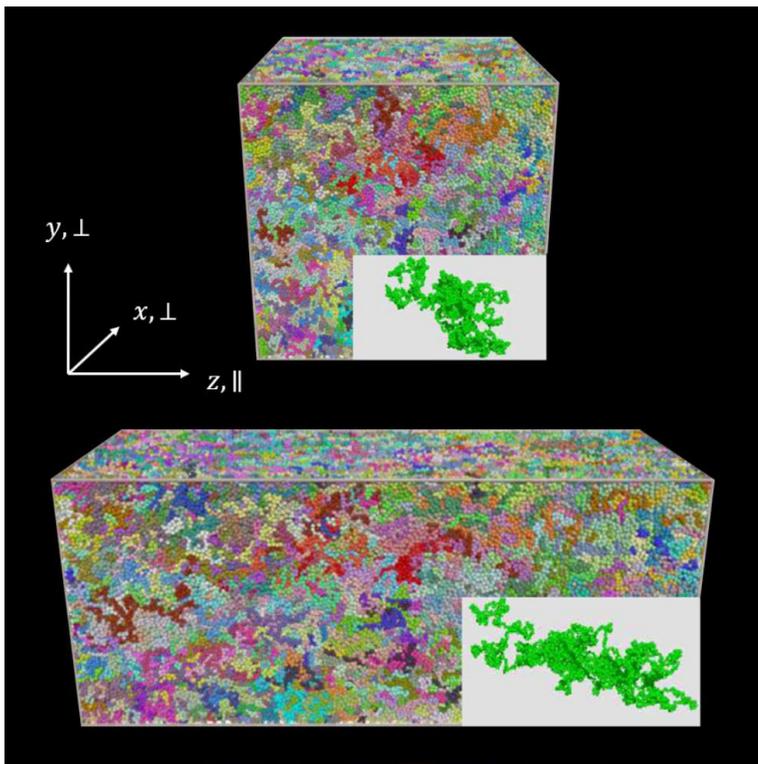
To bridge knowledge gaps about topological constraints in entangled polymers, the team developed both computational and experimental methods to push the limits of an established theory of polymer dynamics known as tube theory, which describes how string-like polymers respond to being deformed. In 1978, a hypothesis by physicists Pierre-Gilles de Gennes, Masao Doi, and Sam Edwards explained polymer motion as restricted within a narrow “tube” of space due to entanglement. The theory has been thought to properly describe nonlinear rheology of entangled polymers, predicting that polymer size will decrease

in all directions following deformation, a phenomenon known as chain retraction. However, the chain retraction mechanism has never been fully validated by experiments. Through cutting-edge neutron scattering experiments and supercomputing simulations, the scientists found conflicting measurements that called for revisions to conventional tube theory. The research also resulted in a new neutron scattering method for polymer dynamics as well as other soft-matter studies—adding another tool to the arsenal of scientific probes at the Spallation Neutron Source and the Center for Nanophase Materials Sciences.

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*Our goal was to understand the complex dynamics in important polymers and soft matter.*

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Molecular dynamics simulation of a well-entangled polymer melt. (Credit: Y. Wang, ORNL)

## THE SCIENCE AND IMPACT

The team began by applying a new mathematical framework called a spherical harmonic approach to analyze polymer relaxation and dynamics from 2D small-angle neutron scattering data. “Our neutron scattering method can help us understand all kinds of complex polymeric materials, including flow and deformation under different processing conditions,” staff scientist Yangyang Wang says. Neutron scattering data revealed how the molecular relaxation of deformed polymers is related in space and time, demonstrating that entanglement has a weaker influence than previously thought. The team

then scaled their investigation to the former Titan supercomputer at the Oak Ridge Leadership Computing Facility. On Titan, the team simulated a highly entangled system of polymers undergoing stretching and watched how the molecules relaxed following deformation. The simulation included 250 polymer chains of 2,000 atoms simulated in 1 billion timesteps to capture the complex interactions. The detailed simulation supplied key measurements that conflicted with the popular tube theory and were also supported by the team’s earlier results from neutron scattering experiments.

## WHAT’S NEXT

The team’s neutron scattering method has been applied to other soft-matter studies for its ability to discern molecular relaxation in

deformed polymers. This project led to a DOE Office of Science Early Career Award in 2019 for an ORNL researcher.

## Publications, Patents, and Videos

Lam, C.N., et al., *Phys. Rev. Lett.* **121**, 117801 (2018).

Wang, Z., et al., *Phys. Rev. X* **7**, 031003 (2017). DOI: 10.1103/PhysRevX.7.031003.

Xu, W.-S., et al., *ACS Macro Letters* **7**, 190 (2018). DOI: 10.1021/acsmacrolett.7b00900.

# Defending High-Consequence Control Systems through Proactive Cybersecurity

PACIFIC NORTHWEST NATIONAL LABORATORY

*Key building blocks for next-generation autonomic cybersecurity solutions were developed and deployed*

## OVERVIEW

The Proactive Adaptive Cybersecurity Framework for Control (PACiFiC) investment leveraged the physics of physical systems to bound cyberspace. Process controls, physical boundaries, and chemical and material laws limit detection and response margins to provide the nation’s high-consequence infrastructure, such as the power grid, with security,

resilience, monitoring/detection, and control. Combining cognitive, social, and psychological understanding adds another dimension by which cyberspace can be bound. Merging physical and social models with a cyber model transforms a currently untraceable problem of cybersecurity detection and automated response into a viable approach and achievable outcome.

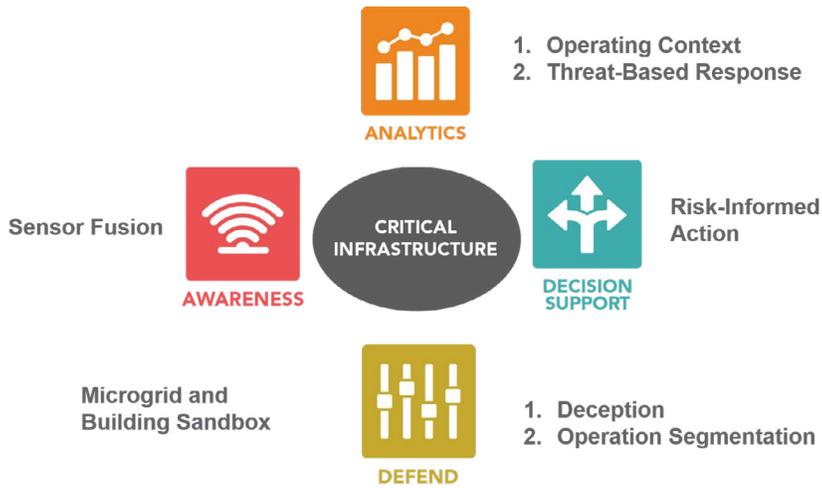
## WHY IT MATTERS

The nation’s high-consequence infrastructure has many systems and devices that monitor and control critical physical processes. However, these operational technologies (OT) are static, have legacy components, and are inherently insecure. Adversaries are highly focused on

exploiting these systems, which could be devastating. The PACiFiC investment sought to demonstrate, for the first time, that OT can be made secure by developing adaptive systems that are proactive, flexible, and dynamic in response to cyber threats and events.

PACiFiC was tested and demonstrated in the environment pictured. (Credit: Pacific Northwest National Laboratory)





Components of PACiFiC's critical infrastructure. (Credit: Pacific Northwest National Laboratory)

## THE SCIENCE AND IMPACT

PACiFiC combines adaptive principles, cross-domain information, and classic security best practices to deliver measurably more secure, reliable, robust, and resilient control systems while retaining strong operational performance.

Key outcomes include:

- Developing adaptive, resilient solutions in cybersecurity at PNNL and through the DOE Office of Electricity Grid Modernization Laboratory Consortium;

- Defining, measuring, and quantifying information technology system resilience, which can be applied to OT systems;
- Investing in mission-relevant cyber test beds;
- Leading the collection and analysis of OT cybersecurity data for DOE;
- Contributing domain expertise with 9 submitted patents, 14 invention disclosures, and more than 20 publications; and
- Building next-generation talent with the addition of more than 15 new and joint hires.

## WHAT'S NEXT

Commercialization and technology transfers continue for several technologies associated with this \$2.7 million project, finished in FY 2019.

Additional critical infrastructure defense development is underway, including for transportation and oil/natural gas infrastructures.

***After viewing a demonstration of the PACiFiC cybersecurity technologies at PNNL, our sponsors at DOE asked if the entire solution could be installed right away at a utility for field evaluation.***

## Publications, Patents, and Videos

Ashok, A., et al., in *Proceedings of the 12th USENIX Conference on Cyber Security Experimentation and Test (CSET'19)*, USENIX Association, 2017, p. 17.

Hofer, W., et al., in *Proceedings of the 2019 IEEE International Symposium on Technologies for Homeland Security (HST)*, 2019, pp. 1–7. DOI: 10.1109/HST47167.2019.9032927.

Rice, T.R., et al., in *Proceedings of the 2019 Resilience Week (RWS)*, 2019, pp. 105–111. DOI: 10.1109/RWS47064.2019.8971821.

[PACiFiC: New Cyber Tools to Protect Critical Infrastructure \(video\)](#)

## Acknowledgments

Investment leads for this project included Paul Skare and David Manz. Key team members were Thomas Edgar, Theora Rice, Aditya Ashok, Bill Hofer, Tom Carroll, Kristine Arthur-Durett, and Sid Sridhar.

# Creating Heat with Hybrid Nano-Antennas

SAVANNAH RIVER NATIONAL LABORATORY

*Nano-antennas can be used to selectively generate heat for thermal processes*

## OVERVIEW

Scientists demonstrated that an electromagnetic field, either as a light or magnetic field, can be selectively coupled to shape-selective hybrid nano-antennas for efficient thermal processes. Localized heating occurs extremely fast, reducing the “wasted” thermal load on the environment. Because the electromagnetic induced heating technology is noncontact, efficient, and highly selective, the required input energy is greatly diminished. By strategically placing nano-antennas at desired locations,

heat can be controlled at the nano-level. The location for nano-antennas, and the subsequent energy deposition, may be fine-tuned through specific chemical, spatial, or magnetic interactions. The nano-antennas, composed of combinations of plasmonic, magnetic, and hydride components, are used for controlled release of hydrogen isotopes, chemotherapy drugs, environmental contaminants, enhanced catalytic processes, and (bio)imaging and therapeutics.

## WHY IT MATTERS

Creation of this new class of shape-selective nano-antennas with tailored properties from abundant and inexpensive materials that serve as local “hot spots” lays the foundation for exciting fundamental scientific discoveries and temperature-controlled applications. These discoveries advance the fields of nanoscience, materials, energy, catalysis, biomedicine, and separations by providing innovative, cost-effective, efficient, and environmentally friendly solutions to meet global energy and societal needs.

SRNL provides a continuous opportunity to develop the future DOE workforce through the Group for Innovation and Advancements in NanoTechnology Sciences (GIANTS) program. GIANTS’ multiyear mentoring and advising program has led to numerous successes and opportunities for postdoctoral researchers and students, including participation in the Nobel Laureate conference.



Scanning electron microscope used to characterize nano-antennas. (Credit: Savannah River National Laboratory)



Shape-selective hybrid nano-antenna materials, including spheres (left), elongated tubes (middle), and equiaxed rings (orange) decorated with nanomaterials (red) (right). The nano-antennas are composed of combinations of plasmonic, magnetic, and/or hydride components. (Credit: Savannah River National Laboratory)

## THE SCIENCE AND IMPACT

This project led to materials discoveries that enable affordable industrial applications and manipulation and control of the thermal process using hybrid nano-antennas. The team successfully demonstrated remote separation and methodical manipulation of hydrogen isotopes using hydride-magnetic storage nanomaterials and use of plasmonic distillation, expanding DOE's energy security, fusion, and defense missions and making separation processes more efficient. This work also delivered enhanced catalytic processes and explored hybrid nanomaterials for biomedical applications. The team also demonstrated rapid techniques for detection and extraction of contaminants using iron

oxide-gold nanomaterials and for remote remediation of locations when exposed to light or a magnetic field.

Twelve undergraduate and graduate students and postdoctoral researchers were provided extensive educational training and experience. Scientific recognition and awards include *Science Daily News*, *PhysOrg* (featured story), *UGA* (featured story), *Energy & Fuels* cover magazine, *Inspirational Woman in STEM* Recognition (DOE), and *U.S. C3E Award Finalist in Research* (DOE/MIT/Stanford University).

## WHAT'S NEXT

The pioneering development of nano-antenna materials has enabled numerous applications for focused noncontact generation of heat, which led to the development of 3D/4D-printed energy storage materials. These unique nanomaterials have untapped potential in advanced (bio)chemical and

catalytic processes, radiation and chemical detectors, advanced manufacturing, environmental stewardship, and biomedical industries (e.g., destruction of bacteria or microbial environments, disinfection by remotely raising temperature, theragnostic).

***Abundant and inexpensive nano-antennas generate heat efficiently through selective and localized noncontact processes.***

## Publications, Patents, and Videos

Hunyadi Murph, S.E., et al., *ACS Appl. Mater. Interfaces* **12**, 9478 (2020). <https://pubs.acs.org/doi/abs/10.1021/acsa-mi.0c00887>.

Hunyadi Murph, S.E., et al., *Anisotropic and Shape-Selective Nanomaterials: Structure-Property Relationships*, Springer, 1–470 (2017). <https://www.springer.com/gp/book/9783319596617>.

Hunyadi Murph, S.E., et al., *J. Phys. Chem. C*, **120**, 15162 (2016). <https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b03733>.

Hunyadi Murph, S.E., et al., *Catalysis Today* (Special Issue), **270**, 51 (2016). <https://www.sciencedirect.com/science/article/pii/S0920586115006847>

“Modern-day alchemy: Researchers reveal that magnetic ‘rust’ performs as gold at the nanoscale,” *Science Daily News*. <https://www.sciencedaily.com/releases/2016/09/160915132444.htm>.

“Controlled Release of Hydrogen Gas from Nano Hydrides via Induced Magnetic Field,” US patent no. US20180319658A1. <https://patents.google.com/patent/US20180319658A1/en>.

“Multifunctional Nanomaterials and Methods of Photothermal Heating and Catalysis,” US patent no. 10,016,745. <http://patentsgazette.uspto.gov/week28/OG/html/1452-2/US10016745-20180710.html>.

“Radiation Detectors Employing Contemporaneous Detection and Decontamination,” US patent no. US20200082954A1. <https://patents.google.com/patent/US20200082954A1/en>.

SRNL: [The Nano Heater \(video\)](#)

## Acknowledgments

Simona Hunyadi Murph, Henry Sessions, Robert Lascola, postdocs, and undergraduate and graduate students conducted this work.

# Using Waste Heat to Generate Electricity and Drive Chemistry

SLAC NATIONAL ACCELERATOR LABORATORY

*Novel heat engines could reduce carbon emissions*

## OVERVIEW

More than 60% of the energy consumed in the United States is wasted as heat. Researchers at SLAC and Stanford University invented an electrochemical heat engine to harvest that waste heat by converting it directly to continuous electric current. They went on to develop a chemical heat engine that uses heat to

split water into hydrogen and oxygen at temperatures compatible with industrial processes. This work led to the discovery of a new class of materials for splitting water 5–10 times more effectively than state-of-the-art materials, and they developed computational methods for identifying the best candidate materials.

## WHY IT MATTERS

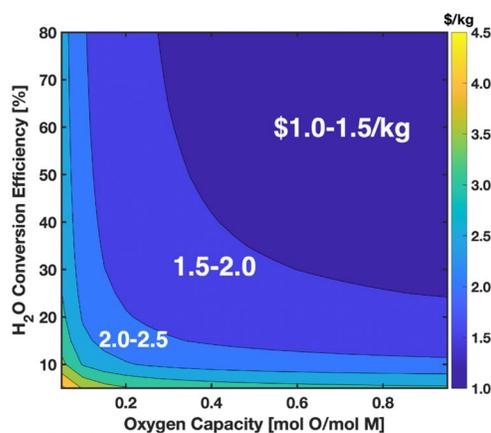
In theory, more than 300 GW of waste heat could be harvested and put to use in the United States alone. If done on an industrial scale, this could significantly

reduce greenhouse gas emissions while generating power and producing chemical feedstocks for making fuel, fertilizer, plastics, and other products.

## THE SCIENCE AND IMPACT

The team's electrochemical heat engine consists of a stack of two electrochemical cells connected in series. One cell runs a chemical reaction at a high temperature, while the other cell runs the reverse reaction at a lower temperature. Excess heat from the high-temperature cells is

used to power the low-temperature chemical reaction. The voltage required by the hot cells is lower than the voltage generated by the cold cells, a difference that produces a continuous electric current. Operating the engine in reverse enables electrochemical refrigeration.



A two-step thermochemical cycle could produce hydrogen at a cost comparable to steam methane reforming, as well as generate pure oxygen or CO<sub>2</sub>. (Credit: J. Rojas et al., 2021)

The team also developed a thermochemical heat engine and discovered a new class of metal oxides—polycation oxides (PCOs)—which are highly active in thermochemically splitting water to produce hydrogen and oxygen. Applications include syngas and hydrocarbon fuel production and thermal energy storage. A computational study of the water conversion capability of metal oxides in the CALPHAD database discovered iron oxides with theoretical yields up to 8× those of state-of-the-art oxides, including one with a theoretical conversion efficiency of more than 50% at 700°C. A techno-economic model found that

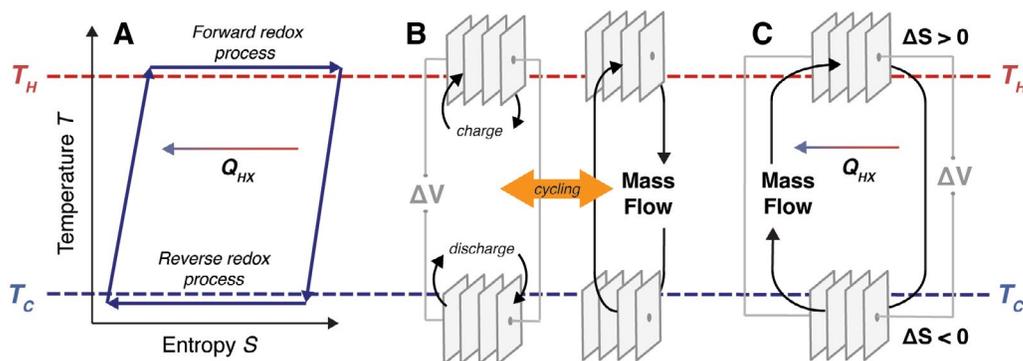
the two-step thermochemical cycle could produce hydrogen at a cost comparable to steam methane reforming, but with the added benefit of producing a pure stream of oxygen. If activated by natural gas, it would produce a pure stream of CO<sub>2</sub>.

“You can basically design a material on a computer, make it in the lab, and it works, because we have figured out most of the underlying fundamental science,” says Stanford professor Arun Majumdar, who led the project with associate professor Will Chueh. “Now we have the world’s record performance for redox activity in these thermochemical reactions, and it all started with the initial LDRD project.”

## WHAT’S NEXT

Work continues in co-PI Majumdar’s lab on novel redox systems and computational approaches for sustainable

energy. A patent has been filed for the PCO-based thermochemical heat engine.



A continuous electrochemical heat engine developed at SLAC and Stanford University uses heat to generate electricity. Run in reverse, it could provide refrigeration. (Credit: A. Poletayev et al., 2018)

## Publications, Patents, and Videos

McKay, I.S., et al., *Sci. Rep.* **9**, 13945 (2019). *Sci. Rep.* **9**, 13945 (2019).

Poletayev, A., et al., *Energy Environ. Sci.* **11**, 2964–2971 (2018).

Rojas, J., et al., *Cell Rep. Phys. Sci.* **2**, 100362 (2021).

Zhai, S., et al., *Energy Environ. Sci.* **11**, 2172–2178 (2018).

Zhai, S., et al., *Energy Environ. Sci.* **13**, 592–600 (2020).

“Thermochemical Gas Reduction Process Using Poly-cation Oxide,” US patent application no. US15/096,368.

## Acknowledgments

The project received follow-on funding from the EERE Fuel Cell Technology Program and the Office of Naval Research, with additional support from Stanford’s TomKat Center for Sustainable Energy and SUNCAT Center for Interface Science and Catalysis.

Parts of this work were carried out at SLAC’s Stanford Synchrotron Radiation Lightsource, a DOE Office of Science user facility.

**When run in reverse, these heat engines can also provide sustainable refrigeration.**

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# Nuclear Security

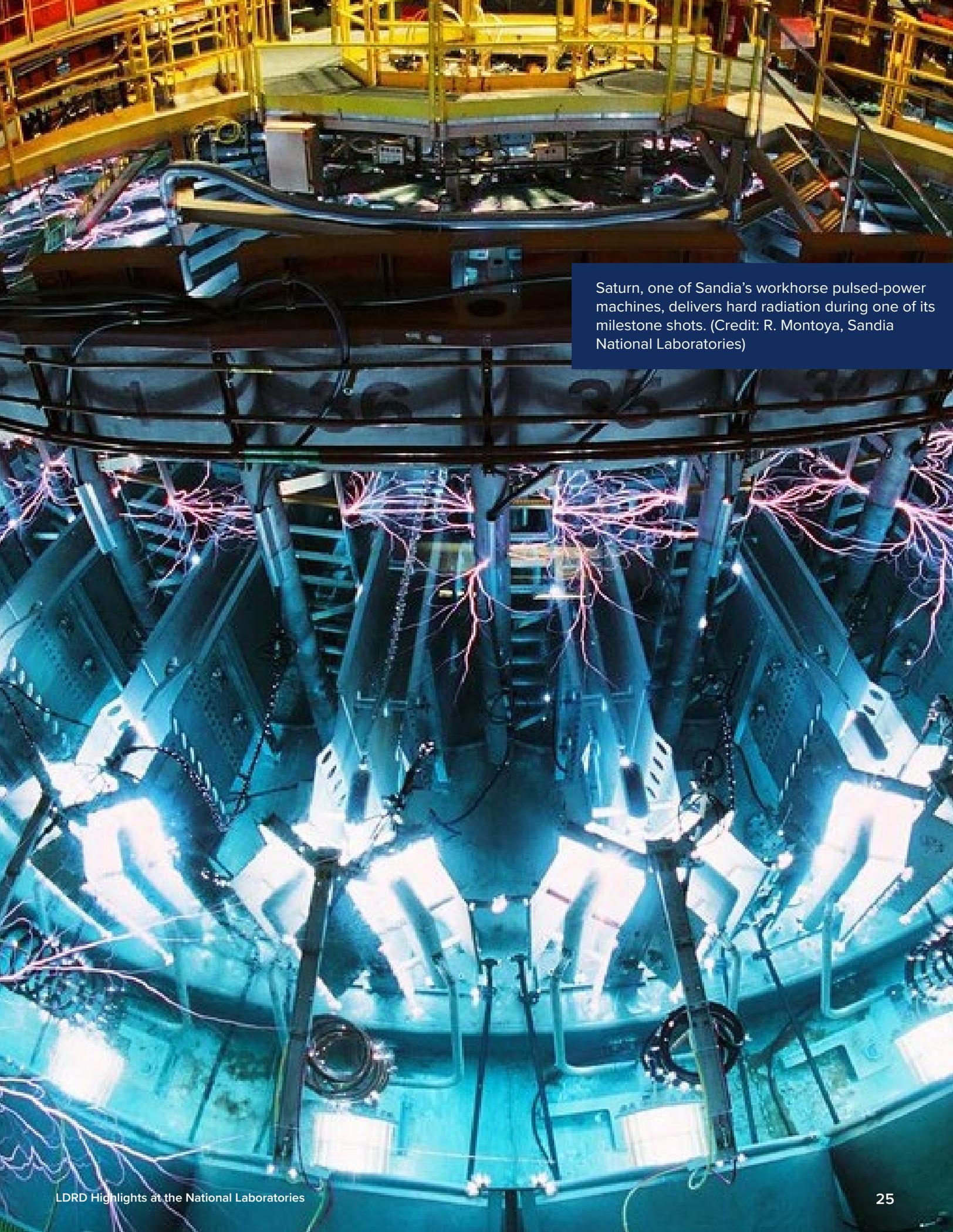
From the program's inception, a priority of LDRD has been to advance basic science and technology to enhance nuclear security through defense, nonproliferation, forensics, and remediation efforts. LDRD projects have made essential contributions to every facet of nuclear security, including stockpile stewardship, high-energy-density research, high-performance computing and simulation, and nuclear and isotopic science.

LDRD researchers have developed unique capabilities to measure microstructural, electrical, and chemical properties of plutonium and its alloys used as the core, or pit, of a nuclear weapon. LDRD projects have examined the effect of decay on crystal structure and resultant changes in material properties, laying the foundations for the weapons laboratories to create "accelerated" aged alloys and thus study the equivalent of 60-year-old plutonium in just 4 years. The most accurate science-based estimates ever obtained for pit lifetimes were derived, with LDRD and subsequent funding, by combining experimental

and computational resources, eliminating the need for a proposed large and costly Modern Pit Facility.

LDRD continues to develop impactful technologies, including proton radiography for imaging materials under shock compression and special materials and processing techniques to make radiation-hardened microchips for use in weapons. LDRD research is also addressing gaps in existing technologies to detect controlled radiological materials that could be smuggled in with cargo at US ports with a new plastic scintillator that responds faster to telltale emissions and discriminates threat materials from benign radiation sources. LDRD is enabling new photonuclear production pathways to make rare and valuable radioisotopes available on demand, as well as modeling of nuclear weapons by studying supernovae. In addition, LDRD continues to play a major role in the next generation of pulsed power.

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  - 30 Uncovering the Mysteries of Supernova Explosions
  - 32 Developing Key Resources in the NNSA Complex
  - 36 Delivering Untold Flexibility for the Construction of Nuclear Deterrence Components with Lattice Metamaterials



Saturn, one of Sandia's workhorse pulsed-power machines, delivers hard radiation during one of its milestone shots. (Credit: R. Montoya, Sandia National Laboratories)

# Making Rare Isotopes that Advance the Science of Energy, Medicine, and Security

IDAHO NATIONAL LABORATORY

*Purified  
radioisotopes  
enable  
breakthroughs  
for nuclear  
energy, medical  
treatment, and  
national security*

## OVERVIEW

Actinium-225 (Ac-225), neptunium-235 (Np-235), neptunium-236 (Np-236), plutonium-236 (Pu-236), and short-lived, low-yield fission product isotopes are critical to nuclear science research areas ranging from advanced nuclear fuels development to astrophysics and fundamental nuclear science. The isotopes Ac-225 and scandium-47 (Sc-47) are needed for new and improved cancer treatments. Increasing

the availability of these isotopes could potentially impact multiple communities of interest. INL scientists are investigating new photonuclear production pathways in combination with novel, rapid chemical separation methods to make rare and valuable radioisotopes available on demand, in larger quantities, at significantly lower cost, and with less radiation exposure than previously possible.

## WHY IT MATTERS

Np-235, Np-236, and Pu-236 are needed as radiotracers for critical nuclear energy research. These isotopes support development of plutonium-238 (Pu-238) power sources for the assessment and development of next-generation nuclear reactor fuels, deep space exploration and research, and material age dating

for nuclear forensics and safeguards. Short-lived, low-yield fission product isotopes are of high interest for expanding the frontiers of basic nuclear science including improving the understanding of the structure of the nucleus. Ac-225 and Sc-47 are highly sought after for providing affordable and effective cancer treatments.

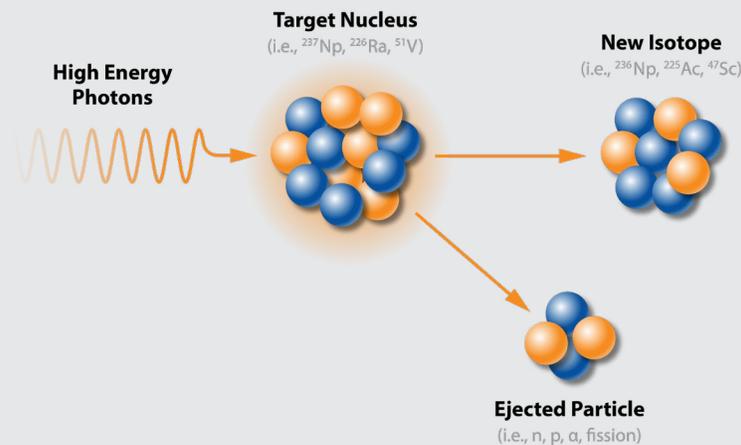


Illustration of the photonuclear reaction process. High-energy photons are impinged on a target material, resulting in the ejection of a portion of that nucleus to produce new isotopes of high value to a range of scientific applications. (Credit: Idaho National Laboratory)

## THE SCIENCE AND IMPACT

Prior to this research, producing large quantities and high purities of critical isotopes and short-lived, low-yield fission products either could not be done or required extremely expensive materials that have limited stockpiles available worldwide. INL researchers developed an innovative approach using high-energy photons that offers high potential for on-site and less-expensive production due to the broader availability of linear accelerators at government laboratories, research institutions, and medical facilities around the world. Many of these new pathways can be designed to use readily available, low-cost, high-purity target materials that produce more pure isotopes of interest when irradiated, resulting in simplified purification processes that reduce the time to purify the isotopes and minimize radiation exposure. For example, the new approach developed through this research to produce Sc-47 utilizes natural vanadium, which is relatively inexpensive and virtually unlimited in supply compared to other techniques. Using a natural vanadium target also avoids harmful gamma radiation from the byproducts produced during Sc-47 production.

As INL proves the viability of these advancements, researchers will expand

into synthesizing heavy lanthanide fission products relevant to the strategic materials needed for energy research and nonproliferation treaty verification. The production pathways developed through this research may provide the only currently viable approaches for access to these rare isotopes.

Researchers at INL have developed and demonstrated many new, tunable chemical separation approaches that are extremely low cost, use commercially available materials, and result in significant breakthroughs in separation timelines. For example, one approach enables isolation of many key fission product isotopes from highly radioactive samples in under 2 hours, instead of 1 week or more using traditional techniques. LDRD-funded work has delivered significant improvement over current techniques in terms of time, chemical recovery, separation, and gamma emissions. The rapid nature, purity, and safety enhancements of the overall processes represents an opportunity for US isotope manufacturers to offer on-demand and on-site rare isotope products and services in the future.

## WHAT'S NEXT

Future work will explore production and scale up operations to harvest these rare and valuable isotopes. The techniques developed through this research can be leveraged by numerous clean energy, nuclear science, medical, and national

security missions. Novel, rapid chemical separations research will also continue to ensure high-quality isotope supply and advance basic actinide science.

***We are improving the supply of critical radioisotopes by creating new production pathways.***

## Publications, Patents, and Videos

Snow, M.S., et al., *Anal. Chem.* **93**(8), 3770–3777 (2021).

Snow, M., et al., *App. Rad. Isot.* (2021, in press).

Snow, M., and Ward, J., *J. Chromatogr. A* **1620**m, 460833–460840 (2020).

Ward, J., et al., *J. Radioanal. Nucl. Chem.* **327**, 307–316 (2021).

Snow, M., and Ward, J., “Methods for Separating Isotopes from a Sample of Fission Products,” US patent no. 10905999, February 2021.

## Acknowledgments

This work was led by PI Mathew Snow and co-investigators Jessica Ward, Jared Horkley, Kevin Carney, and Ari Foley, all of INL. University collaborators included Jon Stoner and John Longley (Idaho State University) and Tara Mastren (University of Utah).

# Enabling the Next Generation of Ultrafast, High-Power Laser Systems

LAWRENCE LIVERMORE NATIONAL LABORATORY

*New capabilities expand mission-critical applications for petawatt-class laser systems*

## OVERVIEW

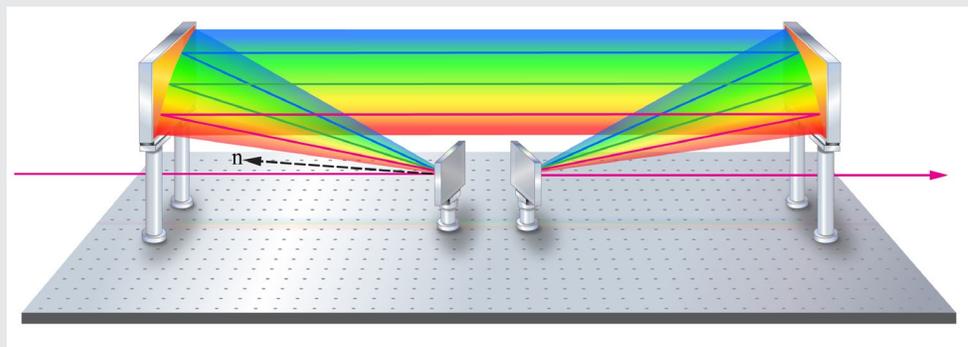
Petawatt (PW) laser technology, developed at LLNL more than 20 years ago, has transformed high-energy-density (HED) science and enabled novel experiments. A pair of LDRD-funded projects started in 2014 explored ways to further advance this technology. Investigators developed two innovations—a new type of diffraction grating and a new pulse-compression

configuration—that enable more than a thousandfold increase in average power for PW laser systems. These solutions also advance PW laser technology beyond providing only a few shots per day to enabling multiple pulses per second, significantly expanding the potential of high-energy PW lasers and ushering in a new regime of high-repetition-rate HED science.

## WHY IT MATTERS

At LLNL, high-power laser systems are used in many mission-critical applications, including generating x-ray and ion beams used for probing, imaging, and radiography in experiments related to stockpile stewardship and HED physics. They also play a key role in

inertial confinement fusion research and its potential to serve as a clean, renewable energy resource. In addition, technology advancements benefit industry in areas such as medical imaging and advanced manufacturing.



The patented out-of-plane pulse-compression method enables use of diffraction gratings at the most efficient angle without causing beam degradation and wasted energy in ultrafast PW laser systems. (Credit: Lawrence Livermore National Laboratory)

## THE SCIENCE AND IMPACT

Investigators addressed two bottlenecks that limited the full potential of high-average-power PW lasers. First, they developed several innovations for diffraction gratings, which are used to compress or stretch a laser pulse. A typical gold grating will absorb 3%–5% of the laser’s energy as it bounces off the grating, leading to beam loss, while also generating heat that distorts the beam. The team demonstrated a new approach to actively cool the gratings, along with a multilayer dielectric design that results in less energy absorption. These solutions make it possible to tolerate much higher laser power without causing thermally induced mechanical distortions that negatively

impact laser beam output. Researchers also developed a new design for chirped-pulse amplification, a technique for stretching out the laser pulse before amplification and providing subsequent compression to achieve very high laser power. This new “out-of-plane” method is now a patented technology. It allows gratings to be utilized at any angle so the most efficient angle can be employed without causing beam degradation and wasted energy. Together, these innovations enable higher-quality PW lasers, with a higher power per pulse, as well much higher repetition rates.

## WHAT’S NEXT

LLNL physicists are working to implement this technology in several new high-intensity laser projects. LLNL scientists leveraged these developments in collaboration with other experts to build the High-Repetition-Rate Advanced Petawatt Laser System (HAPLS) for the European Union’s Extreme Light Infrastructure Beamlines facility. At the time it was delivered to the facility in 2017, HAPLS was the world’s most advanced PW laser system. These concepts are also being integrated into the design for a major upgrade to the Linac Coherent Light Source at DOE’s SLAC National Accelerator Laboratory.

High-intensity lasers with increased power and unprecedented repetition rates will also enable transformational research in HED science, such as providing a substantial increase in data volume to aid studies while opening doors to couple these efforts with emerging technologies such as cognitive simulation. These capabilities will allow for impactful HED assessments on an ever-faster timescale while also fostering our nation’s leadership in laser-driven discovery science.

***Investigators addressed two bottlenecks that limited the ability to fully realize the potential of high-average-power petawatt lasers.***

## Publications, Patents, and Videos

Alessi, D.A., et al., *Opt. Laser Technol.* **117**, 239–243 (2019).

Alessi, D.A., et al., *Opt. Express* **24**(26), 30015 (2016).

“Symmetric Out-of-Plane Configurations of Diffractive Gratings and Method,” US patent no. 10,594,106 B2.

[S&TR Preview: Groundbreaking Laser Set to Energize Science \(video\)](#)

## Acknowledgments

The multidisciplinary team includes staff and postdoctoral researchers from several LLNL research directorates, including experts in HED physics and photon science, as well as staff from LLNL’s National Ignition Facility. Key team members include Emily Link, Constantin Haefner, Michael Aasen, David Alessi, Jerald Britten, Hoang Nguyen, and Paul Rosso.

# Uncovering the Mysteries of Supernova Explosions

LOS ALAMOS NATIONAL LABORATORY

*Multidisciplinary understanding of cosmic explosions leads to advances in nuclear security*

## OVERVIEW

Supernovae—luminous stellar explosions—are among the most powerful explosions in the universe and are produced in the most extreme matter conditions (i.e., a trillion times more dense than anything on Earth). By leveraging LANL physics and computational expertise, LDRD researchers diagnose the details of these explosions and probe the extreme

physics behind them. Decades of LDRD investments in this area have resulted in many applications to nuclear security, directly impacting the National Nuclear Security Administration's (NNSA's) Advanced Simulation and Computing (ASC) program. Work in this area involves training scientists in holistic approaches and recruiting new scientists to the laboratory.

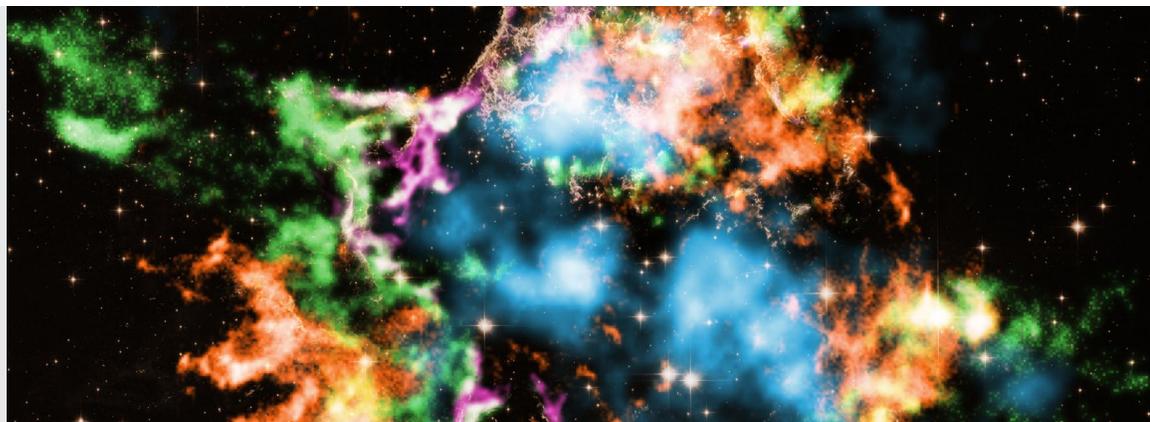
## WHY IT MATTERS

Over three decades ago, astronomers spotted one of the brightest exploding stars in more than 400 years—Supernova 1987A—which revolutionized our understanding of the progenitors and engines of astrophysical transients. Observational evidence of turbulence in all aspects of the progenitor evolution and the explosion mechanism shattered our current understanding, driving computer simulations of these engines and pushing the envelope in multidimensional modeling.

Multiphysics modeling is important in many of the key applications studied at LANL,

from inertial confinement fusion to stockpile stewardship. Like astrophysicists, scientists in national security need to validate their computer codes, and because much of the underlying physics driving these models is the same, scientists working in national security are able to test their codes using supernovae data. Supernovae explore conditions more extreme than any we can generate on Earth, even at the world's brightest lasers like LLNL's National Ignition Facility (NIF), and models are validated against supernova observations like those of the Cassiopeia A supernova remnant.

NASA's Chandra X-ray Observatory has captured unparalleled x-ray images of many supernova remnants, such as Cassiopeia A. (Credit: NASA)



## THE SCIENCE AND IMPACT

LANL researchers developed the first 3D simulations of the inner engine behind supernovae in 2002. Over nearly two decades, LDRD-funded researchers have extended the laboratory's broad expertise to study other transients and follow these explosions from their central engine to the outbursts, studying and probing both HED physics and matter in the extremes.

Understanding cosmic explosions requires combining a broad range of physics expertise—dense matter, neutrinos, plasma physics, radiation transport, and atomic physics—and the computing and computational science to develop the multiphysics simulations that bring the physics together. Observations of these

events include transient outbursts in a wide range of wavelengths, gamma rays from the decay of radioactive isotopes, gravitational waves, cosmic rays, and neutrinos.

Astrophysicist and LDRD researcher Christopher Fryer and collaborators have developed new computational tools, open-sourcing a number of tools to model astrophysical transients (e.g., SNSPH, NuBHlight, SuperNU). The team also works within the ASC program, facilitating information exchange between the computational science community and ASC. This effort has led to the formation of the Center for Theoretical Astrophysics.

## WHAT'S NEXT

Fryer's team is actively building collaborations with scientists at LANL, in the broader DOE complex, and in academia, specifically those working on LANL's ASC effort, the Toward Exascale Astrophysics of Mergers and Supernovae Scientific Discovery through Advanced Computing collaboration, and the Exascale Computing Project. These collaborations will lead to advances across programs, producing bleeding-edge technology to solve problems in science and national security alike and training a new generation of scientists capable of leading this new technology.

Fryer's team is developing next-generation computational approaches, working with DOE's new nuclear physics facility for rare isotope beams and HED physics facilities (e.g., Omega, NIF, z-pinch) and ground- and space-based astrophysics facilities (e.g., LANL's RAPTOR, University of California's Lick and Keck Observatories, Laser Interferometer Gravitational-Wave Observatory). Fryer's team also is working with NASA to address new proposals for transient missions ranging in wavelength from optical to gamma rays.

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***We've learned more about how to model a nuclear weapon by modeling supernovae.***

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## Publications, Patents, and Videos

Korobkin O., et al., *ApJ* **910**, 116 (2021).

Miller J.M., et al., *ApJ* **902**, 66 (2020).

Vance G.S., et al., *ApJ* **895**, 82 (2020).

## Acknowledgments

The LDRD work was led by Christopher Fryer and many other LANL researchers, including Aaron Couture, Aimee Hungerford, Samuel Jones, Sanjay Reddy, and Mike Warren.

# Developing Key Resources in the NNSA Complex

## NATIONAL NUCLEAR SECURITY ADMINISTRATION FACILITIES

***NNSA facilities provide critical national security capabilities***

### OVERVIEW

LDRD-funded research frequently sparks efforts to establish new multidisciplinary capabilities and facilities, which expand research horizons and offer our nation innovative resources that can address emerging national security needs. Time and again, LDRD investments have positioned NNSA facilities at the cutting edge of science, making the agency ready to meet current and evolving mission needs.

#### **National Center Analyzes Atmospheric Releases of Hazardous Materials**

The National Atmospheric Release Advisory Center (NARAC) at LLNL plays a key role in our nation's efforts to predict and respond to atmospheric hazards. Staffed by a multidisciplinary team of experts in data science, physics, chemistry, and atmospheric science, NARAC supports planning, real-time assessment, emergency response, and studies regarding intentional and accidental atmospheric releases of nuclear, radiological, chemical, and biological materials.

NARAC was established in 1979 following the Three Mile Island nuclear power plant accident. Over the last four decades, it has responded to hundreds of alerts, accidents, and disasters, while also conducting studies to enhance its predictive capabilities and refine the nation's consequence

management resources. More than a dozen LDRD-funded projects at LLNL have enabled NARAC to remain at the forefront of predictive modeling and analysis of events with potential national security implications, including nuclear forensics and nonproliferation, as well as industrial accidents, volcanic plumes, and fires.

LDRD funds spanning 2007 to 2016 supported studies of atmospheric source reconstruction, incorporating meteorological data into forecast dispersion models and leveraging LLNL's high-performance computing resources and large datasets to better characterize and quantify uncertainties. Today, these tools are part of NARAC's suite of analytical resources. For one project, investigators developed a nuclear cloud rise and fallout model for use in modeling detonations, building on work from a previous LDRD-funded project for which scientists developed models to improve local-scale simulations of atmospheric flow. For another project, scientists developed a new machine learning capability to quickly estimate and incorporate weather uncertainty into atmospheric dispersion assessments conducted at NARAC. NARAC staff currently serve on LDRD-funded research teams exploring wildfire simulation and postdetonation phenomenology, continuing the legacy of leveraging LDRD investments to enhance mission-critical technical capabilities.



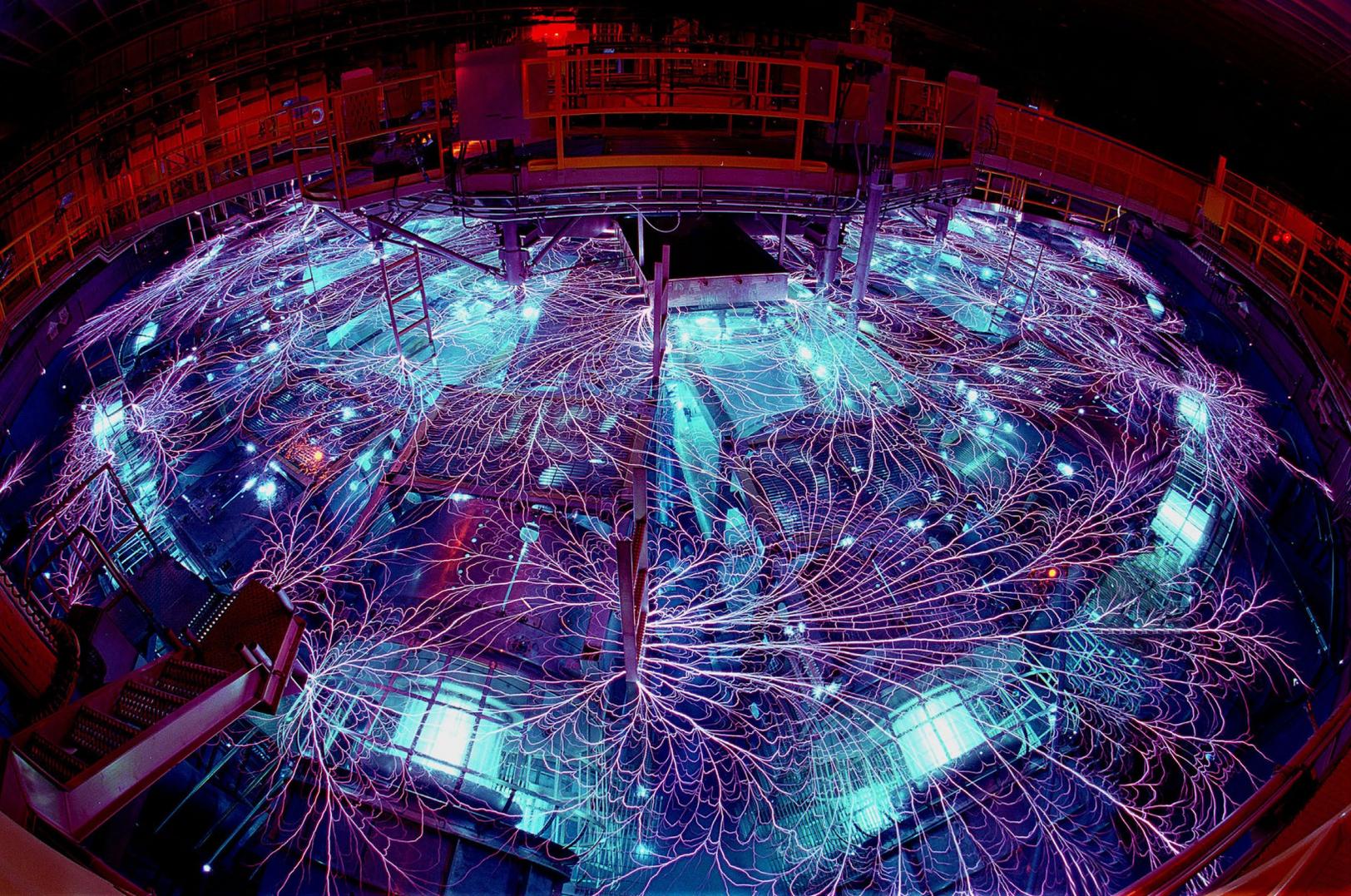
LDRD investments enable NARAC to remain at the forefront of predictive modeling, real-time assessment, and analysis of events with potential national security implications. (Credit: Lawrence Livermore National Laboratory)

### **Nation's Premier Plutonium Manufacturing and Science Facility**

The nation's premier plutonium manufacturing and science facility at LANL supports missions from pit manufacturing and surveillance, to plutonium recovery, to deep space exploration. The Los Alamos Plutonium Facility (PF-4) at Technical Area 55 carries out the chemistry and metallurgy for recovering, purifying, and converting plutonium and other actinides. Doing so requires safely and securely shipping,

receiving, handling, and storing nuclear materials, as well as minimizing the wastes and residues thereby produced. PF-4 was designated the nation's Plutonium Center of Excellence for R&D by NNSA in 2008.

We will succeed at the expanded plutonium pit mission only by making large advancements in efficiency and compliance, and LDRD program funding is integral to both. For example, a team of LDRD researchers has developed a



Created to validate nuclear weapons models, Sandia's Z machine is also in the race for viable fusion energy. (Credit: R. Montoya, Sandia National Laboratories)

solution for safely decontaminating aging gloveboxes, the large containers in which nuclear materials can be manipulated without human contact. Another LDRD team has developed a system for nondestructive testing of containers used throughout PF-4 for nuclear materials storage. Properly tested, the containers can be used for years, but without recertification they join the waste stream.

Sustained investments in LDRD continue to ensure PF-4 remains agile while responding to increased demands. For example, an LDRD-funded Director's Initiative aims to modernize, streamline, and optimize quantitative nuclear material measurements and nuclear material control and accounting.

The team is using modern data analysis and statistical approaches coupled with optimized nondestructive assay instruments. Success will enable continuous materials monitoring, making interruptions for manual inventories a costly thing of the past.

### **Z Machine: The World's Most Powerful and Efficient Laboratory Radiation Source**

Sandia National Laboratories' Z machine uses high magnetic fields associated with high electrical currents to produce high temperatures, high pressures, and powerful x-rays for research in HED science. Part of Sandia's Pulsed Power program, the Z machine creates conditions found nowhere else on Earth. Having a laboratory-based high-yield fusion capability within the nuclear weapons complex creates an experimental platform for assuring the

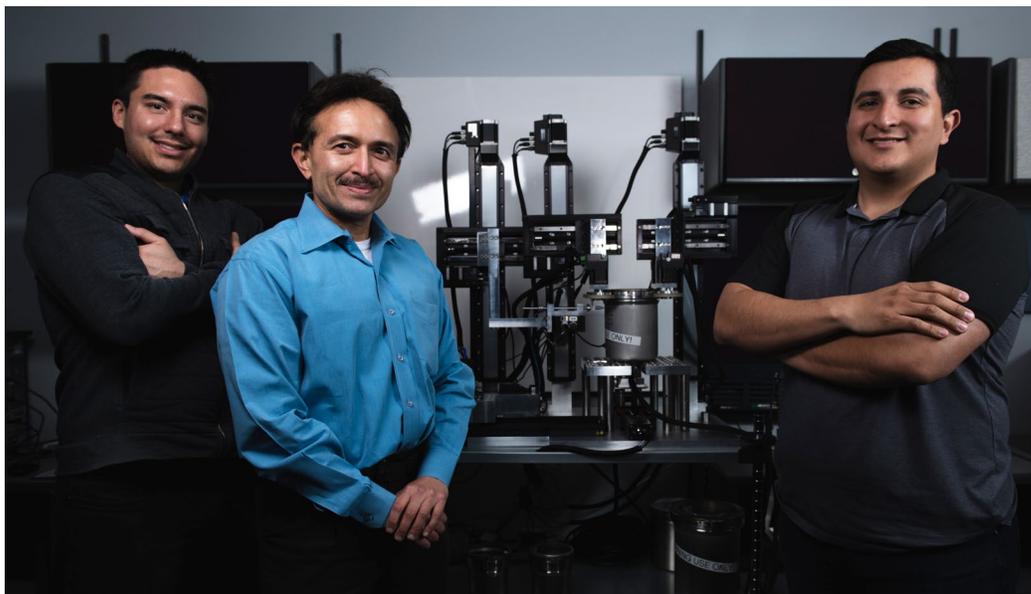
US nuclear weapons stockpile will perform far into the future.

The Z machine creates HED conditions that provide data and experience to the modeling and design community in dynamic material properties, nuclear survivability and radiation effects, and inertial confinement fusion. Because the yield from the nation's nuclear weapons is generated when conditions within the explosive package are in the HED state, proficiency in HED science must remain a core technical competency into the future.

Since 2005, LDRD investments have helped advance new HED platforms, which have subsequently impacted DOE programs and enabled NNSA milestones. LDRD-funded HED research has spanned topics such as advanced fusion concepts, hostile environments, dynamic temperature measurements, high-

pressure/precompression cells for planetary and stellar science, stochastic shock in advanced materials, and certifiable additive manufacturing techniques.

LDRD continues to play a key role in the next generation of pulsed power. The Assured Survivability and Agility with Pulsed Power (ASAP) LDRD Mission Campaign is a set of targeted investments spanning FY 2020–FY 2026 focused on enabling critical testing capabilities, providing validation data for national security threats, and conducting qualification assessments for conventional and nuclear systems in hostile environments. ASAP R&D is expected to help inform the design for a next-generation pulsed power facility providing 10× the energy of the current Z machine. This new facility could address several key issues in weapon science, dynamic materials, effects modeling, and fusion research not possible at existing NNSA facilities.



Jonathan Gigax, Raj Vaidya, and Jose Parga (left to right) stand with their Modular Integrated Non-destructive Test System, or MINTS, which allows for determining structural health of ubiquitous nuclear material containers at PF-4 without ruining the containers. (Credit: Los Alamos National Laboratory)

# Delivering Untold Flexibility for the Construction of Nuclear Deterrence Components with Lattice Metamaterials

SANDIA NATIONAL LABORATORIES

*New multimode metastructures will meet mission requirements and provide flexible implementation for future needs*

## OVERVIEW

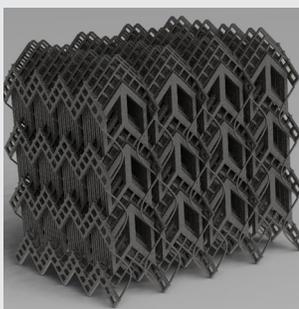
From the printing of a simple eye-wash cup in 1983 to a lattice “metamaterial” in 2020, 3D printing allows visionaries to revolutionize what is possible when it comes to the creation of multi-dimensional objects. By leveraging modern 3D-printing capabilities, Sandia developed programmable materials (i.e., modern versions of foams and

honeycomb structures) that convey extremely beneficial properties such as high strength-to-weight ratio and energy absorption. By adjusting the structure’s shape and topology, in addition to the constituent base material, the lattice metamaterials become tunable, allowing them to be customized for the mission application and its projected environment.

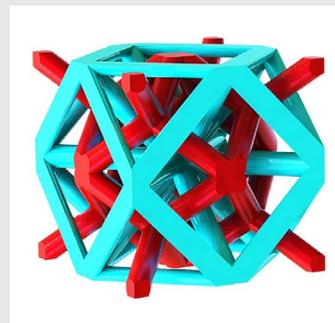
## WHY IT MATTERS

Nuclear deterrence mission applications must be extremely dependable in the harshest environments. Components must perform even when they undergo extreme vibration, experience significant shock/impact, encounter blistering temperatures and intense radiation, or are subjected to crushing. Conventional materials are produced through heat and pressure and

are limited by complex, indirect control of fundamental thermodynamic and kinetic processes, and new alloys often take a decade to develop. Because of the agility provided by this LDRD research, new 3D metamaterials can be rapidly adjusted to address a new set of performance requirements brought about by ever-changing national security threats.



This cathedral-like metamaterial has internal features that rub against each other to naturally absorb shocks and dampen vibration. A Sandia patent now covers the concept of using friction in metamaterials for this purpose. (Credit: Sandia National Laboratories)



CAD model of the dual polyhedra interpenetrating lattice unit cell. Sandia’s interpenetrating lattices are simple adaptations of ancient geometric principles brought to life through additive manufacturing. (Credit: Sandia National Laboratories)

## THE SCIENCE AND IMPACT

Through this project, Sandia also discovered unique lattice topologies, such as one termed an “interpenetrating lattice.” The team tiled this mathematical notion into a physically realized 3D lattice architecture, providing for a completely new way to manage energy transfer, whether it be thermal, mechanical, or electrical. While traditional lattices, such as the honeycomb, transmit energy through their continuously interconnected struts or walls, interpenetrating materials throttle energy

transmission through interactions between surfaces. This remarkable capability limits vibration transmission and stress. The team also found they could control how cracks formed and propagated by embedding intentional porosity into an otherwise brittle lattice. The hierarchical design, which was actually lighter than the original baseline design, resulted in a substantial improvement in the material’s resistance to fracture, more than sixfold in some cases.

## WHAT’S NEXT

The team is evaluating how computational models can be leveraged in the discovery and optimization of structures needed for applications such as a metal with rubber-like properties that can conduct electricity for survivable power grid applications or a high-temperature rocket nozzle that is soft to the touch and survives impact landings. They are also exploring how computational homogenization techniques and emerging machine learning codes might be employed to address a combination of multiple performance requirements while

simultaneously constraining the solutions to only those that are manufacturable.

The benefits of 3D-printed lattice materials are far reaching and could significantly improve applications across the defense, transportation, energy, biomedical, and consumer sectors. Already, this LDRD project has led to full and provisional patents and two spin-off programs. Two postdoctoral researchers hired for the project have joined the Sandia staff.

## Publications, Patents, and Videos

Alberdi, R., et al., *Mater. Des.* **194**, 108883 (2020).

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Garland, A.P., et al., *Additive Manuf.* **38**, 101741 (2021).

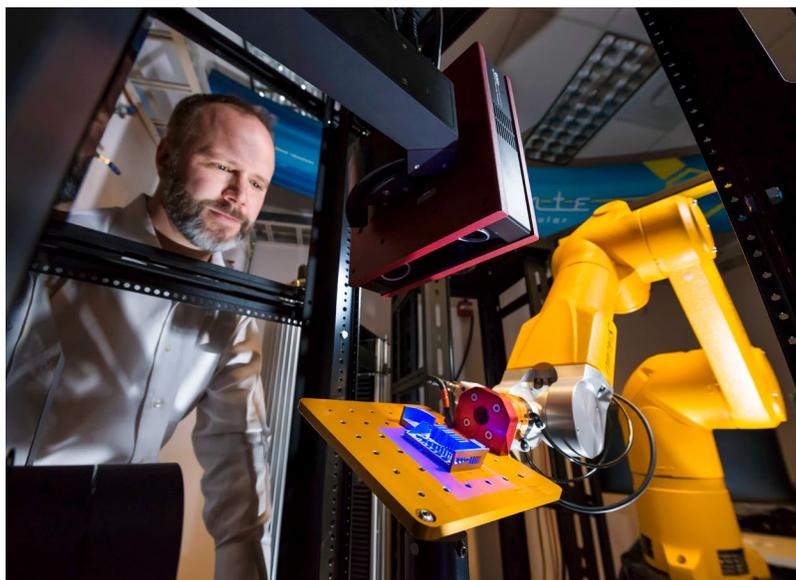
Garland, A.P., et al., *Mater. Des.* **203**, 109632 (2021).

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## Acknowledgments

The multidisciplinary LDRD team was led by PI Brad Boyce, who received the Brimacombe Medal from the Minerals, Metals & Materials Professional Society in 2020 for sustained excellence and achievement related to minerals, metals, or materials science and engineering.



Sandia materials scientist Brad Boyce watches as a 3D-printed part is scanned. Modern 3D-printing capabilities were leveraged to create the interpenetrating lattice metamaterials. (Credit: R. Montoya, Sandia National Laboratories)

***The tuned metal lattice materials will enable greater design flexibility for future weapon systems.***

# Scientific Innovation & Discovery

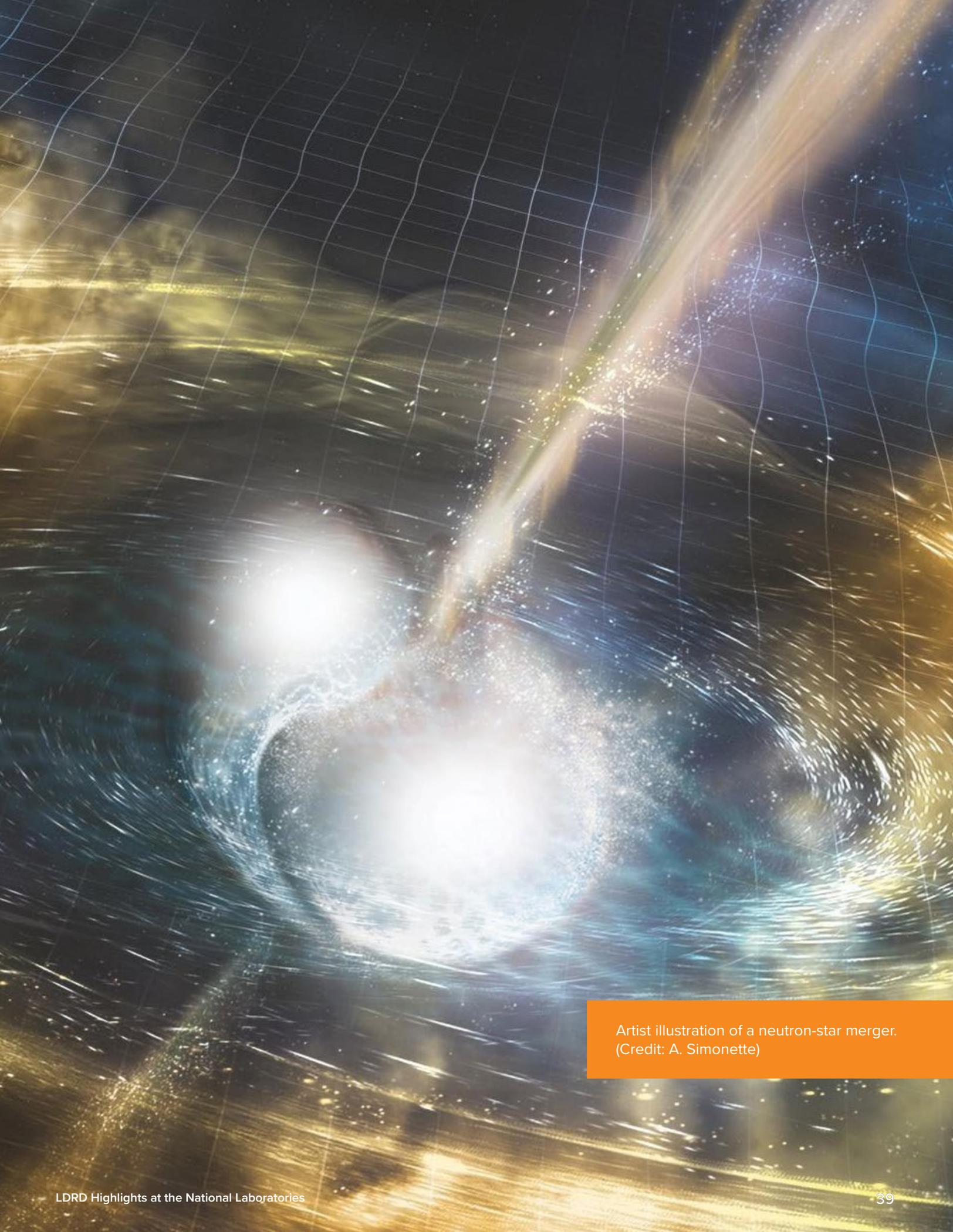
The LDRD Program is a major vehicle of scientific innovation vital to the national laboratories, allowing scientists to respond to national priorities, evolving opportunities, and challenges with speed, flexibility, and rigor. Discovery at such an accelerated pace continues to deliver transformative scientific and technological advances across the breadth of fundamental and applied science programs of the DOE mission, while seeding new scientific directions within them.

As noted in the 2015 DOE Basic Energy Sciences Advisory Committee report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*, “success requires a sustained campaign of strategic investments that initiates new research thrusts, attracts and sustains a leading scientific workforce having the necessary skills, and provides the innovative instruments and tools with which

to carry out the work.” LDRD funds target DOE mission challenges while leveraging the world-class expertise of our national laboratories.

Scientific Innovation and Discovery projects demonstrate discoveries in applied materials sciences, biosciences, and cosmology, as well as important developments in data analysis and materials characterization techniques. Modern silicon sensors for precision applications developed with LDRD funding offer transformative solutions to tracking systems in collider experiments. Breakthrough techniques supported by LDRD to measure vast cosmological distances are providing key insights into the nature of dark energy. Technologies developed under the LDRD Program that can be used to convert municipal waste and biomass into renewable materials are advancing our goals for decarbonization.

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  - 44 Delivering a Breakthrough for Cosmology
  - 46 Enabling Spectroscopy of Quantum Matter under Extreme Pressure
  - 48 Combining Renewable Electrons with Carbon Waste for Sustainable Chemicals and Materials
  - 50 Tuning In to Dark Matter with an Exquisitely Sensitive Radio
  - 52 Increasing Particle Accelerator Reliability with Machine Learning



Artist illustration of a neutron-star merger.  
(Credit: A. Simonette)

# Speeding Up X-Ray Coherent Diffraction Imaging with Trained Neural Networks

ARGONNE NATIONAL LABORATORY

*Artificial  
intelligence  
enables  
real-time  
imaging*

## OVERVIEW

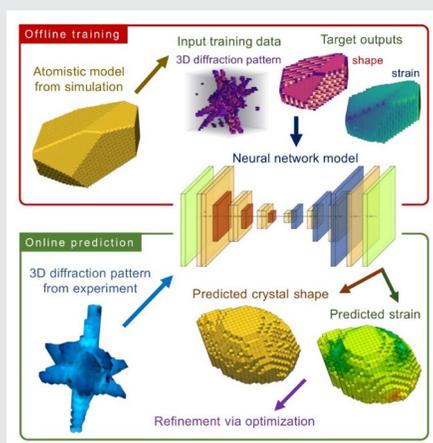
X-ray coherent diffraction imaging (CDI) uniquely provides images of nanometer-scale structures and strains deep inside materials, but the method is currently too slow to yield such images in real time, making experiments involving dynamic processes very difficult. The reason is that one portion of the diffraction data (i.e., the phases) must be calculated

using time-consuming mathematical procedures. This project demonstrated that deep convolutional neural networks (NNs) can reconstruct high-quality images from CDI data in record time by bypassing the mathematical steps. This type of real-time image reconstruction has the potential to revolutionize advanced imaging techniques that rely on such mathematical procedures.

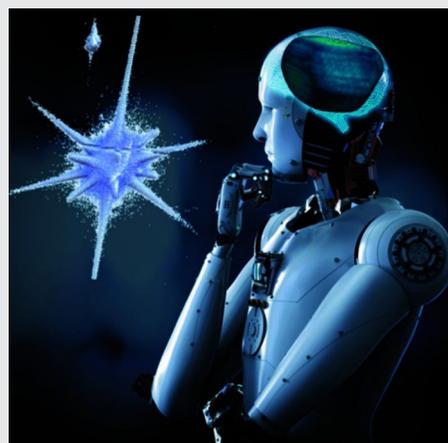
## WHY IT MATTERS

Synchrotron x-ray beamlines dedicated to CDI already produce much more diffraction data than traditional methods of image analysis can handle in real time. The data overload will only worsen as major synchrotron facilities around the world undergo upgrades. Argonne's Advanced Photon Source (APS), for example, will soon undergo a massive upgrade that

will increase the brightness of its x-ray beams by up to 500 times, yielding a similar increase in data production. "We were concerned that after the upgrade, data rates will be too large for traditional methods of imaging analysis to work," explains project member Mathew Cherukara. "Artificial intelligence methods can keep up by producing images hundreds of times faster."



Physics-aware artificial intelligence framework for nanoscale structure and strain reconstruction in 3D Bragg CDI. The artificial intelligence performs rapid predictions after being trained using atomistic simulations. (Credit: H. Chan et al., 2021)



A robot equipped with artificial intelligence inspects a coherent diffraction pattern and directly forms an image of the sample. (Credit: R. Harder, 2021)

## THE SCIENCE AND IMPACT

The project began by developing CDI NN, a deep convolutional NN. Once trained, this network could accurately produce images of test data within a few thousandths of a second on a standard desktop computer, thousands of times faster than with the repetitive mathematical procedures currently in use. CDI NN is not hindered by the presence of large strains in the material being imaged and can operate on coarser datasets.

The project also developed PtychoNN, a deep convolutional NN designed to bypass the repetitive image-reconstruction steps associated with ptychography, which is used to image large volumes in thick samples by scanning a coherent x-ray beam across a sample while measuring the scattered x-ray intensities. Repetitive image analysis methods require that adjacent measured scan points overlap by at least 50%. PtychoNN learns to directly image a sample's structure and strain characteristics and, once trained, is hundreds of times faster than high-performance mathematical software. In addition, PtychoNN does not

require data overlaps, further accelerating data acquisition and reconstruction by a factor of five.

The project's final major activity involved 3D-CDI-NN, which was designed as the most accurate approach to directly imaging a sample's structure and strain characteristics. 3D-CDI-NN is a deep convolutional NN and differential programming framework that can be trained to predict 3D structure and strain characteristics solely from 3D x-ray coherent diffraction data. 3D-CDI-NN is "physics aware" in that the physics of the x-ray scattering process is explicitly enforced in the training of the network, and the training data are drawn from atomistic simulations representative of the physics of the material under study. Predictions are further refined through a physics-based optimization procedure that enables maximum accuracy at lowest computational cost. 3D-CDI-NN can image structures and strains hundreds of times faster than traditional repetitive methods, with negligible losses in accuracy.

## WHAT'S NEXT

The project team is now working to develop a method whereby NNs will train themselves and improve with each subsequent experiment. This will allow the

NNs to become more accurate in their predictions without requiring human guidance or feedback.

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***We are working on a method whereby neural networks will train themselves and improve continuously.***

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## Publications, Patents, and Videos

Harder, R., *IUCrJ* **8**(1), 1–3 (2021). <https://doi.org/10.1107/s2052252520016590>.

Chan, H., et al., *Appl. Phys. Rev.* **8**, 021407 (2021). <https://doi.org/10.1063/5.0031486>.

Cherukara, M.J., et al., *Appl. Phys. Lett.* **117**, 044103 (2020). <https://doi.org/10.1063/5.0013065>.

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## Acknowledgments

This material is based upon work supported by LDRD funding from Argonne National Laboratory, provided by the Director, Office of Science, of the US Department of Energy under contract no. DE-AC02-06CH11357. The team members are Mathew Cherukara (APS, Argonne), Ross Harder (APS, Argonne), Henry Chan (Center for Nanoscale Materials, Argonne), Subramanian Sankaranarayanan (Center for Nanoscale Materials, Argonne), Youssef Nashed (SLAC National Accelerator Laboratory, formerly of the Mathematics and Computer Science Division, Argonne).

# Developing Innovative Silicon Sensors for Next-Generation Particle Tracking Systems for Collider Experiments

BROOKHAVEN NATIONAL LABORATORY

*Modern silicon  
sensor  
technologies  
enable scalable  
and ultimate  
precision 4D  
particle tracking  
systems*

## OVERVIEW

The capability of a precise reconstruction of the position and time of the particles emerging from interactions of colliding beams is a key challenge for future particle and nuclear physics experiments at the next generation of colliders, including the Electron-Ion Collider at Brookhaven and the Future Circular Collider at the European

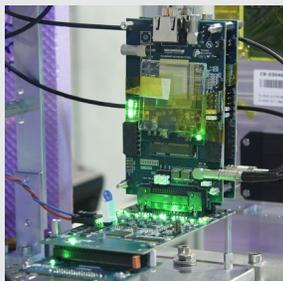
Organization for Nuclear Research (CERN). The project focused on development and evaluation of three innovative silicon-based technologies: high-voltage complementary metal-oxide-semiconductor (CMOS) sensors, low-gain amplification devices (LGADs), and monolithic active pixel sensors (MAPS).

## WHY IT MATTERS

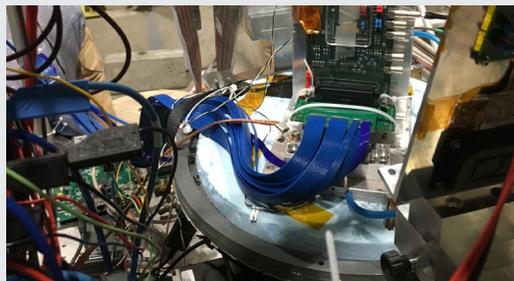
Silicon detector technology is the mainstay of today's collider experiments, enabling precise measurement of the position of charged particles. Since its first use at CERN in the 1980s, incremental steps have been made to improve signal collection efficiency, position resolution, radiation resistance, and production techniques. Future detectors will require faster response and extreme precision, minimal detector mass, and power consumption. Scalability to larger areas (400–500 m<sup>2</sup> of silicon) introduces significant challenges with regard to required performance and production costs.

The different technologies explored in the project target innovative solutions for overcoming the aforementioned challenges:

- CMOS technology enables the use of production facilities with a very high degree of standardization, quality assurance, and production throughput.
- LGADs provide a controlled amplification of the ionization charges, enhancing signal-to-noise ratio and achieving precise timing information (10–50 ps).
- MAPS, integrating the sensing device with the readout, eliminate the need for most of the several billions of pixel interconnecting bondings that would be required with the



LEFT: Dedicated readout boards used for the characterization of the silicon sensor. (Credit: Brookhaven National Laboratory)



RIGHT: Test beam setup at CERN. (Credit: Brookhaven National Laboratory)

current technologies, significantly reducing production costs.

MAPS have been used in experiments at colliders, but their overall performance does not yet compete with traditional sensors for speed and radiation hardness. However, the push toward thinner devices for better performance and the recent availability of fabrication techniques in a wider range of industrial processes

## THE SCIENCE AND IMPACT

The project has pioneered the development at Brookhaven of modern silicon-based technologies for precision applications. BNL researchers, collaborating with US and international organizations, have developed and characterized LGADs. At CERN, they also tested prototypes designed by collaborators in Spain, measuring a time resolution to better than 30 ps on 1.3×1.3 mm<sup>2</sup> pads, suitable for precision timing measurements in high-luminosity hadron colliders. Such devices are an essential tool to mitigate the pileup effects of several hundred interactions in a single collision event.

A dedicated readout system was developed for the characterization of

will outpace and overcome the more traditional approach in the next few years.

These technologies may also impact other fields, such as high-precision/fast-readout sensors for dynamic structural analysis in time-resolved crystallography, beam monitoring at photon science facilities, and medical applications, such as precision timing-based positron emission tomography.

high-voltage CMOS sensors and of a MAPS prototype, ATLASPix1, measuring an in-pixel efficiency of 99.4%. This program supported the PI to initially coordinate the High-Granularity Timing Detector (HGTD) proposal in the ATLAS (A Toroidal LHC ApparatuS) experiment, leading to its technology baseline selection. LGADs have since become the selected technology for the ATLAS HGTD and the Compact Muon Solenoid detector Endcap Timing Layer, approved by the CERN Research Board as part of the official scope of the High Luminosity Large Hadron Collider (LHC) upgrades of the two experiments. The evolution of the ATLASPix1 design is an option for the LHC-beauty (LHCb) Upgrade of the Inner Tracker detector in the early 2030s.

## WHAT'S NEXT

These investigations will naturally lead to development of 4D-MAPS, enabling the simultaneous precise reconstruction of the particle's position and time. This project

has directly seeded another LDRD activity for silicon sensors for photon sciences and the ongoing Early Career Award program of one of the collaborating scientists.

***Space-time reconstruction of extraordinarily complex events occurring in the highest-energy collisions is a key challenge for particle accelerators.***

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## Acknowledgments

The program was carried out by BNL researchers H. Chen, K. Chen, G. Giacomini, J. Kierstead, F. Lanni, H. Liu, E. Mountricha, S. Stucci, A. Tricoli, and L. Xu and was enabled by a prolific collaboration with US and international institutions, including the Universities of Bern and Geneva (Switzerland), CERN, the Institute for High Energy Physics and the Centro Nacional de Microelectronicas in Barcelona (Spain), the University of Heidelberg and the Karlsruhe Institute of Technology (Germany), the University of Liverpool (United Kingdom), Orsay and the University of Paris VI-VIII (France), and the University of California–Santa Cruz (California).

# Delivering a Breakthrough for Cosmology

FERMI NATIONAL ACCELERATOR LABORATORY

*A new scientific field combines optical and gravitational-wave observations*

## OVERVIEW

When the National Science Foundation (NSF)-funded Laser Interferometer Gravitational Observatory (LIGO) and the Virgo Gravitational Observatory in Italy reported the gravitational-wave “chirp” of a binary neutron-star merger in 2017, scientists working with the DOE-funded Dark Energy Camera mounted on the Blanco telescope in Chile sprang into action. The Fermilab LDRD project enabled quick comparison of real-

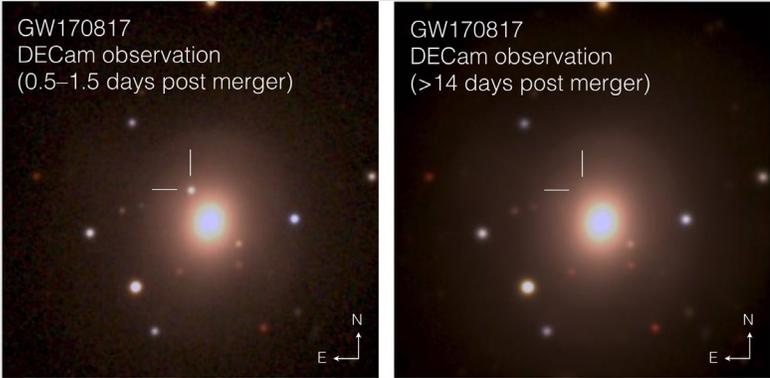
time camera images with previously collected images to flag differences and immediately alert scientists at other telescopes. This led to the co-discovery of the bright optical counterpart of the associated “Kilonova” in Galaxy NGC 4993, the first-ever observation of both optical and gravitational-wave signals of the same cosmic event. These observations initiated the new field of Multiple Messenger Astronomy (MMA).

## WHY IT MATTERS

Dark energy is responsible for the ever-increasing acceleration of our universe. Understanding its nature requires breakthrough techniques to measure vast cosmological distances. Gravitational-wave “chirp” events from the in-spiral of massive bodies are theoretically well understood and can serve as standard distance candles or “sirens.” The project used the DOE-supported Dark Energy Camera to discover and measure probable optical

counterparts of gravitational-wave events enabling optical measurements of the cosmic expansion rate. This effort has grown into a full program to establish optical counterpart red-shift observations as standard sirens with techniques developed in cosmological surveys.

This project supported construction of a “fast difference imaging pipeline” to process real-time images from the Dark



Comparison images before and after the 2017 gravitational-wave event (GW170817) and its host galaxy, NGC4993. (Credit: DES collaboration)

Energy Camera and quickly compare these with previously collected images and flag differences. Once ruled out as possible asteroids, variable stars, or supernova, new objects were passed quickly to collaborating telescopes for fuller astrophysical characterization.

When LIGO first detected a binary black hole merger in 2015, the Dark Energy Camera optical counterpart search validated no optical counterpart, as expected with the dark merger of black holes. When LIGO and the Virgo gravitational-wave observatory in Italy first detected a binary neutron-star merger in 2017, the Dark Energy Camera optical counterpart search detected an expected

bright optical counterpart, leading to co-discovery of the associated “Kilonova” in Galaxy NGC 4993.

These observations initiated the exciting new field of MMA and resulted in a publication with thousands of co-authors in which LIGO, other gravitational observatories, NASA’s space-based Fermi-GRB gamma ray observatory, and many ground- and space-based telescopes reported the joint gravitational wave and electromagnetic observations. PI Marcelle Soares-Santos discussed MMA at the 2017 NSF press conference, announcing observation of the first binary neutron-star merger.

## THE SCIENCE AND IMPACT

The discovery of an optical counterpart to a gravitational-wave event allowed the first cosmological measurement with gravitational waves: a constraint on the expansion rate of our universe independent of previously established cosmic distance metrics based on supernovae and precision fit of Cosmic Microwave Background (CMB) fluc-

tuations. The supernova and CMB measurements of the expansion rate presently disagree at the 3–5  $\sigma$  level. Gravitational-wave measurements of the expansion rate make a promising new tool to further understand and contribute to resolution of this tension.

## WHAT’S NEXT

Having added standard sirens to the scientific lexicon as a powerful experimental cosmology tool, we can perform precise and accurate new measurements using upcoming data from the DOE-supported surveys, Dark Energy Spectroscopic Instrument and Legacy Survey of Space and

Time, and from the gravitational-wave detectors LIGO, Virgo, and KAGRA. These results will shed light on the issue of discrepant expansion rate measurements from traditional methods such as supernovae and the CMB and will advance our understanding of dark energy.

## Publications, Patents, and Videos

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LIGO and 8 partner collaborations including DES, *Nature* **551**, 85 (2017). <https://arxiv.org/abs/1710.05835>.

[LDRD Research highlighted in PBS NOVA presentation “What’s the Universe Made of?” \(video\)](#)

*This is akin to seeing the lightning bolt and hearing the thunder.*

# Enabling Spectroscopy of Quantum Matter under Extreme Pressure

OAK RIDGE NATIONAL LABORATORY

*Researchers  
develop a  
way to probe  
quantum and  
light matter  
at high  
pressures*

## OVERVIEW

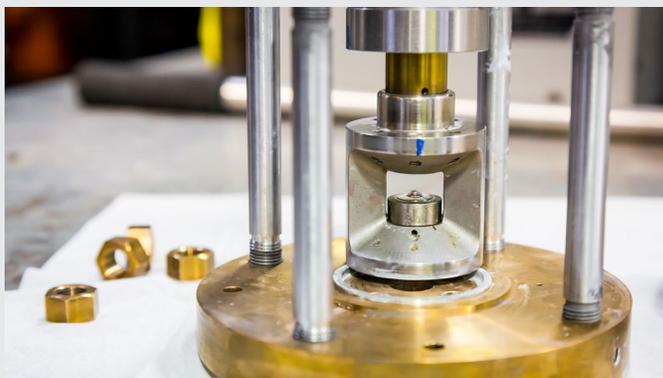
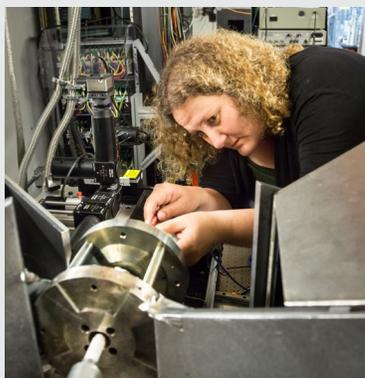
As scientists learn more about quantum behavior in materials, they need increasingly sophisticated methods. High-pressure inelastic neutron scattering is used to measure atomic, molecular, and magnetic motions in materials under extreme pressures. The project focused on applying the technique to two scientific programs: quantum phenomena at very low temperatures and hydrogen-containing materials. Both

areas of research involve interesting properties at extreme pressures and are well suited for investigation with neutrons, electrically neutral particles that can penetrate easily through matter. To achieve their goal, the researchers had to overcome technical barriers, such as designing pressure cells to accommodate relatively large sample volumes and cooling the cells to near-absolute-zero temperature.

## WHY IT MATTERS

High-pressure research provides a clean tuning parameter for probing emergent phenomena in quantum materials and can induce new behaviors and properties. In situ neutron scattering under extreme conditions can add to our understanding of water uptake in Earth's minerals or the pressure-temperature phase diagrams of such minerals, as well as the formation and behaviors of matter in extraterrestrial bodies such as

planetary ices. High-pressure research can also provide insights into the study of water or other absorption in porous materials. Pressurization or pressure-synthesis of pure hydrogen and superhydrides (i.e., hydrogen-rich metal materials) also enables room-temperature superconductivity, a topic for which in situ neutron scattering under pressure could provide unique new information.



Researchers with the SNS at ORNL, including PI Mark Lumsden and neutron scattering scientist Bianca Haberl (pictured left), developed technology to squeeze materials with a million times the pressure of Earth's atmosphere and study them using neutrons. When bombarded with neutrons, these materials provide an unprecedented picture of the changing nature of matter under extreme pressure. (Credit: G. Martin, ORNL)

## THE SCIENCE AND IMPACT

To study quantum materials, the team procured and tested a high cooling capacity dilution refrigerator for measurements at cold temperatures on the Cold Neutron Chopper Spectrometer at the Spallation Neutron Source (SNS). “Pressure cells have a large mass so cooling them is not trivial,” PI Mark Lumsden says. “We also needed to reach very low temperatures below 1 K because the quantum effects we’re trying to observe only exist at very low temperatures.” The team tested nickel-chromium-aluminum clamp cells with the dilution refrigerator and found that pressures of 2–3 GPa were possible at temperatures as low as 200 mK, providing unique capabilities for spectroscopy studies of quantum matter.

To enable measurements on hydrogen-containing materials, the team used the high-flux VISION vibrational spectrometer at SNS to optimize and test a large-volume polycrystalline diamond anvil cell. In testing, the cells pressurized samples as

large as 1 mm<sup>3</sup> up to 13 GPa, providing unprecedented inelastic neutron scattering capabilities for chemical spectroscopy. “Neutron spectroscopy is typically limited to less than 2 GPa, and we achieved more than 5× that pressure,” Lumsden says. The new cells designed for VISION resulted in low neutron background and an open geometry, which proved useful for other high-pressure measurements and have since been used on multiple instruments at both SNS and the High Flux Isotope Reactor (HFIR) at ORNL. Single-crystal diamond anvil cells based on a similar design were able to reach a pressure of 40 GPa on the Spallation Neutrons and Pressure Diffractometer and on previously unprecedented sample volumes. Replacing the polycrystalline diamond anvils with single-crystal diamonds on VISION also enabled the first glimpses of hydrogen under pressures above those possible in typical gas pressure cells when using neutron spectroscopy.

## WHAT’S NEXT

The experience gained from developing these pressure cells has yielded an ongoing capability for users at both SNS and HFIR, and the ORNL team now leads the world in high-pressure neutron scattering. For example, the new diamond cells enabled a record measurement above 60 GPa on a high-pressure polymorph of ice, ice-VII, yielding the first full set of structural data at such pressures. Recently, diamond anvil cells have been designed to enable neutron diffraction at a record pressure of 120 GPa.

Looking to the future of neutron science at ORNL, this project helped demonstrate the gains that could be achieved in high-pressure research with advanced instruments such as those planned for the upcoming Second Target Station (STS). The high peak brightness of cold neutrons available at the STS and the inelastic and elastic instruments that have been proposed can enable measurements on smaller samples, which will expand the accessible pressure range.

## Publications, Patents, and Videos

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## Acknowledgments

The team collaborated with Reinhard Boehler of the Carnegie Institution for Science, who is an expert in the design and fabrication of diamond anvil cells for use with scattering techniques.

***We had an opportunity to leverage world-leading instruments at the Spallation Neutron Source and technical advancements to push the limits of high-pressure neutron scattering.***

# Combining Renewable Electrons with Carbon Waste for Sustainable Chemicals and Materials

PACIFIC NORTHWEST NATIONAL LABORATORY

*Initiative develops catalysis for distributed conversion of carbon into value-added products*

## OVERVIEW

The Chemical Transformations Initiative (CTI) advanced our goals for decarbonization by utilizing catalytic science to discover more efficient means of converting carbon waste into renewable chemicals and materials. Research results indicated the potential to close the carbon cycle by recycling the energy potential of carbon waste

through developing catalysts capable of performing electrocatalytic conversions under low temperatures and pressures. CTI researchers synthesized multifunctional materials with both acid-base and redox centers to extend catalyst lifetimes, enhance reaction rates, and realize novel chemical conversions without the need for high-energy heat sources.

## WHY IT MATTERS

Converting municipal waste and biomass into usable products helps secure our nation's energy independence and advances the goal of achieving a carbon-neutral future. The ultimate goal of the CTI was to provide a basis for producing high-density renewable feedstocks with a low-carbon footprint through the utilization of recycled waste combined with a renewable energy-powered conversion process. The challenge lies in creating a conversion process that is selective yet still active at lower temperatures and pressures.

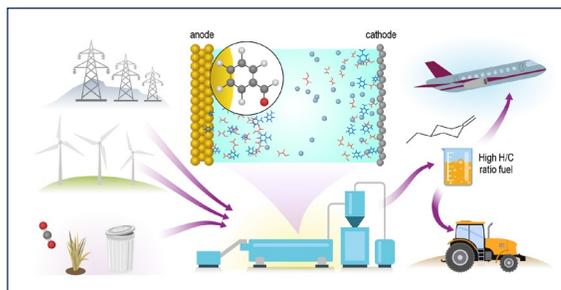
"Research from the CTI has transformed our understanding of an important field within catalysis. We combined advanced multiscale simulations and mechanistic studies with signature capabilities in electrocatalytic reactor design to realize low-temperature conversions and understand the exquisite details of how these processes work and how to control them," Roger Rousseau, CTI director, says.

The capabilities developed under the CTI have built a strong base, both

LEFT: A close coupling of new experimental capabilities with theory and modeling helps us understand how organic molecules are transformed at electrode interfaces to reuse carbon sustainably. (Credit: Pacific Northwest National Laboratory)

MIDDLE: Dr. Vanda Glezakou led CTI's efforts to develop advanced computation and data science techniques to create sustainable carbon technologies. (Credit: Pacific Northwest National Laboratory)

RIGHT: CTI catalysis scientist Oliver Y. Gutiérrez learned how to use renewable electrons to convert waste carbon into valuable chemicals. (Credit: Pacific Northwest National Laboratory)



experimentally and with chemical simulations, for the laboratory and DOE to further explore important chemistry conversions using electrons that are low-cost and harvestable in very distributed locations, rather than at a central refinery.

## THE SCIENCE AND IMPACT

Since its inception, CTI scientists have reimagined chemical catalysis by targeting the conversion of biomass-derived organic molecules to higher-value chemicals and precursors at low temperatures and pressures. Over the past 4 years, this project has resulted in 50 peer-reviewed publications, many in high-impact journals including *Chemical Reviews*.

CTI has (1) established critical mechanistic insights into the electrochemical hydrogenation of organic functional groups; (2) designed zeolite-based catalysts with a high acid content, which are stable in water and can perform reactions such as alcohol dehydration more than an order of magnitude

Because energy-poor waste is often wet and therefore costly to transport, deployment of distributed, small-scale chemical production facilities can target local needs for energy-dense products such as fuels and fertilizers.

faster than mineral acids under the same conditions; (3) created a multiscale modeling approach to understand the role of charge transfer on the rate of electrocatalytic conversions; and (4) evaluated CTI-developed capabilities for uses ranging from wastewater cleanup to fuel production and identified targets for partial electrification of chemical synthesis.

Together, these achievements lay the foundation for optimizing multifunctional catalysts under mild conditions to enable the decentralized conversion of waste carbon sources into high-energy-containing chemicals and materials.

## WHAT'S NEXT

CTI-developed capabilities will continue to benefit DOE and the nation by elevating PNNL's expertise and contributions in catalysis, electrochemistry, and chemical engineering. This initiative provided preliminary results and capabilities to support research and technology efforts for several DOE offices, including the Office of Science (Basic Energy Sciences) and the Offices of Energy Efficiency and

Renewable Energy, Fossil Energy, and Nuclear Energy. CTI researchers will continue to develop catalytic science and technologies for the scalable, distributed conversion of dispersed carbon into energy-dense liquids and solids, as well as other critical areas for accomplishing DOE's mission, including direct air capture of carbon dioxide and fuel cells for heavy-duty vehicles.

***Research from the Chemical Transformations Initiative has strengthened our understanding of an important field within catalysis.***

## Publications, Patents, and Videos

Akhade, S.A., et al., *Chem. Rev.* (2020). doi: 10.1021/acs.chemrev.0c00158.

Nguyen, M., et al., *Catal. Today* **350** (2019). doi:10.1016/j.cattod.2019.05.067.

Qiu, N., et al., *Appl. Catal. B: Environ.* **277**(15), 119227 (2020). doi: 10.1016/j.apcatb.2020.119277.

## Acknowledgments

Portions of this work were supported by user facilities such as the National Energy Research Scientific Computing Center at LBNL, the APS at Argonne, and the Environmental Molecular Science Laboratory at PNNL.

# Tuning In to Dark Matter with an Exquisitely Sensitive Radio

SLAC NATIONAL ACCELERATOR LABORATORY

*Dark Matter  
Radio searches  
for dark matter  
waves at new  
frequencies*

## OVERVIEW

Dark matter makes up 85% of the mass of the universe, but because it interacts with regular matter only through gravity, we only see its indirect effects. Multiple searches for the most popular dark matter candidate, the WIMP (weakly interacting massive particle), have turned up empty. The

Dark Matter Radio (DMRadio) searches for extremely light dark matter candidates that are detected as waves rather than particles. Like an AM radio searching for a station, it will scan a wide range of frequencies for the extremely faint signals of two closely related dark matter candidates: axions and hidden photons.

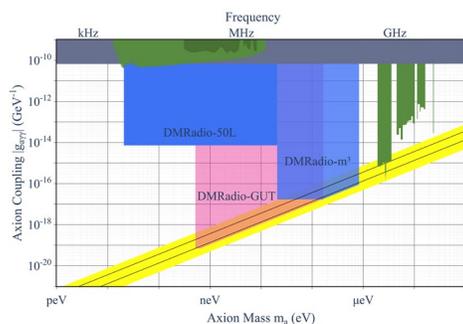
## WHY IT MATTERS

Dark matter has had a profound impact on the evolution of the universe, shaping the formation and distribution of the galaxies we see today, and the quest to understand it dates back decades. The direct detec-

tion of dark matter would be a major breakthrough in both astronomy and particle physics and would fundamentally change our understanding of the laws of nature.



SLAC/Stanford PI Kent Irwin, left, looks at DMRadio equipment with Betty Young, Hsiao-Mei (Sherry) Cho and Dale Li. (Image credit: A. Freeberg, SLAC)



A series of DMRadio experiments will search for extremely light dark matter axions as waves, rather than particles. (Credit: S. Chaudhuri, Snowmass2021 Letter of Interest)

## THE SCIENCE AND IMPACT

Most dark matter searches look for the scattering of massive particles, which requires massive equipment located deep underground to shield it from cosmic rays. If axions and hidden photons exist, they would be so light that they are better described as waves whose associated fields can spread over kilometers. Previous searches for wavelike dark matter, including ADMX-G2, have looked for signals at high frequencies (i.e., a few hundred megahertz or above). DMRadio, which like an AM radio uses an LC oscillator, can search a broad frequency range from kilohertz to 200 MHz.

Because axions would be converted into ordinary photons when placed in a magnetic field, DMRadio will create magnetic fields where those conversions can take place and search those fields for tiny magnetic signals produced by those photons. These signals are so faint that detecting them requires quantum sensors called SQUIDs—superconducting quantum interference devices. The DMRadio Pathfinder, the first experiment, can pick up magnetic signals a hundred million trillion times smaller than those produced by a typical refrigerator magnet.

## WHAT'S NEXT

The DMRadio Pathfinder experiment led by SLAC and Stanford professor Kent Irwin has branched out into a program of planned and proposed experiments aimed at developing ever-more-sensitive detectors for a full-scale axion dark matter search.

Dark Matter Radio 50 Liter (DMRadio-50L) will search for axions below 5 MHz. It will use a 1 Tesla magnet with a 50 L volume to create the magnetic field where axions convert to photons, and also develop new quantum sensors more sensitive than SQUIDs. Dark Matter Radio Cubic Meter (DMRadio- $m^3$ ) will search for axions from

5 MHz to 200 MHz using a more powerful 4 Tesla magnet with cubic meter volume.

The planned DMRadio-GUT would build on the technologies used in previous experiments and implement new technologies to increase the sensitivity of the search. Its magnet would be 10 times larger and generate a field 3× stronger than the one in DMRadio- $m^3$ . This will allow a search for axions created at the energy scale where the strong, weak, and electromagnetic forces all come together into one.

***To search for the faintest signal, we build the most sensitive radio.***

## Publications, Patents, and Videos

Chaudhuri, S., et al., <https://arxiv.org/abs/1904.05806>.

Chaudhuri, S., et al., <https://arxiv.org/abs/1803.01627>.

## Acknowledgments

Construction of DMRadio-50L infrastructure is being funded by the Gordon and Betty Moore Foundation and the Heising-Simons Foundation. Development of new quantum sensors and the conversion of DMRadio-50L into a fully quantum experiment (DMR-Quantum) is being funded by the DOE Office of High Energy Physics under the QuantiSED Program. It will be fully operational in 2 years.

DMRadio- $m^3$  received \$1 million in design funding as part of the DOE Dark Matter New Initiatives Program. The project, which will be constructed in FY 2023, is being carried out by SLAC, Stanford, UC Berkeley, LBNL, MIT, University of North Carolina—Chapel Hill, and Princeton University. It will be ready for construction in FY 2023.

# Increasing Particle Accelerator Reliability with Machine Learning

THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY

*Machine learning helps identify accelerator faults and improve quality of data*

## OVERVIEW

The state-of-the-art particle accelerators used for research by the Office of Science programs typically operate at their systems' performance limits. Tiny fluctuations in the particle-accelerating components can upset operations, wasting precious "beam on" (i.e., facility operation) time and limiting multiple experiments. This project investigated the potential efficacy of

deploying machine learning to identify an impending failure event, the reason for it, and the appropriate preventive measure—all in a fraction of a second for hundreds of systems. Such fault prediction and mitigation would enhance accelerator performance, increasing the vital research output these accelerators facilitate.

## WHY IT MATTERS

The Continuous Electron Beam Accelerator Facility (CEBAF) at Jefferson Lab is a continuous-wave recirculating linear accelerator that approximately 1,700 scientists use to acquire data on the nature of matter. Roughly \$1 billion has been invested in constructing and improving CEBAF, so it is critical to use it efficiently. Several experiments run in parallel, so any loss of "beam on" time affects many

users. The most common reason for loss of beam is a fault in one of the 418 accelerating systems that add energy to the electrons in the beam. Diagnosing and correcting these faults can be slow and tedious, leading to undesirable loss of incoming data for the experiments. Reducing that loss is important for responsible stewardship of the nation's investment in CEBAF.

## THE SCIENCE AND IMPACT

Some of the accelerating systems are instrumented to capture data that can be used to better understand their behavior. A fault event triggers archiving of the data generated prior to the event. Subject matter experts then analyze the time-tagged data, identify which cavity faulted first, and classify the type of fault. This information permits trending analysis

and strategic mitigation of problems. However, manually reviewing the data and classifying the fault events are tedious and time-consuming. Furthermore, unfamiliar patterns in the data raise the question of whether one is a variant of a known fault type or something completely new.

## Publications, Patents, and Videos

Shabalina, A., et al., OSTI ID 1735851 (2020).

Tennant, C., et al., *Phys. Rev. Accel. Beams* **23**, 114601 (2020).



Technician in ultra-clean environment at Jefferson Lab preparing a superconducting radiofrequency cavity. (Credit: Thomas Jefferson National Accelerator Facility)

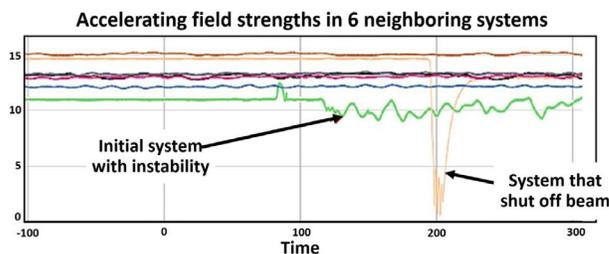
Quickly identifying faltering systems can have enormous impact on improving CEBAF experiments. Machine learning methods permit near-real-time classification of fault events and remove bias from the analysis. Additionally, classification of the

fault type is more accurate for known patterns and can potentially reveal new ones. Artificial Intelligence–assisted activities help reduce CEBAF downtime, thereby making the most of precious, limited research time.

## WHAT'S NEXT

This project was the foundation for a follow-on proposal to explore additional ways artificial intelligence could improve the

operation of the accelerating systems at CEBAF. The new project was awarded \$1.35 million for a 3-year effort.



Data archived for a single fault event. Here, there were two unstable systems, which is perhaps symptomatic of a larger problem outside of either system. (Credit: Thomas Jefferson National Accelerator Facility)

***Machine learning is particularly well suited for finding [fault] patterns, even in noisy data.***

## Acknowledgments

This project was led by Jefferson Lab scientists Anna Shabalina, Adam Carpenter, Chris Tennant, and Lasitha Vidyaratne.

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## Acknowledgments

The DOE acknowledges the contributions of the many authors who provided an LDRD article for this brochure and extends sincere thanks to all laboratory program contacts for coordinating and to the editorial and publication support team from ORNL.

Editorial Support: Laurie Varma, ORNL

Publication Design and Production: Laddy Fields, ORNL

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