



# RESEARCH

Laboratory Directed Research & Development

**FY23** ANNUAL REPORT



BIOSCIENCE | COMPUTING AND INFORMATION SCIENCES | EARTH SCIENCE | ENGINEERING SCIENCE | MATERIALS SCIENCE  
NANODEVICES AND MICROSYSTEMS | RADIATION, ELECTRICAL, AND HIGH ENERGY DENSITY SCIENCE

**ACCELERATING INNOVATION**



LABORATORY DIRECTED  
RESEARCH & DEVELOPMENT  
*WHERE INNOVATION BEGINS*



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT  
**2023 ANNUAL REPORT**

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**FROM THE CHIEF RESEARCH OFFICER**



This is my first year as Sandia's Chief Research Officer, but it isn't my first year working in, supporting, or leading Laboratory Directed Research and Development (LDRD) projects. It's been my privilege to have this experience across multiple national labs including Los Alamos, Lawrence Livermore, Oak Ridge, and now Sandia, and I can tell you that the Department of Energy (DOE) isn't just working to enable the missions of today. Through the transformative LDRD insights, solutions, and technologies delivered at 17 national laboratories, DOE is also providing the innovations to meet the needs of tomorrow's missions.

The DOE mission is broad, which is why so many labs across our country are striving for scientific breakthroughs that address problems of national interest. It takes multidisciplinary teams engaging in trailblazing research to build toward strategic capabilities, however, working at the leading-edge is inherently high risk/high reward. Researchers sometimes don't find the answer they expect, but this isn't failure since the knowledge can guide future inquiries. When outcomes surpass expectations and can be applied in other research or utilized later, the reward is high.

Through the LDRD process this past fiscal year, researchers achieved incredible advances, such as:

- Developing a capability to help radar systems identify targets of interest for national security.
- Predicting possible actions of cyber adversaries through a wargame.
- Evolving future heat shield materials for hypersonic vehicles.
- Creating a technology to precisely monitor rarely used antibiotics in patients recovering from serious infections.
- Determining a method for detecting diseases through compounds in the breath.
- Delivering cyber-resilient techniques to help defend electric grids.

The LDRD program is also a stellar workforce recruitment, retention, and development mechanism. It allows the workforce to sharpen their skills as they cooperate on cross-laboratory projects and acts as a talent pipeline mechanism for university students who learn about Sandia by supporting projects under faculty members collaborating with us. In addition, postdocs who work at Sandia can partner with our experts while utilizing our one-of-a-kind tools and facilities, and this can encourage them to consider Sandia for employment or for future collaborative endeavors.

As Sandia celebrates its 75th anniversary, it's truly my privilege to be the Chief Research Officer and support the LDRD program and researchers here who are providing exceptional service in the national interest.

  
Douglas B. Kothe

Associate Laboratories Director & Chief Research Officer  
Advanced Science and Technology

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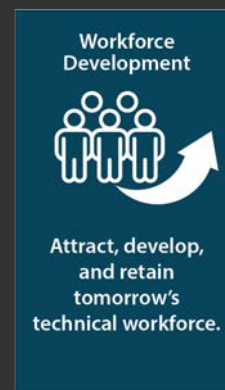
# LDRD PROGRAM OVERVIEW

Sandia is a federally funded research and development center (FFRDC) focused on developing and applying advanced science and engineering capabilities to mitigate national security threats. This is accomplished through the exceptional staff leading research at the Labs and partnering with universities and companies.

Sandia's LDRD program aims to maintain the scientific and technical vitality of the Labs and to enhance the Labs' ability to address future national security needs. The program funds foundational, leading-edge discretionary research projects that cultivate and utilize core science, technology, and engineering (ST&E) capabilities. Per Congressional intent (P.L. 101-510) and Department of Energy (DOE) guidance (DOE Order 413.2C, Chg 1), Sandia's LDRD program is crucial to maintaining the nation's scientific and technical vitality.

## LDRD PROGRAM OBJECTIVES

Sandia's LDRD objectives guide the program overall and align with DOE Order 413.2C and National Nuclear Security Administration (NNSA) guidance. The Mission Agility and Technical Vitality Objectives are supported by the Workforce Development Objective, which is a critical element to affect, grow and leverage the technical experts needed to execute R&D projects.



## SANDIA'S LDRD PROGRAM STRUCTURE

Sandia's LDRD investments are structured around three Program Areas, which are further broken down into Investment Areas (IAs). Each IA is focused on discipline- or mission-based research priorities set by Sandia's leadership. The LDRD program structure and the allocation of funds to the associated IAs are designed to align LDRD investments with Sandia strategy and future national security mission needs.

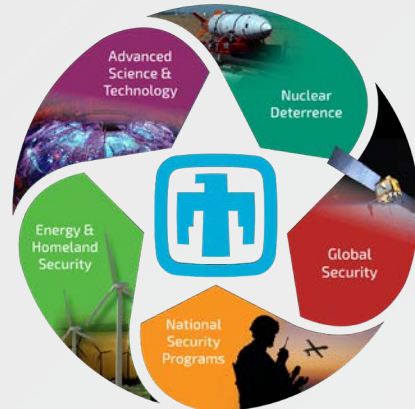
## LDRD INVESTMENT AREA ROLES

### RESEARCH FOUNDATIONS



Research Foundations steward discipline-based ST&E competencies that address the extensive national security challenges within Sandia's mission space. Each of the Research Foundations focuses on stewarding differentiating or unique capabilities in seven areas.

### MISSION FOUNDATIONS



Sandia oversees five major portfolios that address national security mission challenges. LDRD Mission Foundations align with the portfolios and conduct the applied research needed to develop capabilities and demonstrate solutions.

## STRATEGIC INITIATIVES

Strategic Initiatives (SI) promote strategic collaborations and Chief Research Office (CRO)/Labs-directed initiatives.



SI include Grand Challenge projects to solve major research challenges that require large multidisciplinary teams; Mission Campaign IAs to move ST&E intentionally from idea to mission impact; Exploratory Express to execute short-term projects of strategic importance; and New Ideas to pioneer fundamental R&D to discover game-changing breakthroughs. These initiatives also support strategic academic collaborations (126 in FY2023) and both the Harry S. Truman and Jill Hruby Postdoctoral Distinguished Fellowships.

# LDRD PROGRAM VALUE

## PERFORMANCE INDICATORS

While the FY2023 LDRD program represented only about 4.9% of Sandia's total costs, the metrics shown below highlight how LDRD has a much greater relative impact on key performance indicators (KPI) and metrics for the Labs. The bar

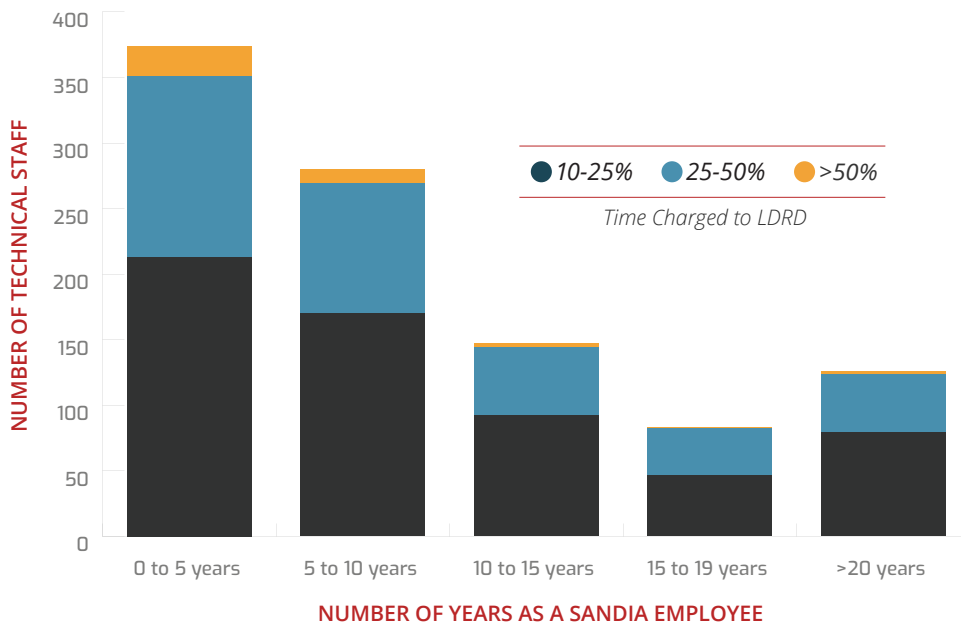
graph illustrates the large percentage of early career staff, thus validating LDRD's important role in attracting, developing, and retaining a world-class workforce to meet our most challenging national security needs.

**\$231.2M**  
Total  
Program Cost  
(not including PM costs)

**\$414K**  
Median  
Project Size

**510**  
Total  
LDRD Projects

**254**  
New Projects  
in 2023



**51%**  
OF SANDIA  
TOTAL  
**231**  
LDRD-  
Supported  
Postdocs

**64%**  
OF SANDIA  
TOTAL  
**54**  
LDRD-  
Supported  
Postdoc  
to Staff  
Conversions

**31%**  
OF SANDIA  
TOTAL  
**409**  
Refereed  
Publications

**43%**  
OF SANDIA  
TOTAL  
**120**  
Technical  
Advances

**38%**  
OF SANDIA  
TOTAL  
**43**  
Patents  
Issued

**17%**  
OF SANDIA  
TOTAL  
**23**  
Copyrights

**67%**  
OF SANDIA  
TOTAL  
**4**  
R&D 100  
Awards

# LONG-TERM METRICS

## The Long-Term Impacts of LDRD Investments

The LDRD program is an investment in the nation’s future, ensuring mission support that is often realized after many years. This section highlights the longer-term (>5 year) impact of LDRD as a national asset. These performance indicators are updated annually. As expected, the data may vary from year to year so long-term running totals will be included and updated every 5 years.

### BACKGROUND

Applying continuous improvement, representatives from each LDRD program at the NNSA laboratories (Sandia, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory) regularly participate in a working group to share best practices and discuss strategies for tracking the long-term impact of LDRD investments. The working group finalized a combination of common quantitative and qualitative long-term indicators, emphasizing a systematic approach to be utilized by each NNSA LDRD laboratory, and acknowledged that individual laboratories may choose to report other long-term indicators that fit their unique missions and capabilities.

### ALIGNMENT WITH LDRD OBJECTIVES

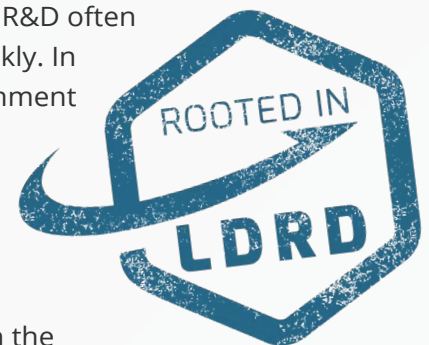
The KPI for LDRD, including numerical KPIs in the form of metrics and qualitative KPIs in the form of project highlights, illustrates the long-term payoffs/success of the program in meeting its three objectives: Technical Vitality, Mission Agility, and Workforce Development. Because KPIs crosscut the three objectives, this report will not provide a 1:1 mapping.

### IMPORTANCE OF QUALITATIVE DATA

Developing numerical indicators for R&D program success is widely recognized as difficult. The NNSA LDRD metrics working group developed numerical success indicators for both Technical Vitality and Workforce Development. Project highlights or “success stories” capture the successes in Mission Agility and some aspects of the other two LDRD objectives not well represented by numerical metrics.

### TRACING IMPACT BACK TO LDRD

Throughout this section, you will see references to “LDRD roots.” LDRD mentors and principal investigators (PI) often discuss what it means for an accomplishment to have LDRD roots. A simple case might involve an idea for an invention that arises during an LDRD project and work on the invention is completed during the period of LDRD investment. But R&D often does not advance quickly. In general, an accomplishment (invention, paper, capability, etc.) is determined to have LDRD roots if there are one or more LDRD projects without which the accomplishment would never have come into being. In other words, if a current LDRD project relies on an earlier LDRD accomplishment, then it is considered to have “roots” in the prior LDRD project. Other relevant definitions for metrics are included in the sections to follow.



# THE INDICATORS

## Top 2%

A relevant indicator of career advancement in an ST&E field is the recognition of individuals as distinguished members of the technical staff, known as Senior Scientists/Engineers and Fellows at Sandia, Fellows at Los Alamos National Laboratory, and Distinguished Members of the Technical Staff at Lawrence Livermore National Laboratory.

The shorthand name used here, “Top 2%,” comes from the intent at each laboratory to limit membership to the top 1% or 2% of scientific and technical staff. Typically nominated and screened by a committee, the Top 2% are recognized for something similar to a lifetime achievement, in this case, for contribution to the mission of each laboratory.

Each year at Sandia, a small number of staff are appointed to the rank of Senior Scientist/Engineer, an honor based on exceptional leadership and consistently outstanding contributions to Sandia’s national security missions. In FY23, 18 out of the

22 staff promoted to Senior Scientist/Engineer were involved in the LDRD program as a PI or team member during their careers. Since FY11, 76% of Sandia’s Senior Scientists Engineers have careers with LDRD roots.

Sandia also reserves a special recognition for an elite group of individuals—Sandia Fellows—recognized for careers of significant accomplishment for the Labs and for the nation. In Sandia’s history, only 21 individuals have held this title (19 individuals with R&D careers and 2 individuals in non-technical positions). In FY23, nine of the R&D Fellows were on staff, and all nine have been involved with LDRD in their careers. The LDRD Program’s Strategic Partnerships pillar funds a set of projects selected and managed by Sandia Fellows. The Fellow projects enable the Labs’ most stellar R&D staff to mentor promising staff as they pursue leading-edge, potentially high-impact R&D. In FY23, there were 29 active Fellows projects across ten IAs.

## LDRD AND TOP 2% TECHNICAL STAFF AT SANDIA NATIONAL LABORATORIES

	SINGLE YEARS			FIVE YEARS		TO DATE*
	FY21	FY22	FY23	FY11-15	FY16-20	FY11-23
TOTAL AWARDS	8	15	26	26	53	131
AWARDS WITH LDRD ROOTS	5	13	21	15	44	100
PERCENTAGE WITH LDRD ROOTS	62%	86%	80%	57%	83%	76%
AVERAGE YEARS FROM FIRST LDRD EXPERIENCE	15.2	19.5	19	9.9	17.8	16.8

\*Initial year to date: Each laboratory has chosen the appropriate lookback period that will ensure data integrity.

## SELECT NEWLY PROMOTED SENIOR SCIENTIST & FELLOW HIGHLIGHTS

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Sandia Senior Scientist **Jeff Koplow** has a long track-record of multi-disciplinary innovations in numerous fields that are based on a first-principles, holistic, and technology agnostic approach to problem solving. He holds over 20 patents and 12 patent licenses and has transitioned many concepts to commercialization. A recipient of a 2015 [DOE SunShot Innovation Fellowship](#), Koplow has also received four R&D 100 awards. He served as the PI of nine LDRD projects and contributed as team member or mentor on numerous others. Read about [Twistact](#), one of Koplow's many LDRD innovations.



In 20 years, Sandia Senior Scientist **Joe Schoeniger** has developed and applied numerous high-throughput screening and biomolecular characterization methods. His research focuses on antiviral discovery, bioconjugate chemistry, and pathogen genome sequence analysis. Schoeniger currently serves as the project manager for the Computational Approaches for Predicting Shared Interactions of Infectious Diseases Grand Challenge LDRD project. He has been the PI on 13 LDRD projects and contributed as a team member to more than 25. Read more about Schoeniger's work [developing a deployable antiviral countermeasure for COVID-19](#).



In almost 40 years, Sandia Senior Scientist **Rex Kay** has developed incredible experience in satellite sensor systems design and evaluation, including focal plane array design. Read more about the [ultrafast X-ray imager](#), an R&D 100 award-winning technology borne out of the Highly Pixelated Hypertemporal Sensors for Global Awareness Grand Challenge LDRD project (FY06-FY09) that Kay led as PI. Kay was also a PI on six additional LDRD projects and a team member on five. He is currently mentoring early career staff on an LDRD project that will develop interface technologies for high data-rate focal plane array imagers.

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Sandia Senior Scientist **Stephen Buerger** excels in novel robotics, unmanned systems, and autonomous and advanced real-time control systems. He provides expertise in advanced mobility systems, small-scale electromechanical systems, and biomedical technologies focused on physically interactive manipulation. He is also versed in energy-efficient and high-performance actuator technologies, as well as biomedical and human-interactive technologies. He has been the PI on nine LDRD projects and a team member on 11.



*LDRD projects have provided me with vital opportunities to explore totally new ideas that can often turn into enduring, sponsor-funded areas of work. I have always appreciated the ability of new connections across Sandia, made via LDRD, to harness the deep, multi-disciplinary power of the Labs and direct it toward new, nationally important challenges.*

*– Stephen Buerger*

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Sandia Senior Scientist **Jacques Loui** currently leads Sandia’s Facility for Advanced Radar and Algorithm Development. He has more than a decade of experience in intelligence, surveillance and reconnaissance sensor technologies and holds multiple patents on ultra-wide-band digital beam steering techniques. He has served as the PI on seven LDRD projects and as a team member on numerous others. Read more about how Loui and his colleagues are [giving radar a digital makeover](#) using LDRD-developed technology.



## SELECT NEWLY PROMOTED SENIOR SCIENTIST & FELLOW HIGHLIGHTS



Sandia Senior Scientist **Alec Talin** is a Fellow of the American Physical Society. His research interests include nanoionics and nanoelectronics for emerging computing and memory, [solid state energy storage](#), photocatalytic and photoelectrocatalytic solar fuels, and coordination polymers and metal organic frameworks for emerging electronics and energy applications. Alec has led nine LDRD projects and contributed as a team member or mentor on 25 LDRD projects.



*I have benefited tremendously from the Sandia LDRD program. First, the LDRD program was instrumental in helping me establish the experimental capabilities, reputation and track record needed to successfully compete for external funding. Second, the program greatly facilitated collaborations with colleagues in NM that persist to the present day.*

*– Alec Talin*



Sandia Fellow **Tina Nenoff** is a [Fellow of both the American Chemical Society and the American Association for the Advancement of Science](#). Her career has focused on the materials chemistry of nanoporous materials, and their chemistry and reactivity at the nanoscale for bulk scale energy and environmental applications. Her research spans the basic to applied research areas of materials synthesis, characterization, and testing. She has given particular focus to understanding the chemistry that occurs in nanoporous frameworks and how that chemistry relates to bulk scale performance. Nenoff has led 12 LDRD projects and teamed or mentored on 10 more.

Sandia Fellow **Cindy Phillips** is a [SIAM Fellow and an Association for Computing Machinery Distinguished Scientist](#). She has contributed to research in combinatorial optimization, algorithm design and analysis, parallel computation, scheduling, network and infrastructure surety, integer programming, graph algorithms, complex and social network analysis, cybersecurity, streaming, neuromorphic computing, and algorithm/architecture co-design. Phillips has led six LDRD projects and served as team member or mentor on over 30 more.



*LDRD has been a fantastic way to learn about new mission/application areas as part of a multidisciplinary team. It's also allowed me to work with amazing professors and their students, taking work from low-Technical Readiness Level (TRL) research-foundation LDRDs to mid-TRL work mission-foundations LDRDs and, at least, to the doorstep of mission use. Now, the relatively new consultant role allows me to learn about and contribute to more projects than ever before. It's hard to imagine where Sandia would be without the knowledge, skills, tools, and connections created by the LDRD program."*

*– Cindy Phillips*

## R&D 100 AWARDS

Another relevant indicator of advancement and leadership in an ST&E field is the R&D 100 Award. The prestigious “Oscars of Invention” honor the latest and best innovations and identify the top technology products of the past year. The LDRD Program Offices at national labs/sites often partner with sister organizations, such as the Intellectual Property Office and Public Affairs, to track whether R&D 100 winners in either the standard category or special awards have “LDRD roots.” Often, because of the long development time from an LDRD idea to practical implementation, the staff who work on an award-winning technology product may not be the same



researchers who initiated the original R&D. Each site’s LDRD Program Office engages in an extensive interview process to uncover the details of how the LDRD work led to the celebrated invention.

Since 1976, Sandia has won 157 awards, illustrating the Labs’ contributions in developing products and technologies with the potential to change industries and make the world a better

place. Over the past three years, 57% of Sandia’s R&D 100 winning contributions have been rooted in LDRD; over the past 18 years, 70% have come from LDRD.

## LDRD and R&D 100 Awards Awarded to Sandia National Laboratories

Counts include standard R&D 100 awards and special recognition awards, as well as awards led by other organizations where Sandia was a key partner.

	SINGLE YEARS			FIVE YEARS		TO DATE*
	FY21	FY22	FY23	FY11-15	FY16-20	FY06-23
TOTAL AWARDS	9	6	6	20	32	92
AWARDS WITH LDRD ROOTS	5	3	4	15	22	64
PERCENTAGE WITH LDRD ROOTS	56%	50%	67%	75%	69%	70%
AVERAGE YEARS FROM FIRST LDRD EXPERIENCE	4.6	4.3	12.5	5	5.6	5.5

\*Initial year to date: Each laboratory has chosen the appropriate lookback period that will ensure data integrity.

## SANDIA WINS SIX 2023 R&D 100 AWARDS, FOUR WITH LDRD ROOTS.

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In 2023, Sandia won [six R&D 100 Awards](#), and four of them were “rooted” in LDRD projects of the past. The R&D 100 Awards, in its 61st year, is a globally prestigious recognition of invention and innovation. It claims entries this year from 15 countries and regions and is sponsored by R&D World Magazine. For the nation, these awards indicate that the research and development done here, in support of the mission, is technologically significant and groundbreaking.

### PRE-SYMPTOMATIC VOLATILE ORGANIC COMPOUNDS (VOC) DETECTOR OF SEIZURE EVENTS. (ANALYTICAL/TEST WINNER)

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*The Pre-Symptomatic VOC Detector of Seizure Events is a portable instrument that can alert the wearer to an imminent seizure more than 20 minutes before it occurs.*

This wearable detector identifies specific skin-emitted VOCs that indicate an imminent seizure. This detector provides a pre-symptomatic warning enabling the wearer to prepare and communicate with family and healthcare providers before the seizure occurs and will dramatically improve the lives of those suffering from unpredictable epileptic seizures. This project has roots in MicroChemLab, Sandia’s first LDRD Grand Challenge. (PI: Philip Rocco Miller) [Watch the video.](#)

### META OPTICS STUDIO (MOS). (SOFTWARE/SERVICES WINNER)

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MOS is a purpose-built software package for the design, simulation, and optimization of flat meta-surfaces, which are artificial structures used to engineer the light wavefront for enhanced focusing, phase correction, and removal of aberrations. MOS is the ONLY software capable of simulating a centimeter-sized meta-surface at nanometer resolution within a few hours. The MOS project developed out of the Metamaterial Science and Technology LDRD Grand Challenge (2009-2011). (PI: Ihab El-Kady) [Watch the video.](#)

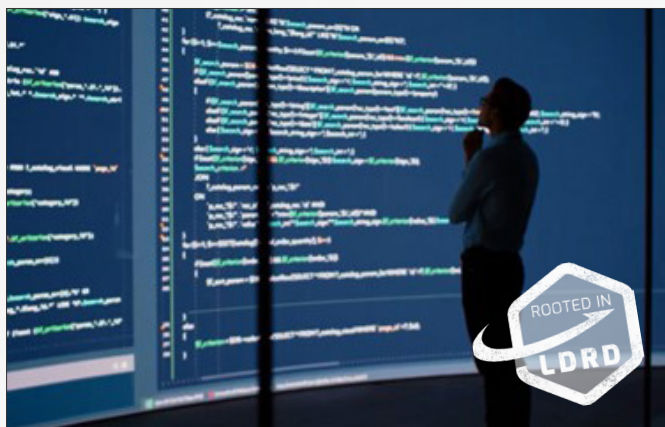


*This software package enables the rapid design and optimization of large-scale meta-optics for integration into optical imaging systems.*

## MATERIALS LEARNING ALGORITHMS (MALA). (SOFTWARE/SERVICES WINNER)

MALA is a software framework that uses machine learning to predict the electronic structure of materials. Electronic structure is fundamental for understanding virtually all molecular and material properties. MALA enables these calculations at length and time scales that were previously unfeasible and was primarily funded out of a Computing & Information Sciences LDRD project, “Accelerating Multiscale Materials Modeling with Machine Learning,” that ended in 2022. (PI: Sivasankaran Rajamanickam)

[Watch the video.](#)

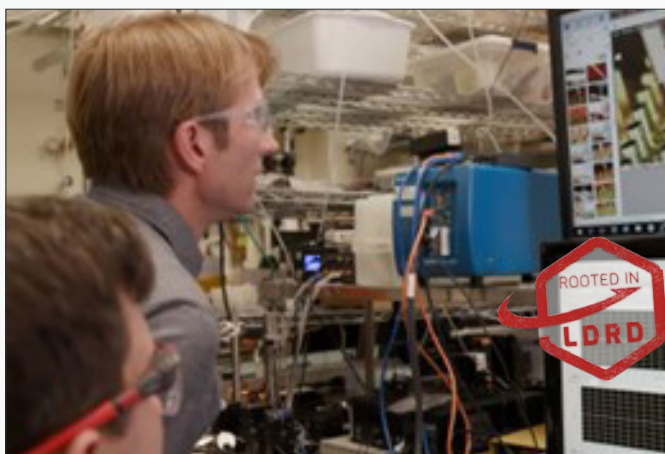


*This software framework uses machine learning to predict the electronic structure of materials faster and at greater scales than what was previously feasible*

## ELECTROCHEMICAL ADDITIVE MANUFACTURING (ELECTRO3D). (PROCESS/PROTOTYPE WINNER)

Electro3D is an additive manufacturing process that simultaneously analyzes and manufactures materials. This platform is more energy efficient than current metal 3D printers, and the technology is scalable, deployable, and can print multi-materials (metals, semiconductor, polymers) with rapid transition and seamlessly integrate with machine learning techniques to address the needs of many customers. This project is rooted in the recent LDRD “Advanced Manufacturing Techniques of Thermoelectric Modules.” (PI: Karl Walczak)

[Watch the video.](#)



*Electro3D allows for new and exciting possibilities in the world of electrochemical metal 3D printing. Not only does it allow users to print materials into less extreme environments, but it eliminates cost and transport limitations that no other technology can offer. With Electro3D, 3D metal printing can enable endless new possibilities for users.*



## PROFESSIONAL FELLOWS

One relevant indicator of advancement and leadership in an ST&E field is the election of individuals as fellows of professional societies. This indicator reflects success for both the individual researcher and the affiliated laboratory. Researchers at Sandia have been elected as fellows to over 25 prestigious scientific and engineering societies, with the most fellows elected to the societies listed below.

- American Association for the Advancement of Science
- American Institute of Aeronautics and Astronautics
- American Physical Society
- American Society of Mechanical Engineers
- Institute of Electrical and Electronics Engineers
- Society for Industrial and Applied Mathematics

## FELLOWSHIP AWARDS

	SINGLE YEARS			FIVE YEARS		TO DATE*
	FY21	FY22	FY23	FY11-15	FY16-20	FY06-23
TOTAL AWARDS	7	4	8	39	39	100
AWARDS WITH LDRD ROOTS	4	4	8	30	33	82
PERCENTAGE WITH LDRD ROOTS	57%	100%	100%	76%	80%	82%
AVERAGE YEARS FROM FIRST LDRD EXPERIENCE	15.2	17	18.5	12.5	14.6	14.1

Read about individuals at Sandia who have been elected fellows of professional societies in the [Workforce Development](#) section of this Annual Report.



# SHORT-TERM METRICS

## Intellectual Property

### PATENTS

Number of U.S. and foreign patents issued in a given FY.

	FY19	FY20	FY21	FY22	FY23
SANDIA PATENTS	159	131	120	92	114
LDRD SUPPORTED	76	67	63	40	43
% DUE TO LDRD	48%	51%	53%	43%	44%

*LDRD supported: Patents issued that would not exist if not for initial work funded by LDRD.*

### COPYRIGHTS

Number of copyrights created in a given FY.

	FY19	FY20	FY21	FY22	FY23
SANDIA COPYRIGHTS	97	151	170	146	135
LDRD SUPPORTED	18	40	34	26	23
% DUE TO LDRD	19%	26%	20%	18%	17%

*LDRD supported: Copyrights issued that would not exist if not for initial work funded by LDRD.*

### INVENTION DISCLOSURES

Number of declarations and initial records of an invention (a new device, method, or process developed from study and experimentation).

	FY19	FY20	FY21	FY22	FY23
SANDIA DISCLOSURES	252	299	295	280	277
LDRD SUPPORTED	102	111	128	117	120
% DUE TO LDRD	40%	37%	40%	42%	43%

*LDRD supported: Disclosures issued that would not exist if not for initial work funded by LDRD.*

## Peer-reviewed Publications

### PUBLICATIONS

Number of peer-reviewed publications, as a function of publication year.

	FY19	FY20	FY21	FY22	FY23
SANDIA PUBLICATIONS	1399	1299	1493	1456	1372
LDRD SUPPORTED	366	343	379	380	408
% DUE TO LDRD	26%	26%	25%	26%	30%

*LDRD supported: Publications that would not exist if not for initial work funded by LDRD.*

## Science and Engineering Talent Pipeline

### STUDENT INTERNS SUPPORTED BY LDRD (>10%) AT SANDIA

Number of graduate and undergraduate students working full- or part-time for the Labs, who charged at least 10% time to LDRD.

	FY19	FY20	FY21	FY22	FY23
GRAD STUDENTS	106	127	139	147	158
UNDERGRAD STUDENTS	115	100	84	110	118
SANDIA R&D STUDENTS	733	722	711	841	857
% DUE TO LDRD	30%	31%	31%	31%	32%

### POSTDOCTORAL RESEARCHER SUPPORT

Number of postdoctoral researchers working full- or part-time for the Labs.

	FY19	FY20	FY21	FY22	FY23
SANDIA POSTDOCS	388	350	428	459	453
LDRD SUPPORTED >10%	148	163	196	209	231
% DUE TO LDRD	38%	46%	46%	46%	51%

*LDRD supported: Postdoctoral researchers charging at least 10% time to LDRD.*

### POSTDOCTORAL RESEARCHER CONVERSIONS

Number of conversions from postdoctoral researcher to a member of the staff.

	FY19	FY20	FY21	FY22	FY23
SANDIA CONVERSIONS	68	47	61	94	85
LDRD SUPPORTED >10%	34	25	32	42	54
% DUE TO LDRD	50%	53%	52%	45%	64%

*LDRD supported: Conversion of postdoctoral researchers who charged at least 10% time to LDRD in the fiscal year preceding the conversion.*

## LDRD IMPACT STORY

### ADVANCING HIGH-PERFORMANCE HETEROGENEOUSLY INTEGRATED LASERS FOR RF PHOTONICS AND QUANTUM SENSING.

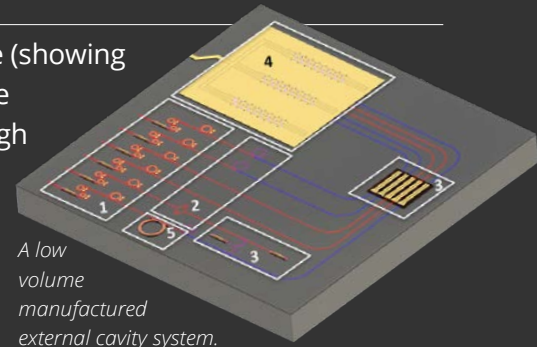
Sandia produced a high performance heterogeneously integrated laser for RF photonics and quantum sensing. To achieve this result, the team explored the fundamental limits to spectral purity of hybrid and heterogeneously integrated lasers. Through fundamental understanding of the governing physics, the team investigated

unique integrated laser architectures and characterized frequency noise and line width. In parallel, the team explored new scientific concepts of the Brillouin processes and demonstrated the first direct proof of plasma enhancement of Brillouin interactions in a suspended

silicon waveguide (showing modulation of the interaction through a voltage bias).

Through a productive collaboration with the Alliance partner

University of New Mexico (UNM), Sandia explored the interaction of acousto-electric gain and stimulated Brillouin scattering. The fundamental laser theory work conducted under this LDRD was featured on the front cover of the [Laser & Photonics Reviews](#). Overall, ten papers were published on various aspects of this LDRD project and three invited talks were held at IEEE, Compound Semiconductor Hub, and UNM. Multiple efforts moving forward make use of the capabilities developed under this LDRD and which continue the larger vision of developing a unique photonic platform for scalable quantum information and processing applications. (PI: Michael Gehl)



A low volume manufactured external cavity system.



### Bulding on LDRD roots

These new discoveries are rooted in Sandia's longstanding work in this area and enhanced through multiple LDRD-funded projects focused on developing elements necessary to realize underpinning technologies. Successes in these

### CMOS-compatible integrated photonics

The *Germanium on Silicon Optoelectronics* LDRD project (FY11-FY13) demonstrated a high speed, ultra-compact integrated waveguide germanium-on-silicon photodetector. This ultra-compact device represented an essential building block in developing a CMOS-compatible silicon photonics platform.

The *Silicon Microphotonic Backplane for Focal Plane Array Communications* LDRD project (FY09-FY11) developed a silicon microphotonic communications platform, demonstrating several technological firsts,

including a world-record low-energy optical silicon photonics modulator with low voltage CMOS drive.

including a world-record low-energy optical silicon photonics modulator with low voltage CMOS drive.

The *Coherent Phonon Generation Through Nanoscale Enhanced Light-Matter Interaction: Towards Novel Silicon Lasers, Broadband Phononic Signal Processing and Optically Powered Micromechanics* LDRD project (FY11-FY13) developed an optomechanical device platform, and experimentally demonstrated the first instance of stimulated Brillouin scattering in silicon as well as forward stimulated Brillouin scattering on a chip.

## Quantum photonics

Sandia increased quantum photonics efforts through two three-year LDRD Grand Challenges—SECANT and SIGMA. The SECANT ([Sandia Enabled Communications and Authentication Network using Quantum Key Distribution](#)) Grand Challenge (FY14-FY17) focused on the construction of chip-scale, handheld quantum transceivers and a hybrid quantum key distribution network with chip-scale transceiver nodes. SECANT enhanced Sandia’s photonic integrated circuits and fabrication capability in the context of quantum and photonic integrated circuits, as seen, for example, in fiber-to-chip coupling efficiencies, results on high-speed modulators, polarization control, and polarization control, and polarization grating couplers.

Through the SIGMA (Strategic Inertial Guidance of Matterwaves) Grand Challenge (FY18-FY21), Sandia

## Capability Deployment

The capabilities achieved through these projects are being leveraged across a variety of mission spaces:

- The heterogenous integration and epitaxial regrowth capabilities are being leveraged in Air Force Research Lab projects focused on the development of photonic integrated circuits and other LDRD projects.
- The ultra-low loss silicon nitride photonic platform is being used by the [National Quantum Information Quantum Systems Accelerator](#), the Robust Optical Clock Network (ROCKN) program out of DARPA and the Entangled Logical Qubits

## Mission Application

The narrow linewidth laser that evolved through a decade of LDRD work is being applied in a range of defense and security sensing systems that must operate reliably in demanding environments.

RF spectral superiority provided by photonic processing will maintain the nation’s advantage over adversaries through unprecedented instantaneous bandwidth and frequency agility.

developed the world’s first low size, weight, and power inertial sensor based on atom-interferometer technology (cooling and readout of rubidium atoms with session initiating protocol). The project developed a [photonic integrated circuit](#) that can provide the required control, which, when integrated with SIGMA’s chip-scale optical amplifiers and frequency doublers, will provide the world’s first integrated laser system for an atom interferometer.



*Sandia scientist Ashok Kodigala aligns a fiber to a chip-scale, heterogeneously integrated laser under a microscope at the MESA complex.*

- (ELQ) program out of the Intelligence Advanced Research Projects Activity (IARPA).
- The new Brillouin physics is supporting a thrust of the Science and Technology Advancing Resilience for Contested Space (STARCS) Mission Campaign at Sandia, which is focused on advancing the nation’s capabilities to maintain and expand freedom of action in space.

Atomically referenced systems with integrated photonics provide the necessary size, weight, and power and robustness needed for fielding next generation strategic navigation and timing.

Integrated photonics provide the only practical route toward system scaling for quantum computing.

(See the [full timeline of development and impacts](#).)

## PROJECT HIGHLIGHTS – MISSION AGILITY

Sandia's LDRD program is organized around three themes: mission agility, technical vitality, and workforce development. Mission agility and technical vitality are closely related but differentiated by the technical readiness levels (TRL) of the research outcomes. The research outcomes in this section have a higher TRL and could impact Sandia's mission work more quickly.

Unless otherwise noted, these highlights are for projects that ended in FY23.

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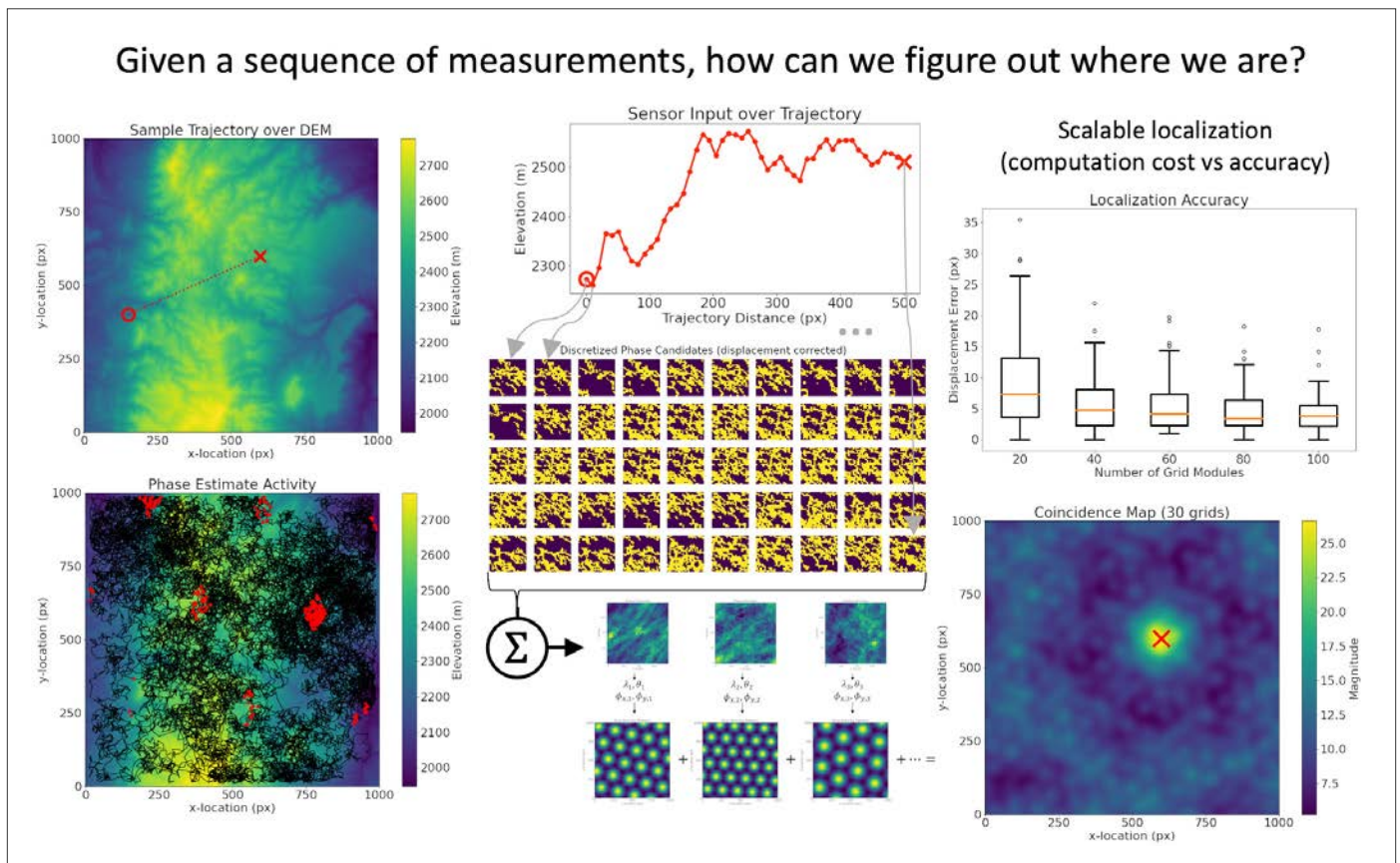
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## IMPROVING TERRAIN-AIDED NAVIGATION THROUGH A NEURO-INSPIRED ALGORITHM.

A research challenge to intelligent navigation in the absence of GPS is that the location of a vehicle must be computed with information gained from onboard sensors, while also considering the size, weight, and power hardware limitation. The interdisciplinary NeuroGrid LDRD was focused on meeting that challenge through the development of a neuro-inspired distributed algorithm for robust terrain-aided navigation suitable to emerging power-efficient neuromorphic computing (NMC) hardware. This project was part of an initial laboratory effort to develop spiking circuits on the Intel Loihi 2 NMC platform, which was supported by a collaboration with Intel

through the Neural Exploration & Research Lab at Sandia. Application of the localization approach to an estimation model was performed through Alliance partner University of Texas at Austin with support by a graduate student. Sim-to-real implementations were also explored at the AutonomyNM Robotarium testbed. The project produced four publications including [ICONS: International Conference on Neuromorphic Systems](#), [NICE: Neuro-inspired Computational Elements](#), and [IEEE/ION Position, Location and Navigation Symposium \(PLANS\) and a patent application](#). (PI: Felix Wang)



The NeuroGrid LDRD team developed a neuro-inspired distributed algorithm for robust terrain-aided navigation suitable to emerging power-efficient neuromorphic computing hardware.

## ENABLING ADAPTIVE GUIDANCE THROUGH CARRL: CONTROL WITH ADAPTIVE ROBUST REINFORCEMENT LEARNING.

More flexible guidance, navigation, and control architectures are needed in hypersonics. The Sandia project team investigating this need discovered that recurrent reinforcement learning could perform coupled adaptive guidance and control of systems with uncertain dynamics and external disturbances and demonstrates much better performance compared to classical techniques. Using a simulated mass-spring-damper system, the team benchmarked this method against idealized omniscient interior point trajectory optimization, robust gain optimization, model reference adaptive control, and sliding mode control. Implementation of CARRL enabled dynamic trajectory replanning with optimal control solutions and minimal online computation cost. The Sandia LDRD team also made encouraging progress in extending these results to simulated and real hexrotors, which enable aerial manipulation. A close collaboration with Sandia Alliance partner University of Illinois at Urbana-Champaign was beneficial to the project. (PI: Rachel Schlossman)

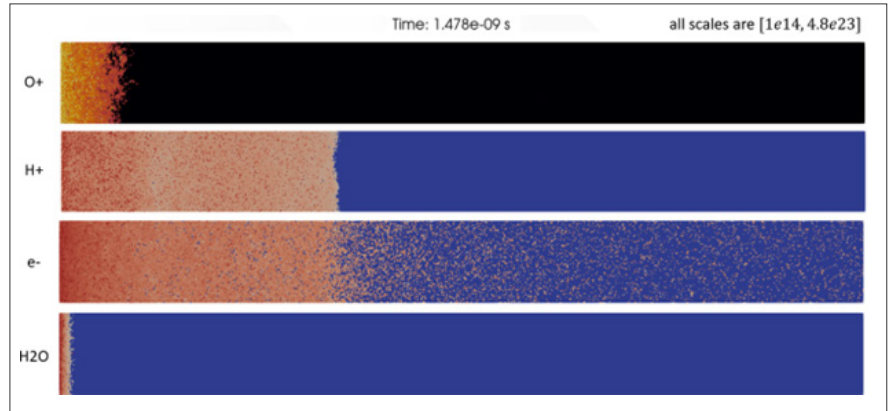
## NON-IMAGING TARGET RECOGNITION FOR HYPERSONIC ENDGAMES.

The hypersonic flight environment and associated vehicle geometry create uniquely challenging constraints for forward-looking seeker technologies that provide high resolution imagery. Given these realities, researchers in this LDRD project developed techniques that allow low-resolution radar systems to identify and home in on targets of interest without using high resolution radar imagery. A robust targeting system, special targeting algorithm, and radar measurements help create a map of the target scene with relative states that converge to provide sufficient levels for a successful engagement. (PI: Jeff Spooner)

## EMPIRE PLASMA SIMULATION CODE SHOWS ADVANCEMENT IN CELL MODELING AND AN INCREASED ROLE IN PULSED POWER APPLICATIONS.

Pulsed-power machines such as the Saturn accelerator predict simulations of high-current diode operation and require self-consistent modeling for a set of highly coupled physics processes. This LDRD team, in collaboration with Alliance partner University of Texas at Austin, demonstrated advanced electromagnetic particle-in-cell modeling capability in the EMPIRE plasma simulation code. These advancements included: (1) a set of verification problems covering all key processes in gap closure physics was designed, (2) a new EMPIRE exemplar (the RITS-6 diode), and (3) a Saturn accelerator exemplar that was enabled by models matured under this work and simulated further into the pulse than previously possible. These developments have led to the highest

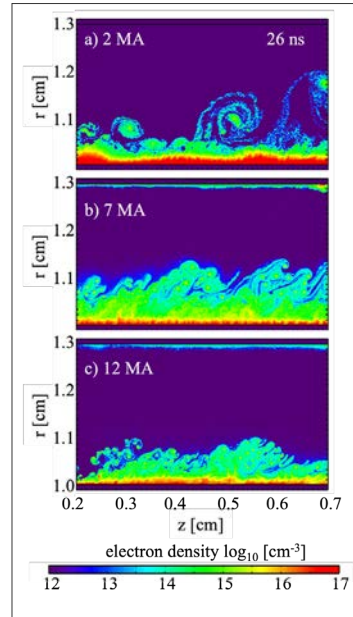
confidence EMPIRE power flow predictions of Saturn to date and provide radiation field predictions within <15% of thermoluminescent dosimeter measurements. The results show the EMPIRE state-of-the-code taking on an increased role in pulsed power applications. (PI: David Sirajuddin)



Electrode-plasma-verification tests for the EMPIRE plasma simulation code.

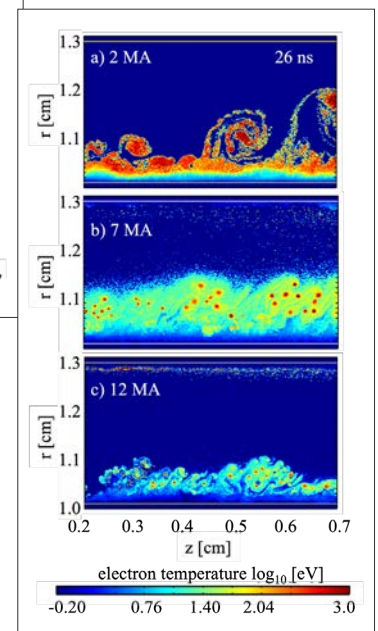
## DEVELOPING AN IMPROVED MELT MODEL FOR POWER FLOW.

Accelerators that drive z-pinch experiments transport high current densities at 1 MA/cm<sup>2</sup> to melt or ionize the target and implode it on its axis. These high current densities stress the transmission lines upstream from the target, where rapid electrode heating causes plasma formation, melt, and possibly vaporization. These plasmas negatively impact accelerator efficiency by diverting some portion of the current away from the target, referred to as “current loss.” Through this LDRD project, a simulation capability was created that captures this wide range of physics and advance the understanding of plasma generation, transport, and scaling in pulsed-power systems. The new model is being used to improve the efficiency of existing accelerators and to design new systems that operate at ever higher current densities. The results were shared at three invited talks and published in [Journal of Physics: Condensed Matter](#) and [Physical Review Accelerators and Beams](#). (PI: Nicki Bennett)



The electron temperature contours corresponding to the densities above. The same 5-mm segment of Fig. 1(b) simulation is used and the currents at 26 ns are (a) 2, (b) 7, and (c) 12 MA for the three pulse rises. (Temperatures are plotted on a log scale from 10<sup>-2</sup> – 10<sup>3</sup>.)

The electron density contours in a 5-mm segment of the simulation illustrated in Fig. 1(b) at 26 ns reaching currents of (a) 2, (b) 7, and (c) 12 MA for the three pulse rises. (Densities are plotted on a log scale from 10<sup>12</sup>–10<sup>17</sup>.)



## INVESTIGATING ALTERNATIVES WITH LESS GLOBAL WARMING POTENTIAL THAN SF6.

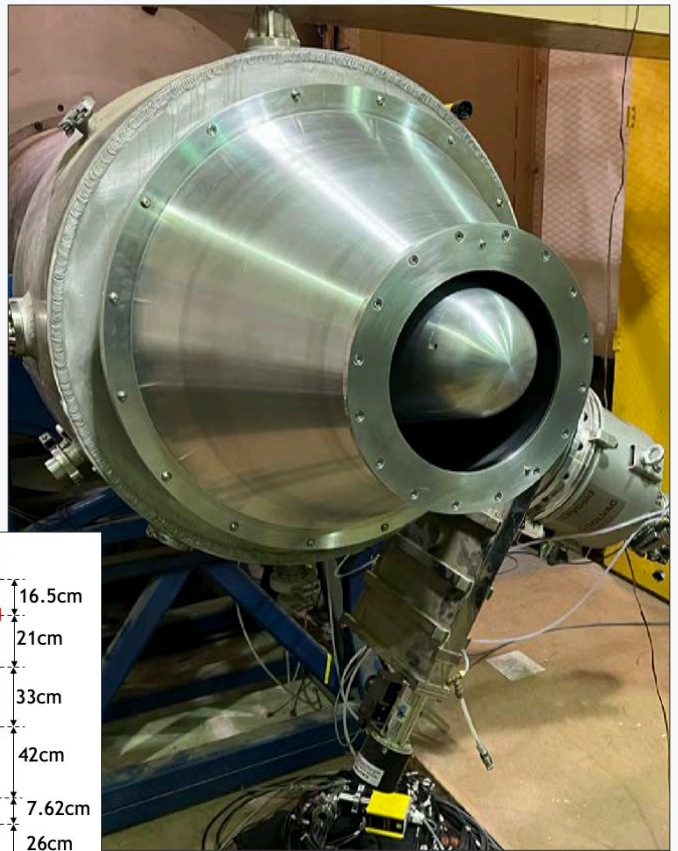
Sulfur hexafluoride (SF6) is widely used in pulsed power switching and high voltage insulation due to its high dielectric strength and stable breakdown distribution, among other favorable properties. However, SF6 is also the most potent greenhouse gas, with a global warming potential (GWP) 23,500 times that of carbon dioxide. Sandia researchers and academic partners at Texas Tech University investigated novel gas mixtures containing the

perfluoronitrile C4F7N. Mixtures with GWP 250 times lower than SF6 demonstrated superior stability and recoverability under switching conditions relevant to large-scale pulsed power facilities. This work resulted in publication in [Journal of Physics D: Applied Physics](#) and a Laboratory Residency Graduate Fellowship for Andy Castillo under his advisor Matt Hopkins. (PI: Adam Steiner)

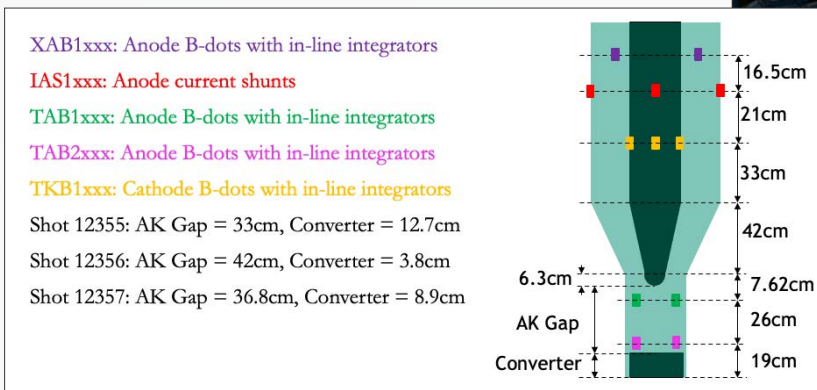
## FROM CONCEPT TO FIELDING A NEW DIODE AT HERMES IN TWO YEARS.

This LDRD project coupled EMPIRE (an electromagnetic plasma code) and ITS (a radiation transport code) and predicted the output of Bremsstrahlung converters, like those fielded at Sandia's High Energy Radiation Megavolt Electron Source (HERMES). The project went from an initial Bremsstrahlung diode concept to fielding a new diode at HERMES in just over two years by utilizing the optimizer from DAKOTA to improve the radiation output of this coupled set of codes and change the geometry parameters of the Magnetically Insulated Transmission Line (MITL) and diode. This LDRD, in collaboration with Alliance partner Purdue University, also exposed where improvements were needed to better simulate the time dependent output required for a Bremsstrahlung diode fielded on HERMES. This work resulted in one staff hire and five

publications, including three publications in the 2022 IEEE International Conference on Plasma Science (ICOPS), one in [Applied Physics Letters](#), and another in [Scientific Reports](#). (PI: Keith Cartwright)



*Bremsstrahlung diode dose improvements were achieved using shaped anode and cathode geometries on Sandia's HERMES III accelerator, the world's most powerful gamma simulator.*

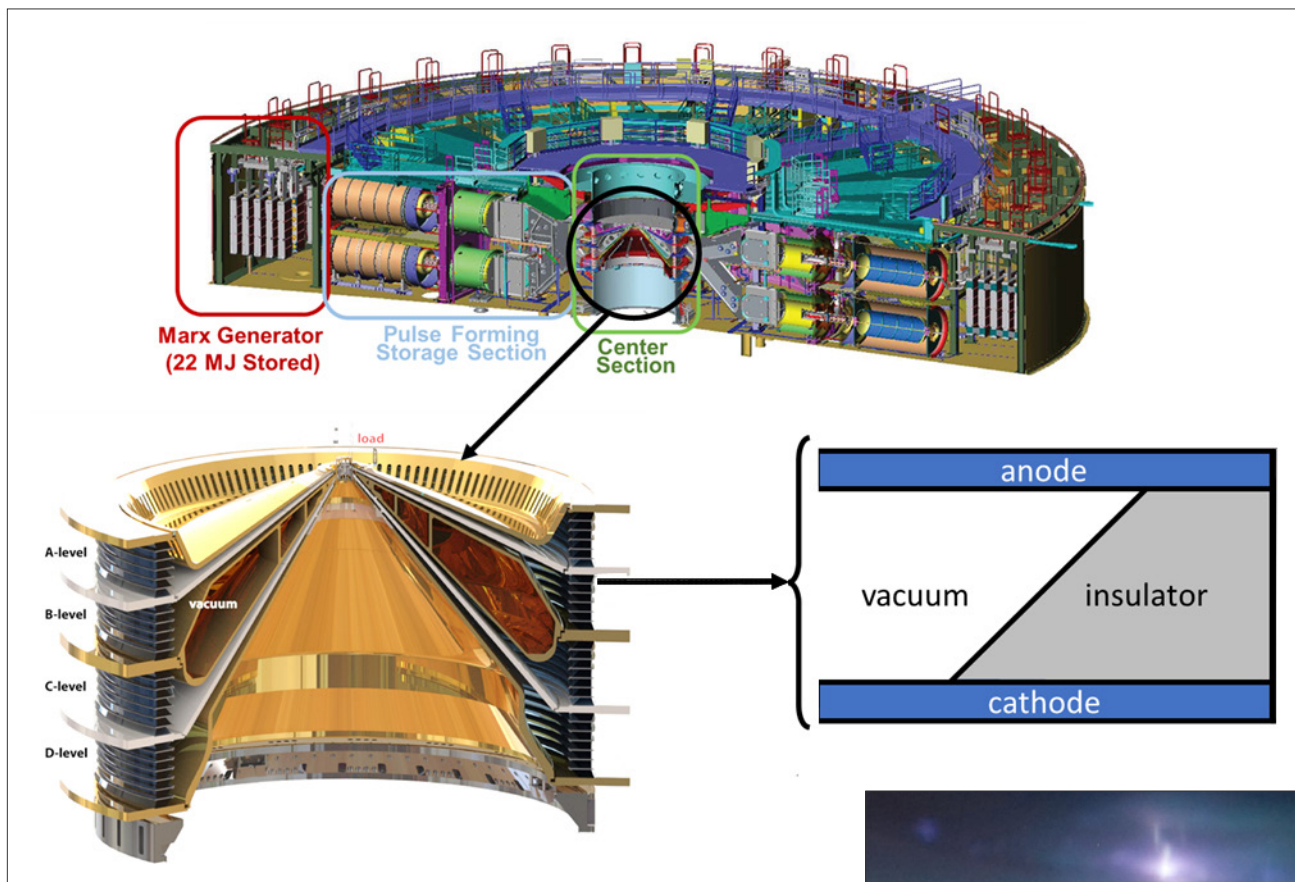


*The optimizer improved the radiation output of this coupled set of codes by changing the geometry parameters of the MITL and diode.*

## PREVENTING DAMAGE CAUSED BY ELECTRICAL DISCHARGE TO PULSED POWER SYSTEMS.

Insulator flashover is a critical failure mechanism in pulsed power systems. If an electrical discharge across the insulator surface occurs during power delivery, the shot may fail, and catastrophic damage may occur to the insulator itself. This LDRD investigated a hypothesized critical insulator failure mechanism, the anode-initiated insulator flashover. Through a combination of experiment, diagnostic development, and computational simulation by a collaborative team of Sandia, Texas Tech University, and Utah State University scientists and students, new insights were achieved, and potential design changes

were proposed. Key insights include clarifying the very early participation of insulator material (not electrode material), in the initiation process through detailed spectral analysis at Texas Tech's flashover test stand. Another key advancement was identifying a mechanism through modeling with Sandia's Aleph code that can cause a discharge to travel from the anode towards the cathode—opposite the usual direction. This work was published in [IEEE Transactions in Plasma Science](#), included in numerous conference proceedings, and covered in conference presentations around the world. (PI: Matt Hopkins)



(Top) Full schematic of Sandia's Z Machine. (left) Close-up of Z center section showing the 4-level insulator stack, each level has 6-7 insulator segments with interlaced field shaping electrodes. (right) A schematic representing each of the insulator segments.

Full time exposure of electrical discharge between hemispherical anode (upper region), intervening insulator, and planar cathode (bottom region). Perspective is looking directly at insulator, "face on."



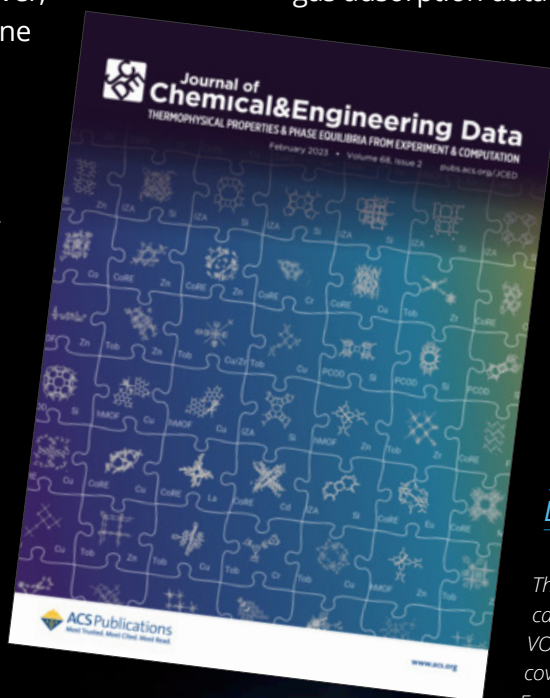
## DETECTING DISEASES THROUGH BREATH.

Biochemical reactions in the body produce small molecules known as volatile organic compounds (VOC), which are exhaled through your breath and can possibly detect different diseases. These VOCs can provide information about infections, diseases, or metabolic process in the body. However, it is difficult to detect VOCs and determine a possible diagnosis. Collaborating with Alliance partner Georgia Tech and Securing Top Academic Research & Talent at Historically Black Colleges and Universities partner North Carolina A&T University, the LDRD team developed highly selective nanoporous sorbents (or molecular sponges), also known as metal-organic frameworks (MOF), to look for these VOCs in the breath. MOFs can be in many different sizes and shapes and tailored to adsorb a target molecule. Molecular modeling is used to design MOFs and can target the VOCs. The MOFs capture desired VOCs from the breath

and separate them from other molecules. This concentrates the VOCs so they can be detected by a portable, inexpensive detector. This technology can help detect different diseases by choosing MOFs that target specific VOCs. A database of gas adsorption data in thousands of MOFs

was developed and published. This data contains millions of data points about adsorption in MOFs and can help researchers choose a good MOF for a specific target application.

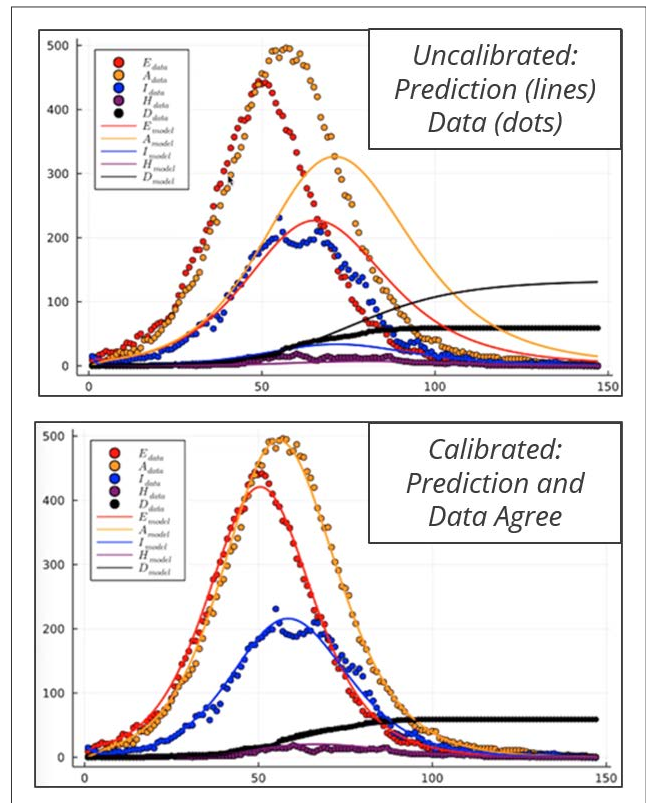
This article made the front cover of [Journal of Chemical & Engineering Data](#). (PI: Scott Bobbitt)



*The Sandia project focused on the capture and detection process of VOCs and was highlighted on the cover of Journal of Chemical & Engineering Data.*

## SHOWING PANDEMIC OUTBREAKS THROUGH MODELS AND AI.

Designing new mathematical and AI methods to shorten pandemic outbreaks was the focus of the Sandia Pandemic Endgame LDRD project in which models are used early in pandemics to predict the location and severity of an outbreak. Endgame's revolutionary AI-driven calibration methods increase model accuracy, and new optimal control methods can help with response to different specific communities. Sandia is validating Endgame models against disease outbreaks in the U.S. and developing countries, and scientists from National/Regional partners Arizona State University and North Carolina State University are collaborating on public-health messaging, developing new spatial models, and building calibration methods into the next-generation pandemic models by DOE. The Endgame team is actively collaborating with the Center for Disease Control on improving accuracy and credibility of national-scale disease models. These results were published in [Applied Network Science](#), and the team gave an invited talk at the Society of Engineering Science. (PI: Patrick Finley)



*Data-driven Calibration of Epidemiological Model: top figure shows uncalibrated information, bottom figure shows calibrated information.*

## EFFICIENTLY SOLVING LARGE OPTIMIZATION PROBLEMS FOR NATIONAL SECURITY APPLICATIONS THROUGH CI-MOR.

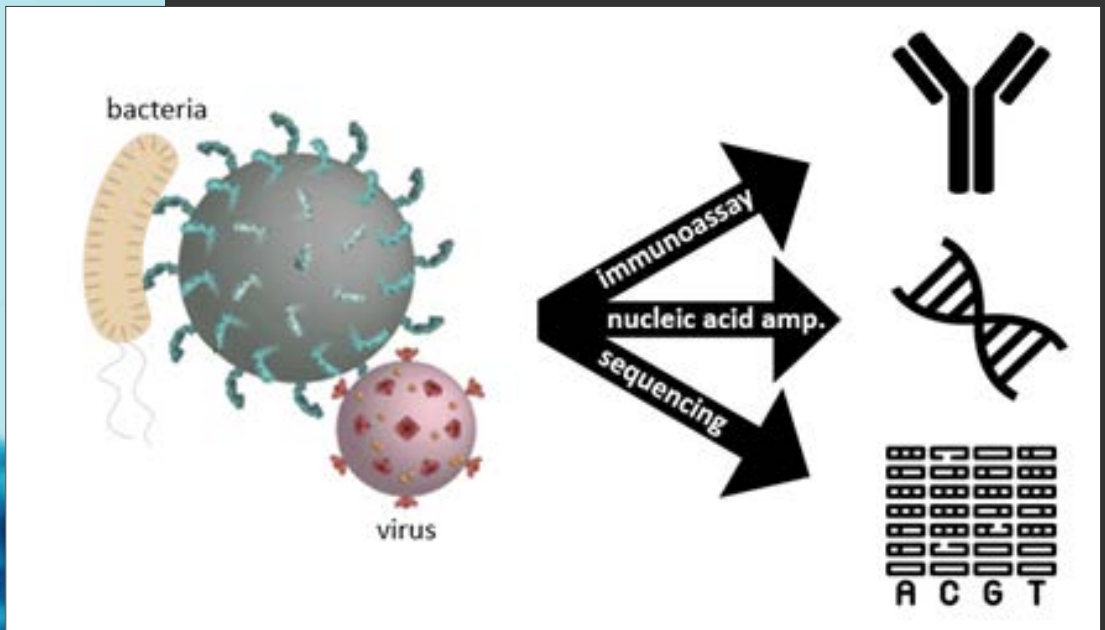
Critical Infrastructure-Model Order Reduction (CI-MOR) LDRD researchers collaborated with Sandia National/Regional partner Carnegie Mellon University to develop methods for efficiently solving large optimization problems occurring in critical infrastructure and engineering designs. This was done by using optimization formulations in machine learning models and leveraging model decision trees. This research confirmed that the ML-based

approximations provided high-quality solutions to these difficult applications. For example, optimal designs were explored for a heat exchanger and a family of refrigeration systems by analyzing variations in a chemical process. These results will be incorporated in the Critical Infrastructure Hidden Markov Model toolkit that will be publicly released in the future. Follow-on funding was secured by IARPA and industry. (PI: William Hart)

## DEVELOPING A QUICK AND EASY UNIVERSAL TEST FOR BIOTHRREATS.



When a bioterrorist endangers the economy, national security, and health, accurate tests need to be developed and distributed quickly throughout the United States. Isothermal assays are fast and easy to operate; however, they struggle to detect ultralow levels of pathogens. The goal of this LDRD project with ApoH Technologies and Alliance partner University of Texas at Austin was to develop a universal pathogen enrichment mechanism that would improve the sensitivity of these alternative assays. Using ApoH protein-coated nanoparticles, the team demonstrated an enrichment of SARS-CoV-2 and *Burkholderia thailandensis* and confirmed the ApoH beads could successfully concentrate pathogens in both human saliva and urine. The ApoH beads are also simple enough to move to a portable platform for accurate biological testing. This advancement will significantly impact our nation's ability to monitor bioterrorists and quickly prepare for future outbreaks and bioterrorism incidents. These results were published in *Expert Review of Molecular Diagnostics*, and the team was asked to participate in an invited talk at the Cambridge Innovation Institute. (PI: Taylor Moehling)

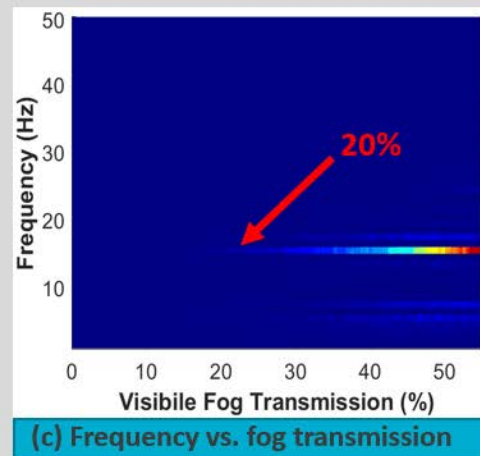
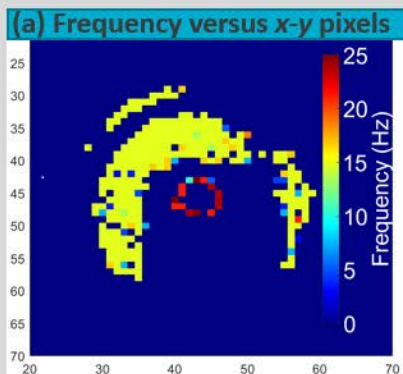


*ApoH magnetic beads provide pathogen-agnostic enrichment and simplify the analysis.*

## UNDERSTANDING REAL-WORLD COMPLEXITIES IN EVENT-BASED SENSING.

Many national security applications/scenarios could face devastating impacts when visibility decreases in weather events such as fog. Event-based sensors (EBS) are novel high-speed asynchronous cameras with high dynamic range. EBSs only read out pixels that sense changes in the scene, dramatically reducing output bandwidth and power as compared to the current state-of-the-art imaging systems used for remote sensing mission applications.

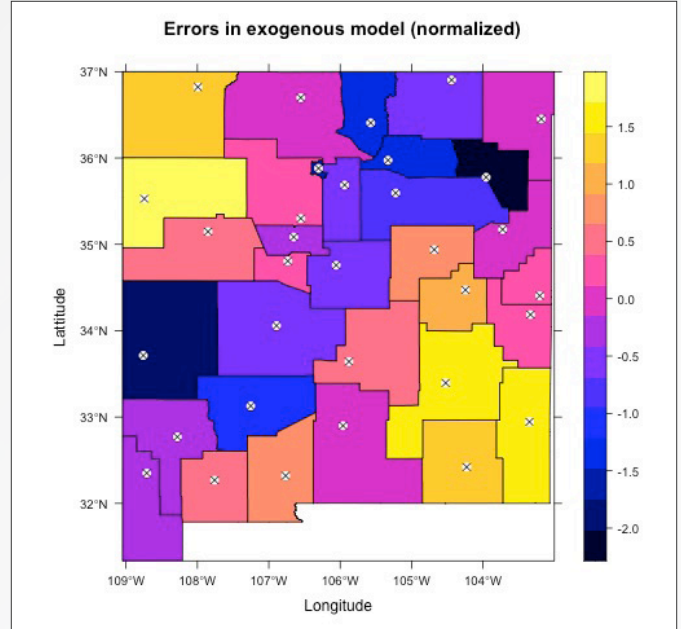
This Sandia LDRD team focused on tackling a key data-science deficiency in using these novel sensors, specifically, a lack of algorithms that operate on EBS output while handling real-world mission-applicable degraded visual environments such as fog. The researchers delivered an EBS frequency detection algorithm pipeline that handles fog environments while evaluating a variety of commercial off-the-shelf EBSs. This project, which resulted in the hiring of one postdoc, provided groundwork to a set of ongoing projects funded by NNSA's Office of Defense Nuclear Nonproliferation Research and Development. The project's frequency detection algorithms are being inserted directly to externally funded projects tackling further development/refinement specific to nonproliferation site monitoring tasks. Results were presented at [SPIE Defense + Commercial Sensing and Optica Imaging Congress](#) and the 2024 Military Sensing Symposium (PI: Lilian Casias)



Results from one of the temporal characterization event-based sensing algorithms. (a) Spatial distribution of detected pixel frequencies demonstrates the algorithm can identify the 15 Hz ground truth signal throughout the chopper body and 23 Hz for the center bolts. (b) An image of the optical chopper. (c) A 3D histogram of tracked frequencies as the fog dissipated and visibility increased. The algorithm was able to pick up the 15 Hz signal at around 20% visibility.

## USING A SPREAD-RATE DETECTOR TO DETECT POSSIBLE DISEASE OUTBREAKS.

Early detection of outbreaks through daily case counts is difficult because of noisy data. In contrast, the spread rate of the disease tends to behave. This LDRD developed a method based on variants to estimate the spread rate. It was tested on New Mexico COVID-19 data to detect the arrival of the Fall 2020 COVID-19 wave. The method correctly detected the arrival of the Fall 2020 outbreak wave a week ahead of time, but it underestimated the spread-rate field over a collection of counties. This joint project with Alliance partner UC Berkeley showed a new theoretical framework for detecting and characterizing outbreaks. Follow-on funding was secured to continue investigation and development of this detector, and one staff member was hired to support the effort. (PI: Jaideep Ray)

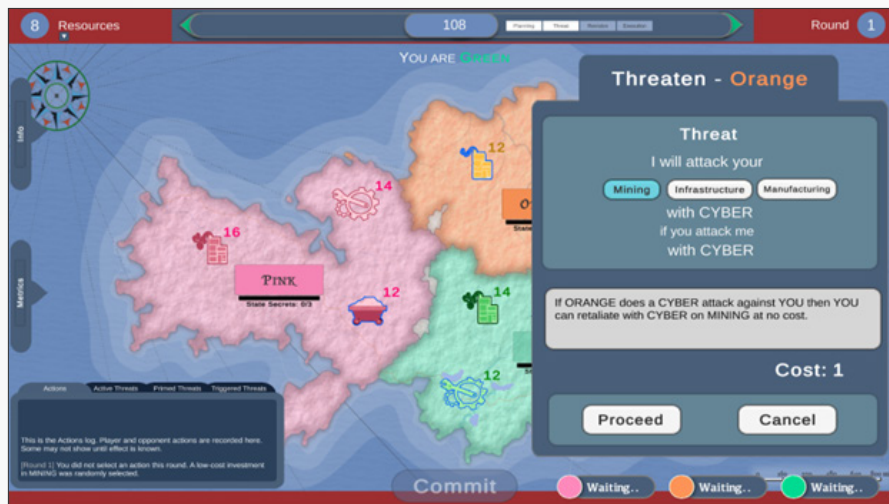


The method shows the detector of the model of the COVID-19 outbreak in New Mexico.

## DEVELOPING CYBER-CAPABILITY WARGAME TANTALUS TO IDENTIFY CYBER ADVERSARY STRATEGIC RESPONSES.

Using cyber-capabilities to deter adversaries provides a potentially powerful new method for addressing national security challenges. Policymakers and academics often debate if cyber deterrence is even possible, and if it is, are these dynamics similar to those in other domains? Sandia collaborated with Alliance partners Purdue, the University of Illinois Urbana-Champaign, and the UC Berkeley to develop an [experimental](#)

[wargame](#) called TANTALUS to study the trade-offs between revealing or concealing cyber-capabilities. With data from over 1,090 players from across the world, results suggested that cyber threats are used just like nuclear threats, but they are less likely to induce deterrence effects. These results can help policymakers better understand the use of cyber threats in deterrence situations. This project developed a foundational software

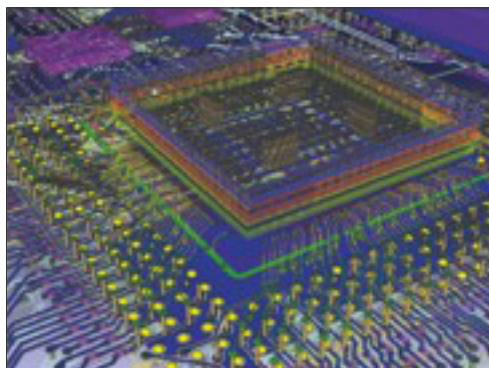


platform, CASTLE, to facilitate the development of online experimental wargames. (PI: Kiran Lakkaraju)

TANTALUS was developed to show how cyber deterrence success or failure is within a player's reach.

## IMPROVING IMAGING RESOLUTION AND MATERIAL IDENTIFICATION FOR EVALUATION OF MICRO COMPONENTS.

Developing an innovative X-ray Computed Tomography Anode that allows for dramatic improvement in imaging resolution and material identification within components undergoing inspection is critical to national security. In this LDRD project, this was achieved by developing fabricated multi-metal patterned anodes using Sandia's world-class fabrication research facilities combined with Sandia's innovative Hyperspectral Computed Tomography Systems. Through this work, the Sandia LDRD team



*Imaging at nanometer scale was the largest challenge the team overcame in creating a robust capability that can be utilized in many areas, including material identification for quality and counterfeit inspection.*

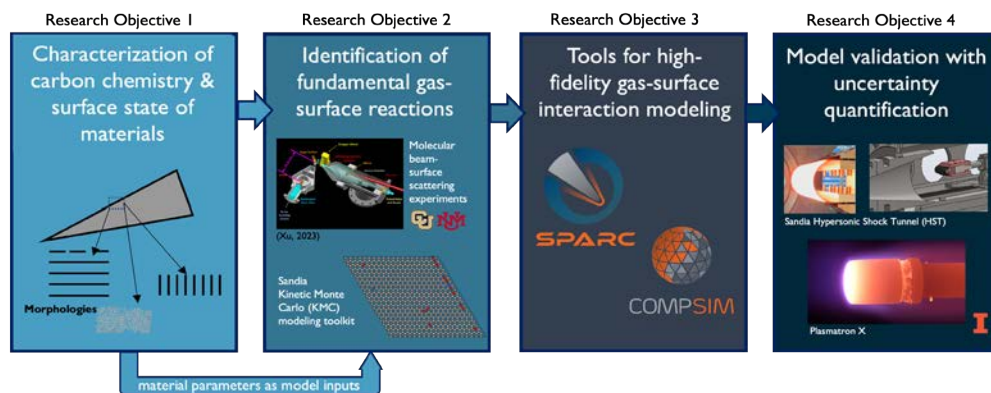
successfully achieved resolutions and image quality metrics that were once infeasible with current X-ray sources. This approach is also readily available for retrofit applications allowing for rapid deployment of these discoveries. This work is expected to allow Sandia to nondestructively inspect microelectronics at scale without modifying or altering the objects to be inspected. Results include seven invention disclosures (two of which are currently under patent review), five conference proceedings, and two journal articles. (PI: Edward Jimenez)

## ADVANCED FINITE-RATE ABLATION PREDICTIONS WITH QUANTIFIED UNCERTAINTY FOR HYPERSONIC FLIGHT.

Accurate predictions of ablation and thermal performance of heat shield materials are critical to the design of thermal protection systems for hypersonic vehicles. This LDRD sought to advance the state-of-the-art and develop an innovative Gas-Surface Interaction (GSI) model development framework for materials for flight regimes that require a finite-rate approach. The team created a multi-disciplinary framework to build and calibrate surface chemistry models through new materials characterization data, molecular beam-surface scattering experiments,

theory, and an optimization toolkit. A validation framework was demonstrated to assess ablation product predictions and uncertainty under realistic high-enthalpy environments in collaboration with Sandia's Hypersonic Shock Tunnel team. The team also leveraged newly implemented finite-rate models to support sensor instrumentation design on an A4H flight test. Partnerships with National/Regional partner University of Colorado Boulder and Sandia Alliance partners University of New Mexico and University of Illinois Urbana-Champaign were instrumental to model development. Results

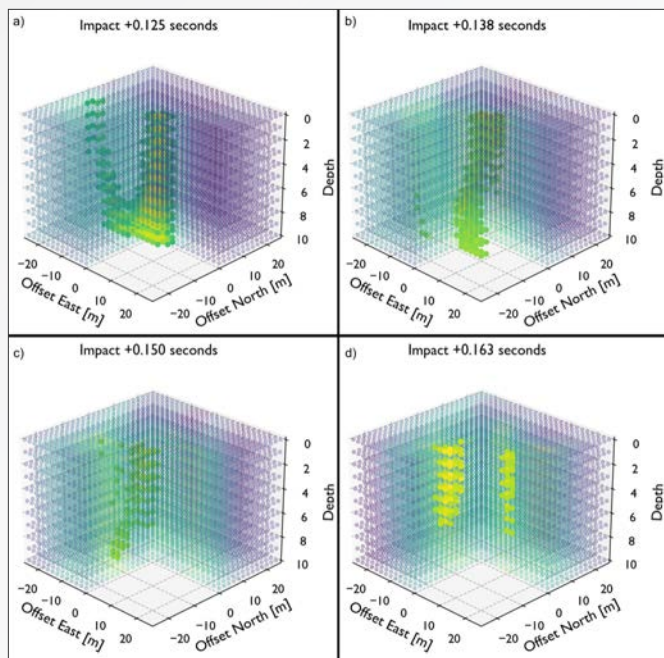
were published in [Physical Chemistry Chemical Physics](#) and [Aerospace Research Central](#). (PI: Erin Mussoni)



*The four research objectives addressed through the LDRD project led by Mussoni.*

## USING DISTRIBUTED ACOUSTIC SENSING TO ACQUIRE SUBSURFACE TRAJECTORY OF EARTH PENETRATORS.

Earth-penetrating weapon development applies numerical modeling to simulate the expected acceleration, stress, and strain of a penetrator, and to predict the penetration depth and target survivability. Evaluation of design performance would be enhanced with detailed knowledge of the penetrator's subsurface Time Space Positional Information (TSPI). This project deployed distributed acoustic sensing (DAS) at Tonopah Test Range to evaluate the efficacy of DAS for acquiring subsurface TSPI. The DAS array successfully recorded the propagations of airborne shockwaves from the transonic munitions and distinct seismic phases from the impacts, with spatial and temporal resolutions of 3 m and 1000 Hz, respectively. Point of impact was successfully triangulated to within 2 m error. Subsurface trajectories were obfuscated by post-impact breakups of the munitions. However, results were promising enough to motivate pursuing further testing to acquire baseline seismograms from an intact penetration. (PI: Romy Frederick)



Distributed acoustic sensing (DAS) demonstrated the efficacy of DAS for acquiring subsurface Time Space Positional Information with the DAS array successfully recording the propagations of airborne shockwaves from the transonic munitions and distinct seismic phases from the impacts, with spatial and temporal resolutions of 3 m and 1000 Hz, respectively.

## ENABLING AM ELECTRONICS WITH HOT ISOSTATIC PRESS METHODOLOGIES.

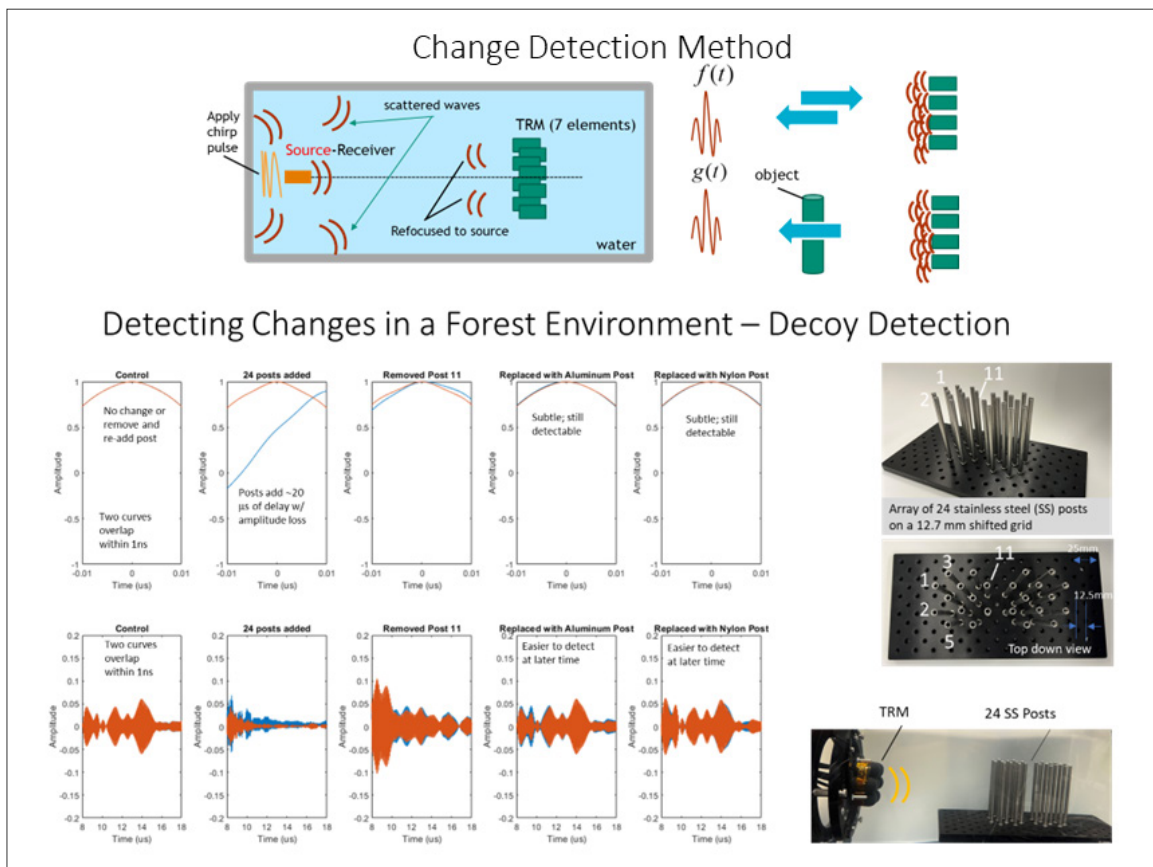
Additive manufacturing (AM) of copper has the potential to accelerate the product development cycles while also enabling previously inaccessible design freedom. These benefits support NNSA priorities of anticipating future threats, surveillance, and formulating responsive solutions. Sandia uses several AM copper parts, but sintering leaves voids that negatively affects the electrical, thermal, and corrosion properties. This leads designers to choose traditional copper manufacturing routes. Currently, most successes in AM have been with colloidal silver-ink printing (inkjet, screen, etc.); however, silver is not ideal (dendrite-growth) for many applications in the

Nuclear Security Enterprise (NSE). Through this LDRD project, Sandia demonstrated that the Hot Isostatic Press (HIP) can induce chemical sintering by applying isostatically-high pressure under controlled temperature to reduce oxide formation and consistent resistivity performance via increase densification; synergistically the isostatic nature of the pressure applied yielded avenues to lower porosity and surface roughness. The ability to process AM electronics copper circuitry will yield reproducible electrical conductivities that meet nuclear deterrence and broader national security mission needs. (PI: LaRico Treadwell)

## USING TIME-REVERSAL ACOUSTICS TO DETECT ASSET TAMPERING.

This study investigated the ability of time reversal acoustics (TRA) to detect change events in complex environments and understand the key parameters that influence the detection event. The complex environment consisted of numerous objects that increase the difficulty of tracking changes to the primary object where line-of-sight prevents direct viewing. A TRA system measured the spatial sensitivity and object tampering sensitivity, where computational tools were used to understand data encoding in the time signals. The team performed change detection studies where objects were moved, removed, added, altered, replaced with decoys, or hidden in complex environments with nearly identical features. Using a computational

approach, the team validated several hypotheses regarding the placement of the sensor Time Reversal Mirror vs. the spatial sensitivity, the impact of closed vs. open boundaries, and the role of open boundary conditions vs. closed for change location detection. As part of the study, the team developed a hardware system with a software application (patent pending) that detects subtle sub-wavelength changes in a water environment. The study also resulted in two pending publications, and interest expressed from the private sector in investigating tamper indications in advanced nuclear power reactors. (PI: Darren Branch)

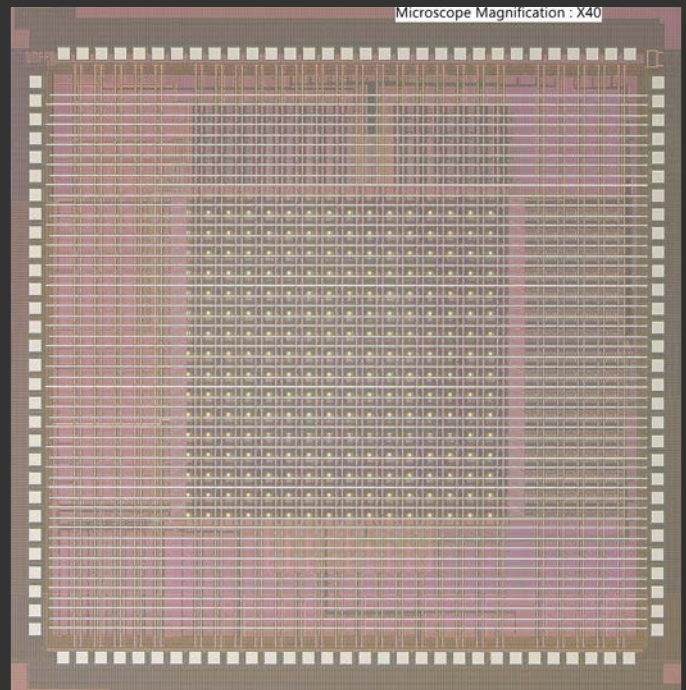


(Top) Change detection method. (Bottom) Detecting changes in a forest environment using decoy detection.

## IMPROVING PERFORMANCE AND SCALING OF GLOBAL COVERAGE REMOTE SENSING SYSTEMS.

Focal plane arrays (FPA) are the critical component that limits the performance and scaling of global coverage remote sensing systems. Low power, area-efficient, embedded signal processing to compress image data near its source is needed to allow efficient movement of data from the interior of the FPA to the data transmission system, so the Sandia LDRD team focused on asynchronous spike-based processing to achieve this objective. A wavelet transform was implemented using rate encoding pixels which asynchronously emit spikes to drive integrate-and-fire processing circuits. Coefficients were stored using Ta-TaOx Resistive Random Access Memory (ReRAM) to program the quantity of charge a spike will place on a neuron integrating circuit. Sandia collaborated with Northwestern

University to develop low conductance ReRAM for more energy and area efficient computing. This project demonstrated operation of neural circuits, coupled with programmable ReRAM elements, and these were implemented in small demonstration FPAs. (PI: Rex Kay)



*Sandia created a neuromorphic focal plane array with programmable spatial and temporal filtering, using asynchronous, spike-based processing.*



## TITANS PROJECT SEEKS TO OPTIMIZE REMOTE SENSING SYSTEMS IN CONGESTED ENVIRONMENTS.

Future remote sensing systems will require high bandwidth communication links operating in congested or contested environments. While optical communication is attractive, the size, weight, and power of existing systems is large. The Transmitters for Applications of National Security (TITANS) project (2.2 $\mu$ m integrated transmitters for applications of national security) sought to create a chip-scale optical transmitter operating at 2.2 $\mu$ m wavelengths leveraging heterogeneous integration of laser materials with silicon photonics. Historically, most optical communication has occurred at

1.55 $\mu$ m wavelengths. However, for high-power density systems, this wavelength is lossy due to two-photon absorption in silicon photonics. The 2.2 – 2.4 $\mu$ m wavelength range avoids this loss mechanism but introduces new research and development challenges in designing the silicon photonics, processing the laser materials, and heterogeneous integration to create a compact chip-scale device. This project demonstrated each of the system components, the integration process, and an initial integrated light source. (PI: Joshua Shank)

## IMPROVING MUNITIONS TRACKING TO ENHANCE BOTH LETHALITY AND SURVIVABILITY.

Tracking low-signal, high-speed objects remains difficult despite the technological progress in imaging systems. This project develops novel 3D tracking techniques to enable passive detection of small, high-speed, low-contrast incoming and outgoing targets. The ability to successfully track munitions throughout their path would enhance both the system lethality and survivability. These

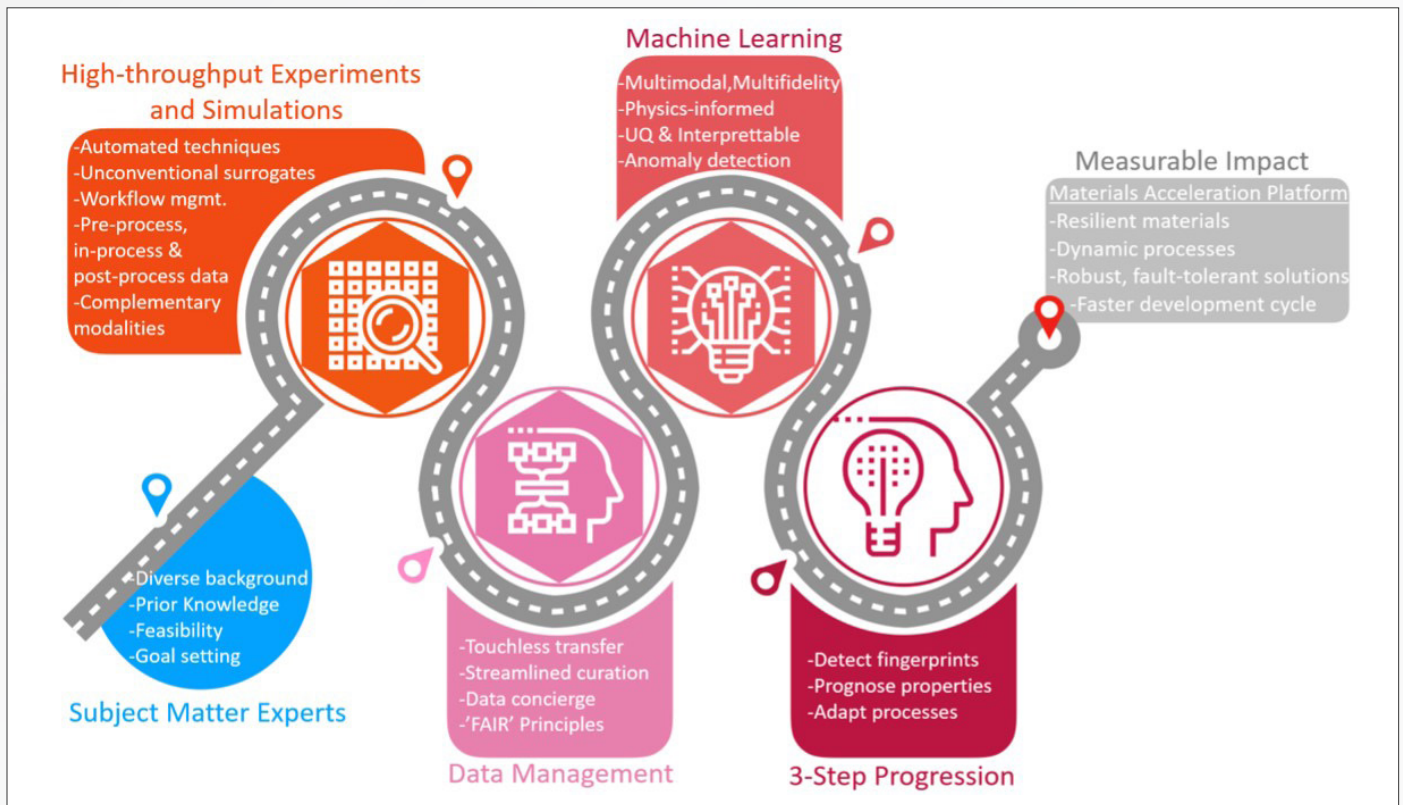
same enhancements would benefit multiple mission domains and also enable autonomy and engagement against autonomous systems. Sandia collaborated with Securing Top Academic Research & Talent at Historically Black Colleges & Universities partner Alabama A&M, which has experience with stereo imaging, multi-object tracking, and real-time data filtering. (PI: Jaclynn Stubbs)



## BEYOND-FINGERPRINTING: AN AI AND ML-GUIDED DISCOVERY OF ROBUST MATERIALS AND PROCESSES.

Imagine a world where robust materials and processes are discovered by semi-autonomous platforms with embedded subject matter expert (SME) knowledge through AI and ML. Beyond Fingerprinting, a Sandia LDRD Grand Challenge, is exploring this realm using a ML-guided approach that integrates expertise with algorithms enriched with physics-based constraints to unearth process-structure-property correlations. The key technical innovations developed under this program include novel high-throughput testing methods, multimodal data fusion, a patented physics-informed multimodal autoencoder, a new physics-based ML algorithm (that speeds up simulations by a thousand times), and a multi-objective Bayesian

optimization. Sandia component engineers recently used the Beyond-Fingerprinting approach to accelerate the development of production protocols for an additively manufactured Kovar alloy used in Sandia products. The project's capabilities, enhanced through collaborations with National/Regional partner Arizona State University, Alliance partners University of New Mexico, Georgia Tech, and UC Berkeley, and Brown University, have already translated beyond materials science into domains ranging from climate change to medical triage. This information has resulted in 18 journal publications, with ML for materials science being published in Matter. (PI: Brad Boyce)

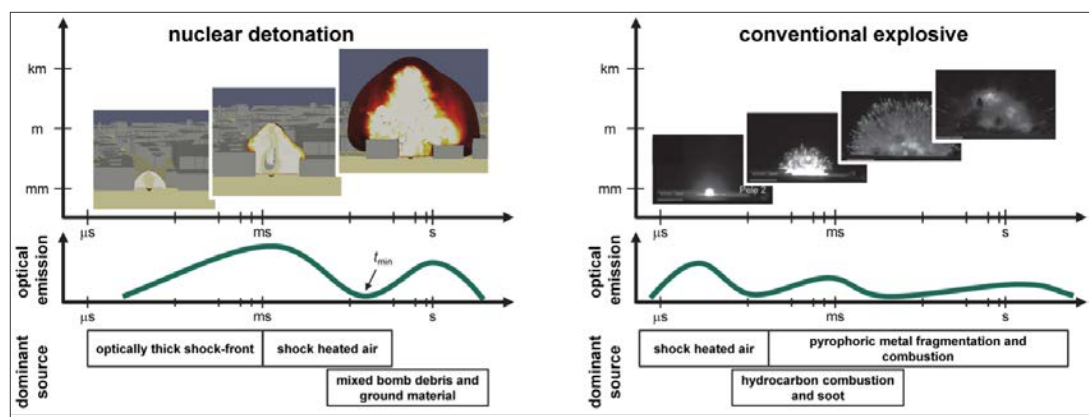


Outcomes from Beyond Fingerprinting have been used in many different technologies.

## LIGHT SPEED GRAND CHALLENGE: ACCELERATING FUNDAMENTAL PREDICTIONS OF EXPLOSIVE OPTICAL EMISSIONS.

Nuclear detonations and chemical explosives produce optical emissions detectable by satellites, and NNSA analyzes these signals to quantify the yield and identify the design heritage. State-of-the-art methods to predict and interpret optical signatures require High Performance Computing simulations that can take weeks to months to be analyzed for complex scenarios such as an urban nuclear detonation or detailed prediction of proliferation signals. Rigorous verification and validation and uncertainty quantification analyses

did not exist for these missions, which resulted in poorly defined simulation accuracy requirements. The Light Speed research team, which included students from five universities, managed to speed up (at least a hundred times) and advance the accuracy (at least ten times improvement) of the optical modeling and simulation capabilities. This cross-functional LDRD team was able to provide quantifiable uncertainty and improved confidence for the first time. (PI: Marc Welliver)



*The Light Speed LDRD Grand Challenge at Sandia sped up and improved the accuracy of optical modeling and simulation capabilities, which can be utilized in nuclear monitoring and proliferation detection.*

## ENABLING A NEW CLASS OF RF-ENABLED MAGNETOELECTRIC DEVICES.

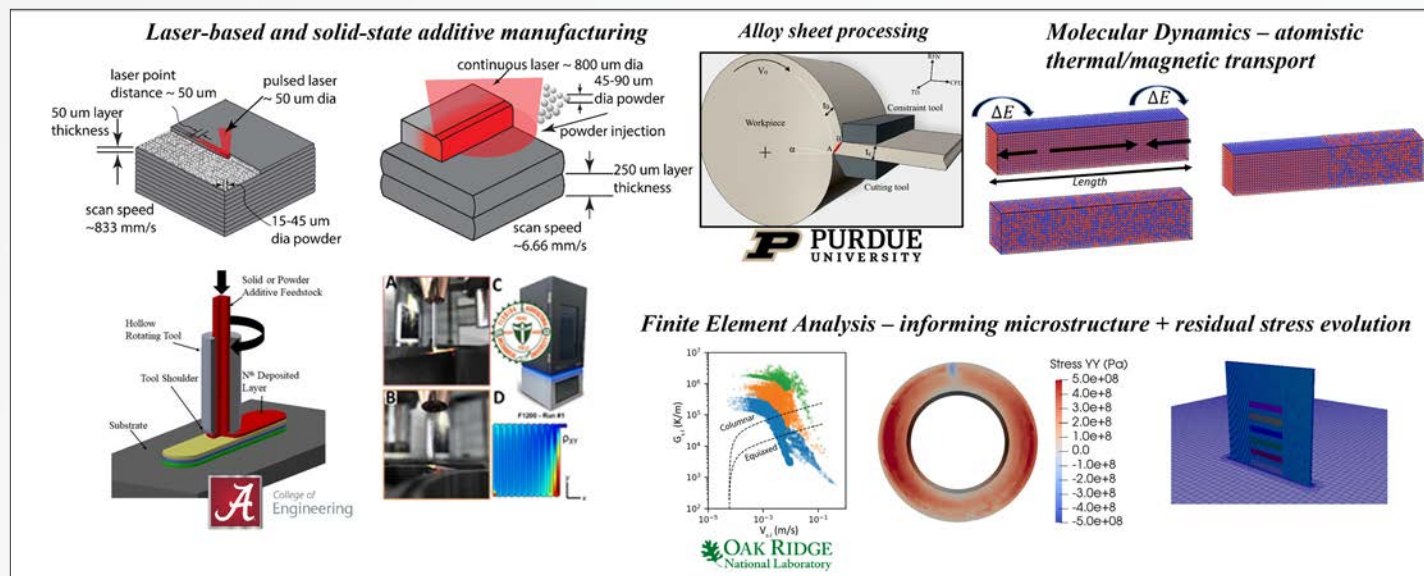
Multiferroic thin-film composites are promising for a broad suite of RF-enabled magnetoelectric devices due to their large magnetoelectric (ME) effect, enabling non-reciprocal physics in a smaller format than previously achievable. In this project, Sandia developed a P-matrix description that captures the physics of an Acoustically Driven Ferromagnetic Resonance (ADFMR) element and used it to simulate surface acoustic wave devices and tunable Bragg reflectors on YZ lithium niobate. Using a delay-line based lithium tantalate ADFMR device, the team demonstrated an insertion loss of -13.7 dB and an ADFMR attenuation constant of -71.7 dB/mm, making this device one of the best performing ADFMR devices to date. To enhance energy coupling, the team developed a sputter-based deposition method to deposit FeGa and

FeGa films onto piezoelectric substrates. The best magnetic properties were obtained using a single-phase FeGaB target (Fe<sub>0.7</sub>Ga<sub>0.17</sub>B<sub>0.13</sub>). Finally, the density functional theory was applied to predict the magnetostriction of ADMFR materials. This work, done in collaboration with Penn State and Alliance partner University of Texas at Austin, resulted in three publications (in process) and a conference paper presented at the 2023 Institute of Electrical and Electronics Engineers International Symposium on Applications of Ferroelectrics. The team also participated in four invited talks, including the Nanoscale Multiferroic Systems Annual Research Strategy Meeting, the Institute of Electrical and Electronics Engineers, the National Science Foundation, and at the Translational Applications. (PI: Darren Branch)

## OVERCOMING CONVENTIONAL MAGNETIC-MECHANICAL PROPERTY TRADEOFFS IN ALLOYS VIA ADDITIVELY MANUFACTURED NANOSTRUCTURES.

Soft-magnetic alloys possess exceptional functional properties for electromagnetic devices. However, these alloys are also characterized by low ductility and strength, limiting device performance. This LDRD used advanced/additive manufacturing (AM) processes and computational tools toward enabling alloys that overcome the inverse relationship between mechanical and magnetic properties. AM was demonstrated as a viable route to produce a range of soft-magnetic alloys, and models were developed that informed experimental process-structure-property relationships. Strong collaborations were established with four universities, including Alliance partner Purdue and Securing Top Academic Research & Talent at Historically Black Colleges & Universities partner Florida A&M, and two national labs, enabling the use of several

unique advanced manufacturing processes and characterization tools. The LDRD generated 10 submitted/published manuscripts, including those in *Manufacturing Letters* and *The Journal of The Minerals, Metals & Materials Society, Journal of Magnetism and Magnetic Materials, Tribology Letters, CIRP Annals, Additive Manufacturing Letters*, four technical advances, a submitted patent application, and the hiring of one postdoc in support of this effort. The LDRD also supported staff participation in a study on AM of functional materials with The Minerals, Metals & Materials Society. Government collaborations included Jet Propulsion Laboratory and Oakridge National Lab, and a few other faculty collaborations occurred with University of Alabama, University of Wyoming, and Colorado School of Mines. (PI: Andrew Kustas)

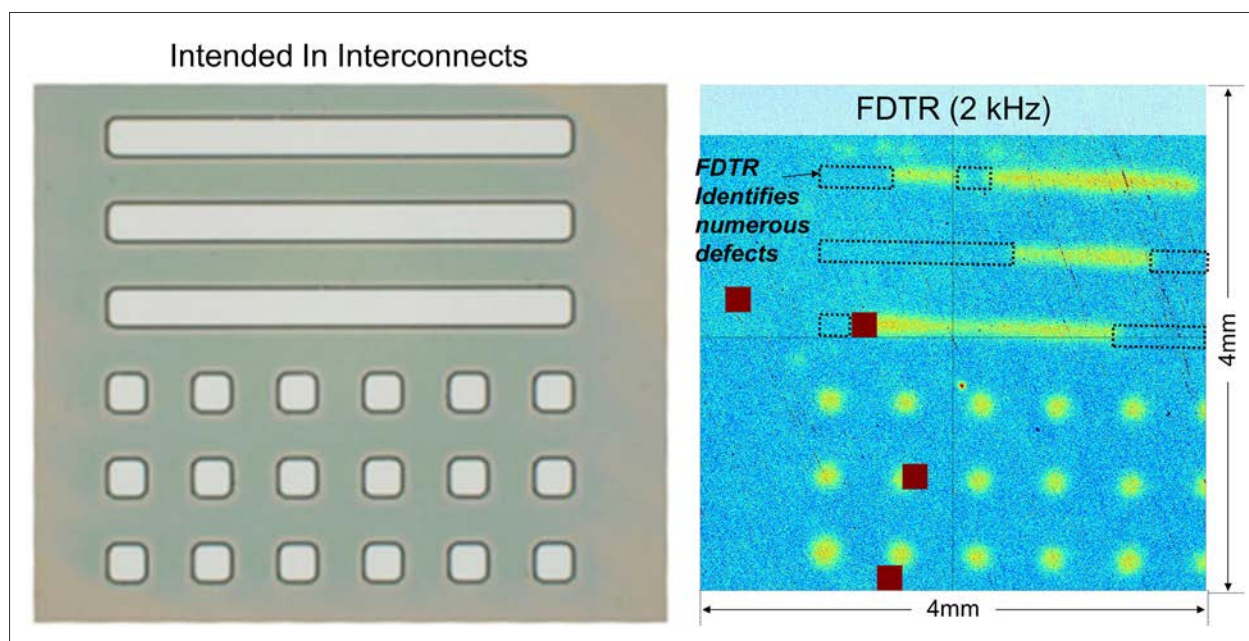


Collaborative interdisciplinary and multi-institutional approach combining advanced manufacturing, process modeling, and materials modeling.

## NEW ROBUST DEVELOPMENTS OF DESIGN IN HEID MICROSYSTEMS.

The Heterogeneous Ecosystem Interconnect Design (HEID) LDRD project focused on the development of design and characterization techniques to realize robust thermomechanical designs for heterogeneously integrated (HI) microsystems. This work, through collaborations with Fabio Semperlotti's group at Alliance partner Purdue University, demonstrated a physics-informed neural network approach to optimize the layout design of an HI microsystem for a power conversion circuit using thermal, mechanical, and size constraints. In addition, innovative thermal characterization capabilities, coupled with high-fidelity thermomechanical models, were demonstrated using Frequency Domain

Thermoreflectance (FDTR) to image the state-of-health of metal interconnects between bonded chips and the interposer non-destructively. This progress led to multiple follow-on efforts targeting the improvement of HI design and characterization capabilities towards the realization of robust, compact HI microsystems for high-consequence applications. This work also resulted in new capabilities that are critical to future Creating Helpful Incentives to Produce Semiconductors (CHIPS) partnerships, six additional follow-on projects, four journal publications, and 10 conferences where papers were presented and invited talks were attended. (PI: Greg Pickrell)



Intended in connects shown (left), with the same in connects showing defects identified through state-of-health FDTR imaging (right).

## MAGNETO-OPTIC LOGIC ENABLEMENT FOR BETTER STRONGLINKS.

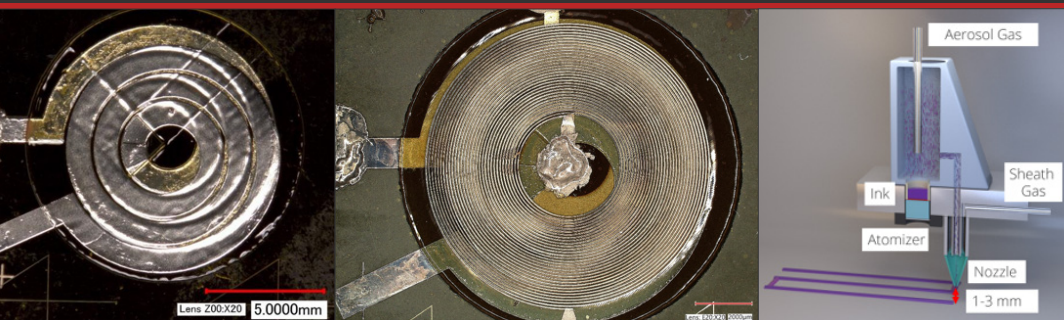
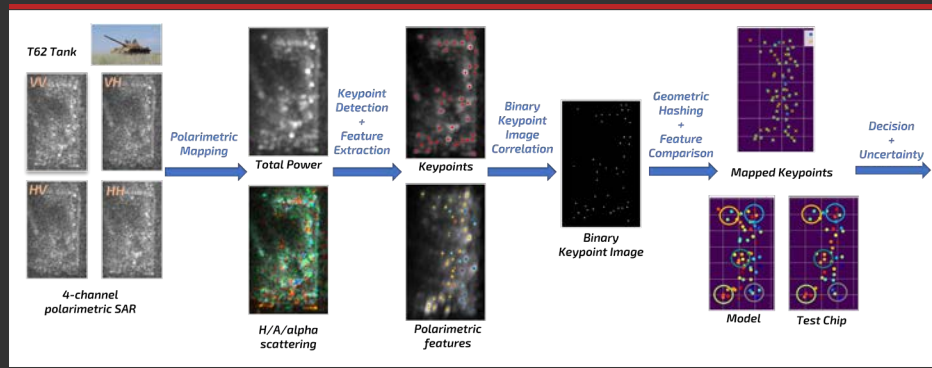
The magneto-optic logic enablement (MOLE) project goal was to realize an unprecedented solid-state, high-power, optical-switch technology for use in extreme environments. The MOLE team established a fundamental understanding of on-chip silicon photonics with integrated magneto-optics to realize high-extinction-ratio, low-insertion-loss, latched-switch capabilities, and

a platform to realizing on-chip optical isolators and circulators for active signal isolation and routing in optical networks. This integrated magneto-optic technology uses on-chip heterogeneous bonding to drastically reduce size, weight, and power. This technology can be utilized across numerous advanced national security components. (PI: Ashok Kodigala)

## GENERATING HIGH VOLTAGES FOR FUZING/FIRING ELECTRONICS WITH TRANSFORMER TECHNOLOGY DEVELOPED USING AM.

Flyback transformers are the component of choice for generating high voltages for fuzing and firing electronics. They have varying requirements and constraints, dependent upon the application, including the output voltage, input voltage, available power, and mechanical environments. Transformers meeting these requirements can be limiting in overall size and weight, taking up valuable real estate in space-constrained designs. This project evaluated the use of additive manufacturing processes to fabricate a flyback transformer in a miniaturized package. Aerosol jet deposition was used to print both conductive and insulative materials on a magnetic substrate. Transformer windings were stacked into several planar layers, achieving high voltage at the secondary from a low-

voltage input on the primary. This technology has demonstrated a promising future where both transformer and inductor volumes can be reduced, designed in a highly configurable package, and aligned with mission roadmaps. Results were published in [IEEE Transactions on Components, Packaging and Manufacturing Technology](#) and highlighted at numerous conferences. (PI: Joshua Dye)



(Left) Primary winding printed on magnetic material substrate, (center) secondary winding printed on top of primary winding, and (right) aerosol jet deposition diagram.



## REDUCING TIME AND COST TO PRODUCE MECHANICALLY ROBUST NEUTRON TUBES FOR NUCLEAR WEAPONS.

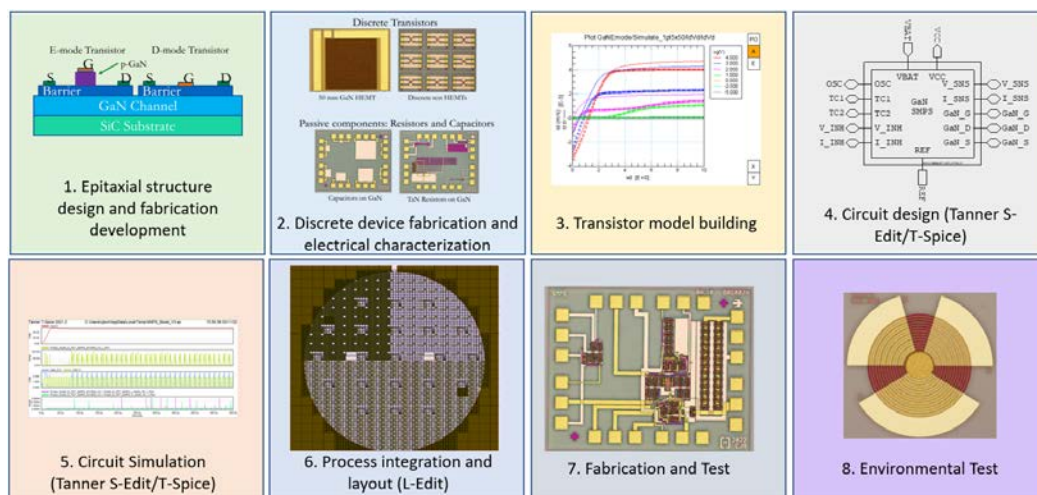
Neutron tubes (NT) are complex vacuum devices in nuclear weapons that historically took more than a decade and over \$30 million dollars to develop. Through a combination of additive/advanced manufacturing (AM) with digital design (DD), there is a potential to significantly reduce development time by minimizing design iterations and supply chain-related delays. However, variability in AM material properties, tolerances, and surface finish can create problems. These features may be hard to capture in a finite element mesh and could make fabrication difficult. Attempts to minimize these problems (e.g., post

processing of printed parts) can add time and cost back into design iterations, thereby eroding the advantages of this approach. This LDRD project team showed that imposing the proper constraints on NT design features and manufacturing methods enabled them to use the DD/AM approach to design, fabricate, and successfully test two different mechanically hardened neutron tubes in three years for a cost of \$2.2 million. A journal article on the AM ceramics that enabled this achievement was published in [International Journal of Applied Ceramic Technology](#). (PI: Dan Kammler)

## IMPROVING MODULARITY, MINIATURIZATION, AND RELIABILITY FOR FUTURE MISSION APPLICATION ARCHITECTURES.

Currently available commercial power supply circuitry consists of bulky, discrete components that lack the modularity required for future architectures. Custom gallium nitride (GaN) monolithic circuits offer technological advantages that currently aren't commercially available. In this research effort, the team developed an all-in-one, monolithically integrated, switch-mode power supply controller consisting of enhancement-mode power switches and their control circuitry on GaN high electron mobility transistor epitaxial layers. A GaN epitaxial structure capable of supporting all needed functions was designed

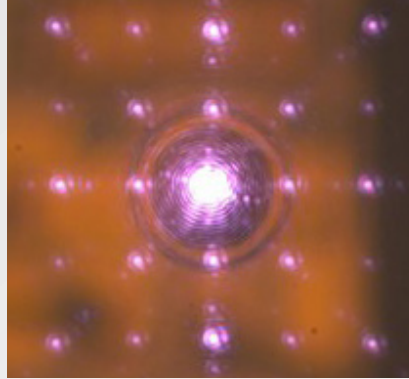
and grown; discrete components were fabricated on this foundational material. The electrical characterization results were used to build device models that paved the way for small-scale integrated circuit design. Valuable insights in design, fabrication, and test were gained. The capabilities developed from this work are being applied to the next generation of projects resulting from this effort and could be used in Sandia mission applications. Alliance partner Texas A&M faculty collaborated with Sandia on aspects of this project. (PI: Brianna Klein)



Creation of monolithic gallium nitride integrated circuit.

## IMPROVING DESIGN AND FABRICATION IN RADIATION-HARDENED PULSED LASERS FOR LASER DIODE IGNITION.

Sandia now leads the world in the understanding of rad-hard semiconductor light emitters and has built a lasting capability to design and fabricate custom rad-hard semiconductor lasers to meet a wide variety of application needs. Through this LDRD project, the team developed quantitative differential-equation models of radiation effects on semiconductor lasers, and also designed and fabricated innovative high-power vertical cavity surface emitting lasers and amplifiers for



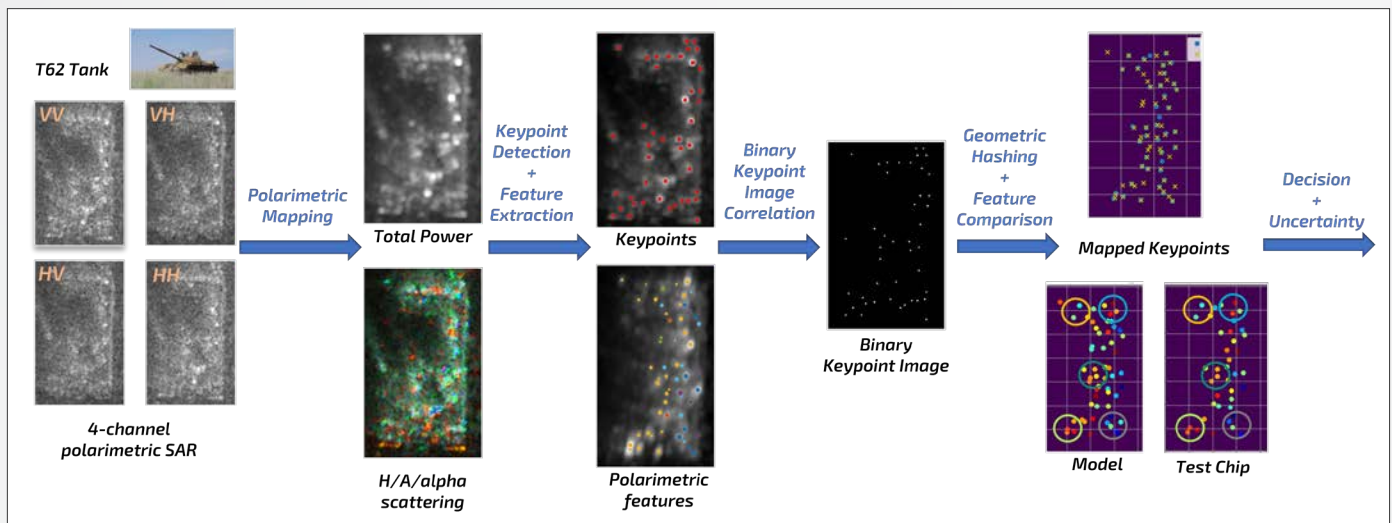
laser diode ignition of chemical reactions. The work yielded new semiconductor laser fabrication capabilities, new staff development, two publications, and two invited talks at [SPIE OPTO Photonics West](#) and [SPIE OPTO](#). (PI: Darwin Serkland)

*Coupled optical cavities offer additional constraints that can select a single optical mode and make brighter lasers.*

## DEVELOPING NOVEL AUTOMATIC TARGET RECOGNITION TO HANDLE RAPIDLY CHANGING TARGET ENVIRONMENTS.

The identification of emerging threats and the generation of actionable intelligence from the vast amounts of collected synthetic aperture radar (SAR) imagery is critical to our national security mission. This Sandia LDRD team developed novel automatic target recognition algorithms that advance the state-of-the-art by incorporating polarimetric SAR features, thus leveraging Sandia's world-renowned expertise in the area. This project takes initial steps toward giving analysts a quick-turn capability that is better able to handle

the rapidly changing target environment. The algorithm was designed to function with limited exemplars to address emerging adversarial threats, for which there is little available data, and to iteratively update as more data becomes available. The team developed a unique target representation or "feature constellation" that captures the relative locations of prominent target features, as well as their underlying scattering properties. (PI: Mindi Koudelka)



*Feature constellation that captures the relative locations of prominent targets as well as their underlying properties.*



## FINDING ADVERSARY CORRUPTION IN TESTERS (FACT).

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The world depends heavily on third party software for which no scalable risk assessment techniques exist, thereby accepting unmeasured risk. For example, a maliciously modified tester could corrupt stimuli, measurements, or reporting, leading to a cascade of costly failures. By creating an evolving set of diagnostics that provide evidence about concerning behaviors like these, Sandia can better inform decisions about the risks that software might introduce to missions. FACT demonstrated a narrow but scalable diagnostic analysis for tester software, collaborating with RAMSeS and tester experts to create one such diagnostic. FACT's prototype multi-language data flow analysis detects evidence of specific adversary-triggered corruption in third-party tester software—despite missing control flow and system models. Team members were invited to represent their expertise at the first Software Understanding for National Security government workshop, hosted by Sandia and convened by the Department of Homeland Security, the National Security Agency, and the NNSA. (PI: Shelley Leger)

## ENABLING AN OVER-WATER NAVIGATION SOLUTION THROUGH TAG-BASED AUTONOMOUS PSEUDOLITES.

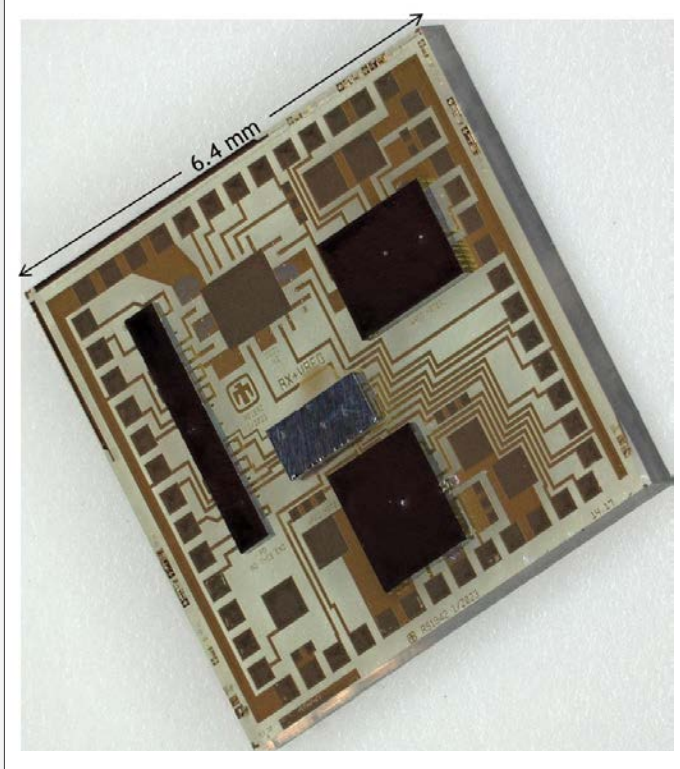
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To enable robust navigation in highly contested environments, this project explored an over-water navigation solution that can take advantage of both stationary (terrestrial) and non-stationary (oceanic) RF transmitters to provide GPS-like accuracy. The Sandia LDRD team created and demonstrated a real-time simultaneous localization and mapping strategy for hypersonic vehicles that leverages both non-cooperative and cooperative RF transmitters to form a high-accuracy navigation solution over-water. This project was performed in collaboration with Alliance partner University of New Mexico and Ohio State University. (PI: Anh Luong)



## HETEROGENEOUS INTEGRATION FOR HARSH ENVIRONMENTS.

Exploring heterogeneous integration for miniature optical data busses in harsh environments is key to delivering future microsystems. This LDRD



project demonstrates key components of an optical receiver capable of power conversion and optical-to-electrical data transmission. The module integrates emerging silicon and compound semiconductor devices using flip-chip assembly onto a glass interposer, serving as a pathfinder for future microsystems. Testing has provided insights into the interactions between different technologies in harsh environments, and learnings will be applied to future microsystems. Partnerships with 3D Glass Systems and National/Regional partner University of Colorado Boulder are providing insight into the potential of photosensitive patterned glass interposers for RF heterogeneous integration applications. (PI: Christopher Nordquist)

*3D heterogeneously integrated microsystem assembly.*

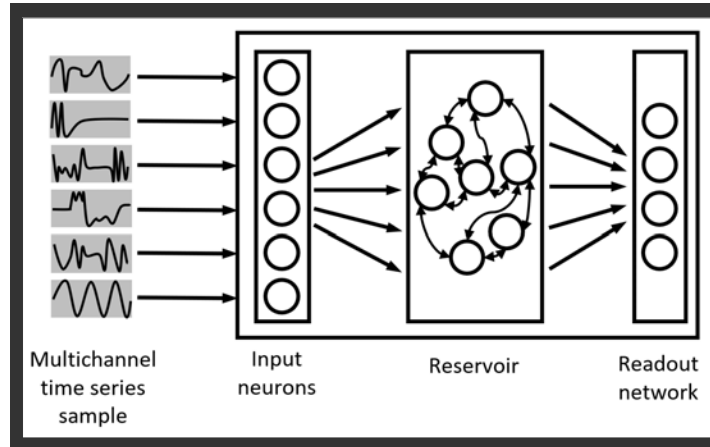
## EARLY DETECTION OF NOISE-HIDDEN ANOMALIES IN FAST DYNAMIC ENVIRONMENTS.

Enterprise networks are constantly attacked by a variety of advanced adversaries that evade existing detection techniques, leading to compromises. This Sandia LDRD team proposed techniques aimed at accurate and timely detection of host-based attacks targeting enterprise security and critical infrastructure; this is known as TreeClock. The team focused on investigating and developing methods to identify signal in the timing difference between events on a host or an endpoint using a novel Bayesian hierarchical model. The timing

information contains sufficient metadata to detect indicators of compromise per their analysis of the results. Directly applying Bayesian methods (e.g., Markov-chain Monte Carlo) to model all time sequence combinations is computationally intractable. As a result, they employed a novel mathematical framework and aggregation techniques to remain scalable. The algorithm was developed and applied to datasets from cybersecurity exercises and a production network. (PI: Mayuri Shakamuri)

## DEPLOYING AUTONOMOUS RECONFIGURABLE NEURAL INTELLIGENCE AT THE EDGE (ARNIE).

Although modern AI is achieving impressive performance, it requires extensive power and training and does not adapt easily. These drawbacks prevent the use of AI in many mission-critical applications, especially those in edge computing scenarios where implementation is required near the sensors and is constrained by size, weight, and power. In collaboration with the University of Texas, San Antonio, the Sandia LDRD team behind the ARNIE showed that brain-inspired AI networks known as liquid state machines (LSM) can perform well, minimize resource requirements, and use the same network to process information that has different meanings in different contexts. In addition, this project implements LSMs on cutting-edge, proprietary neuromorphic hardware. These achievements help Sandia deploy compact, low-power, computationally flexible, AI systems at “the edge.” The results were presented at [ICONS: International Conference on Neuromorphic Systems '23](#). (PI: Corinne Teeter)



An LSM consists of an input layer, a recurrent spiking reservoir, and a readout network. Connections from input to reservoir and between reservoir neurons are sparse, randomly initialized, and fixed; only output connection weights are trained. Samples of multichannel time series data are fed to the input neurons, which project the received values onto the reservoir, resulting in spiking activity. Once a sample has been fully processed, the readout network classifies the resulting reservoir state and outputs its predicted label for the sample.

## COMPONENT-SCALE OBJECT SURVIVABILITY DEMONSTRATED AT Z MACHINE.

Experiments at Sandia's Z machine support stockpile stewardship, providing experimental validation of simulated shock response of materials under extreme environments. Recently, shock-measurements of penny-sized material coupons at Z have supported experimental validation of shock physics simulations. Such simulations consider coupled photon and electron transport, energy deposition, and mechanical response.



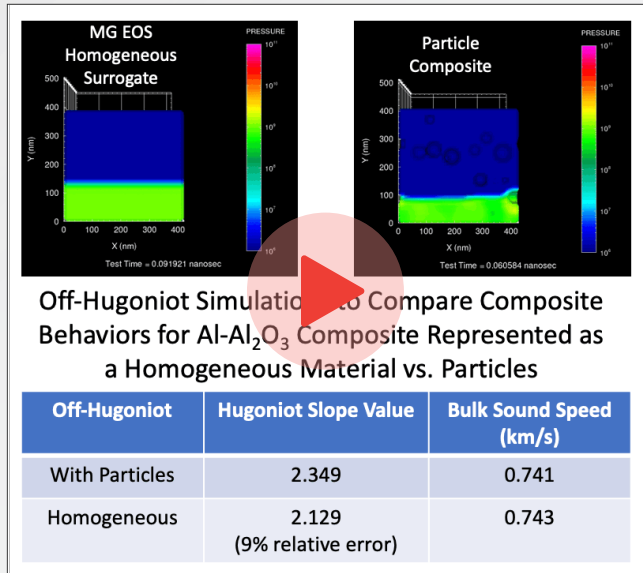
In July 2023, Sandia demonstrated the first 3D component-scale test object at Z machine.

Recent experiments demonstrate a new paradigm for component qualification to harsh environments. In July 2023, Sandia demonstrated the first component-scale testing of fully 3D test objects. These 4-inch-tall test objects were exposed to thermomechanical shock from the warm x-ray radiation at Z, while shielded from hazardous material contamination and debris damage by a novel large-area cassette. Concurrent multiphysics simulations predicted survivability to this harsh environment; no post-shot damage to these test objects was detected. Recovery and post-shot analysis of fielded coupons and test objects is a critical step in experimental validation. The work done on this project was showcased in [Extreme Mechanics Letters](#) and resulted in follow-on funding. (PI: Laura Biedermann)

## MACHINE-LEARNED MODELING OF NOVEL BARRIER MATERIALS.

Creating and calibrating thermomechanical material models for composites cannot utilize the same approaches used for homogeneous materials. This Sandia LDRD team created a novel hybrid equation-of-state (EOS) material model for composite barrier materials in radiation-shock environments. The research done by the team will enable better material modeling for advanced design and qualification of composite barrier materials. This hybrid model will correct a classical model, with a physics-informed machine-learned discrepancy model. This project created a modeling paradigm, the approach to microstructural direct numerical simulations (DNS) for calibrating the models, and an optimal experimental design approach that both selects the most useful calibration DNS to run based in information gain and calibrates the model with uncertainty. The figure shows how the Mie-Gruneisen EOS does not lead to the same

off-Hugoniot behavior as that from DNS of the composite, requiring correction. The results from this project also include an invited talk given at JASON Study on AI. (PI: Sharlotte Kramer)

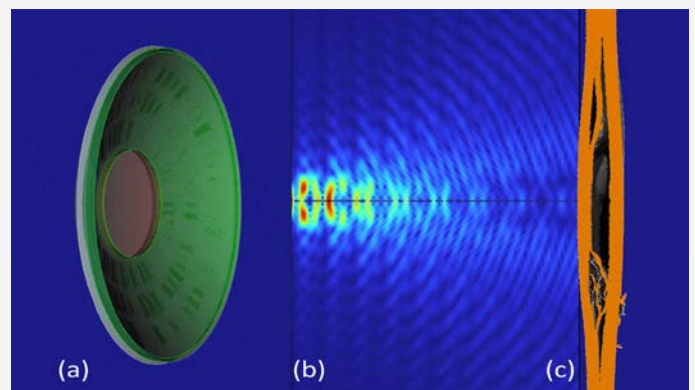


Off-Hugoniot simulations.

## FOCUSING SOUND WAVES TO EMULATE LOW PRESSURE SHOCK DAMAGE IN MATERIALS.

Materials designed to withstand the harshest conditions—from commercial products to defense articles and even fusion reactors—require specialized testing facilities that can be expensive or difficult to schedule. In this LDRD project, the team demonstrated an inexpensive method for rapidly shocking materials using high-intensity focused ultrasound. By focusing short pulses of ~few MHz frequency acoustic waves, small regions of a material can be repeatedly compressed and stretched at different strain rates, comparable to many impact scenarios. Mechanical energy can be targeted at interfaces, joints, or other areas of concern to identify deformation mechanisms and damage thresholds, allowing new materials to be screened for unique applications. High-fidelity computational models were also developed to allow optimization of test conditions. This project

was conducted in collaboration with Alliance partner Georgia Tech and University of Texas at Dallas. (PI: Nathan Moore)



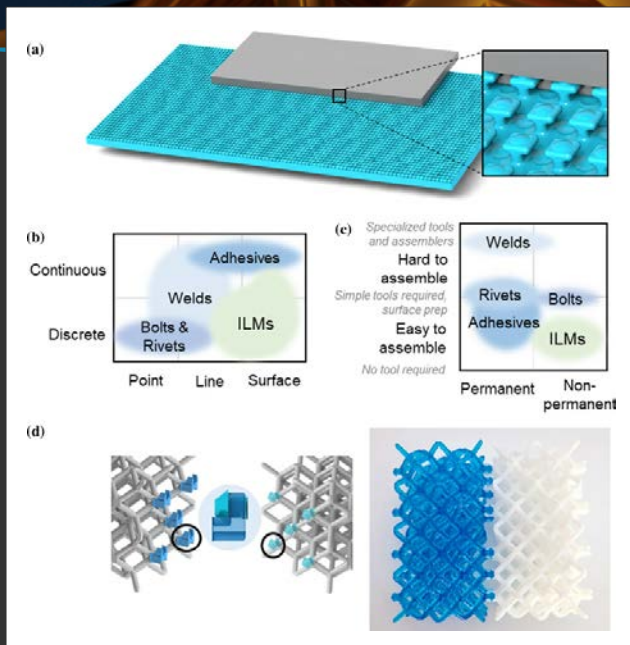
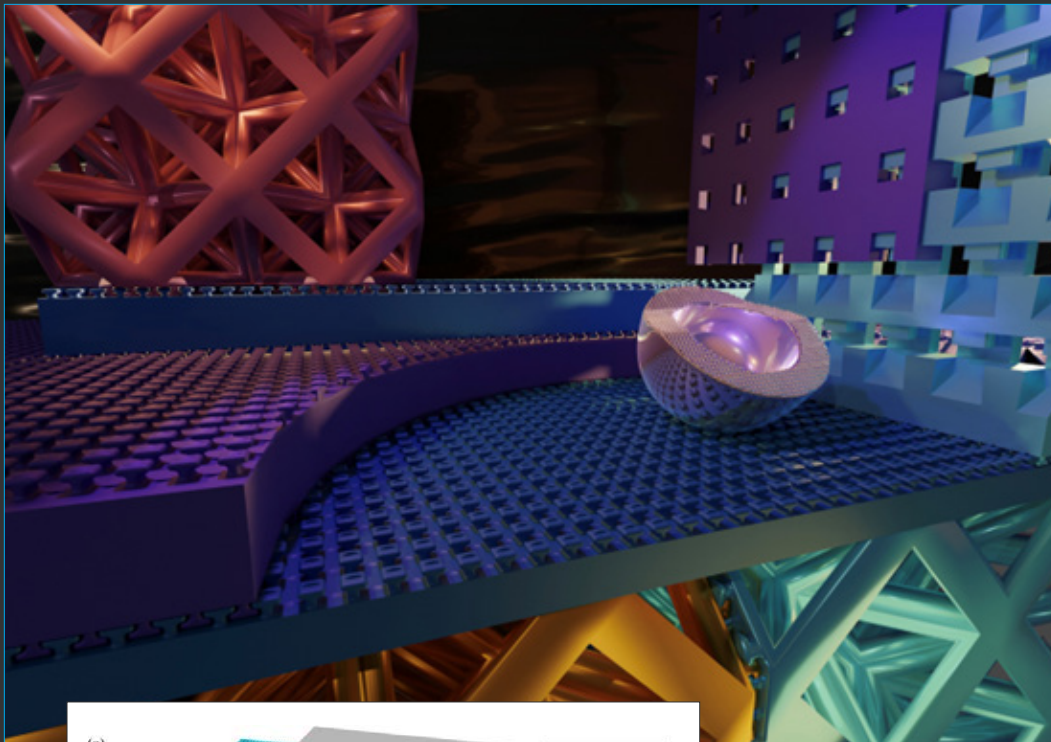
By focusing (a) short pulses of ~few MHz frequency acoustic waves, (b) small regions of a material can be repeatedly compressed and stretched at strain rates up to  $\sim 10^5 \text{ s}^{-1}$ , comparable to (c) many impact scenarios.

## INTERLOCKING METASURFACES PROVIDE UNMATCHED COMBINATION OF PROPERTIES.

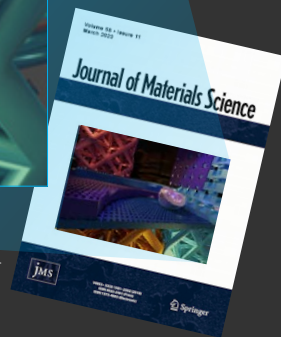
Joints are universal in engineering design, yet current joining technologies struggle to meet many critical needs like creating a structural, remateable joint between a ceramic and a metal. This LDRD created interlocking metasurfaces (ILM), a new joining technology, that provides a combination of properties unmatched by existing joining options. The team demonstrated that the structural properties of ILMs are controlled

through a combination of unit cell topology and unit cell interactions and can readily join dissimilar materials. Data-driven design methodologies were used to rapidly customize unit cell topologies for specific needs. The technology developed through this work is enabling for Sandia and has the potential for broad industrial appeal. The work, done in collaboration with Alliance partner Texas A&M, resulted in a journal cover on the March 2023

issue of the *Journal of Materials Science* and was selected as the January finalist for the 2023 Cahn Prize. Work from this project was also featured in *Materials & Design*. (PI: Philip Noell)



The March 2023 cover of *Journal of Materials Science*.



ILMs are patterned surfaces that imbue adhesive-like properties to otherwise non-adhesive surfaces.

## MULTIFUNCTIONAL, MICROSTRUCTURED POLYUREA-BASED BARRIER COATINGS FOR PROTECTIVE BARRIERS.

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Novel, multi-functional polymeric nanocomposites were developed through this LDRD to absorb and dissipate multiple forms of energy for protective barriers. By engineering polymer and particle nanostructures, the team was able to demonstrate superior energy transfer performance in multiple combined environment test campaigns, including at the Z machine, SPHINX electron source, shock tube, Hopkinson bar, and at the National Ignition Facility. The nanocomposite science developed in this project tested multiple hypotheses and demonstrated that the technology is ready to

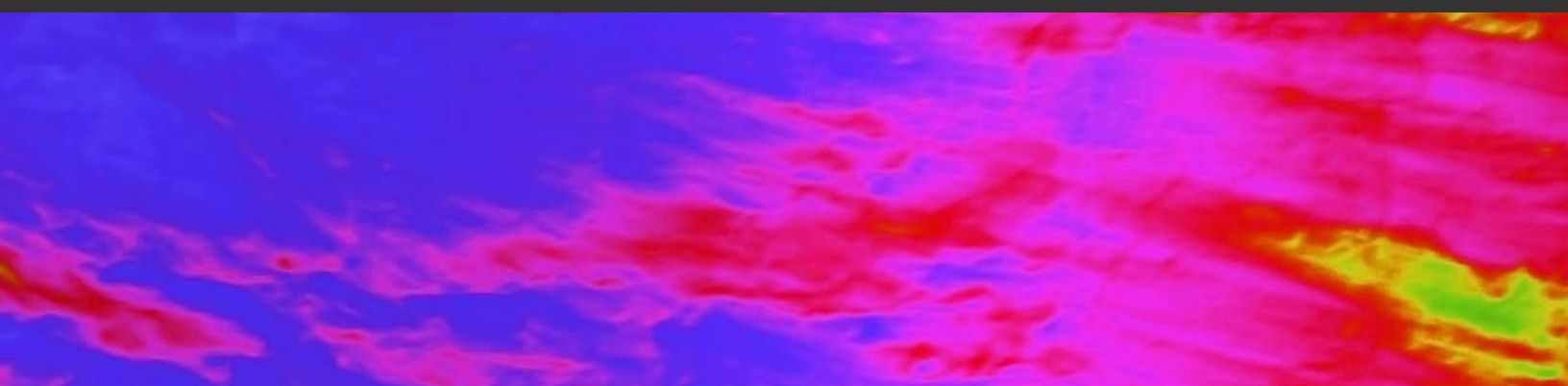
transition to mission applications at Sandia and throughout the NNSA enterprise. The work, which utilized faculty collaborations with National/Regional partner Carnegie Mellon and University of Texas at Dallas, was published in the *Journal of Radiation Effects: Research and Engineering*. The team, which included a new staff member and a postdoc hired in support of this project, received a Sandia Employee Recognition Award for technical achievement, and follow-on funding was received for further development. (PI: Christine Roberts)

## RADIOIMAGING FOR REAL-TIME TRACKING OF HIGH-VOLTAGE BREAKDOWN.

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Radioimaging detects and locates corona discharge, providing screening for early life failure and/or weakness in electrical components and devices. Corona is an undesirable plasma discharge often caused by manufacturing defects. This project demonstrated that corona onset is consistently detectable at GHz radiofrequency and can be imaged at 1-mm resolution with 32 10-GHz sensors arranged in a 1-meter-diameter network. The number of sensors, however, is limited by laboratory space restrictions and signal-to-noise ratio (SNR), requiring sensor and data-acquisition miniaturization. An ongoing collaboration with Alliance partner University of New Mexico

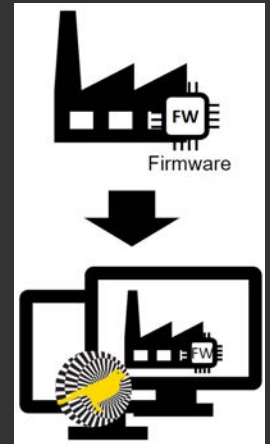
seeks to understand and leverage RF emission characteristics and SNR of plasma discharge. A radioimaging prototype is already operational and serving customers in detecting ion trap breakdown for Microsystems Engineering, Science & Applications, locating capacitor partial discharge for TPL Inc., and determining corona onset voltage for TSS USA Manufacturing. The radioimaging project team was awarded the NNSA's prestigious Defense Programs Award of Excellence for technology transfer of a radio-imaging analysis method to image and detect discharge and breakdown in commercial capacitors. (PI: Julia Tilles)



## HALLUCINATING CANARIES: DEVELOPMENT OF INSTRUMENTED FIRMWARE RE-HOSTING FOR CYBER RESILIENCE IN ENERGY SYSTEMS.

Today, there is a gap in our ability to defend Operational Technology (OT) from cyber threats. The OT devices are computer systems that sense and actuate on the physical world. They control the electric grid, manufacturing, and other critical systems. These devices are difficult to defend because they have limited computation resources, use non-traditional operating systems and software, and have long life cycles (20+ years). The Hallucinating Canaries LDRD team at Sandia developed techniques to leverage firmware emulation to create virtualized instances of OT devices. The virtual devices are instrumented with detectors for different classes of cyber attacks to create cyber canaries. The canaries decouple defense of the OT devices from the physical constraints of the devices. This provides a path to

continuously upgrade the defenses on OT devices and has the potential to transform OT devices from some of the least protected systems to some of the best protected systems. Capabilities developed through this LDRD contributed to Sandia programs, a core tool adopted by a third party for further development, and the ability to use “Firmware in the Loop” for emulation experiments has potential to be a significant advance in Sandia’s Emulytics capabilities. (PI: Abe Clements)

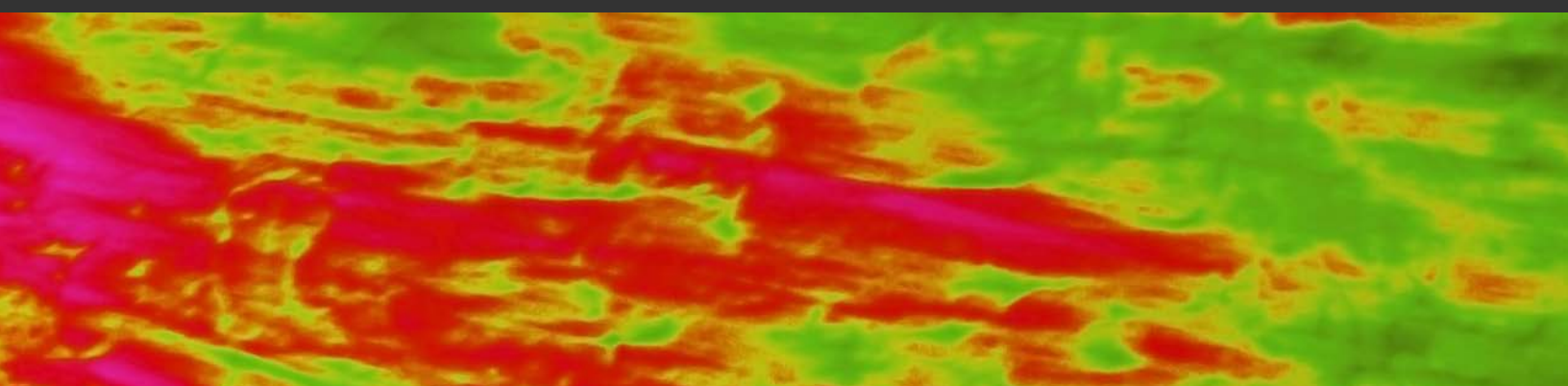


*Devices to defend against cyber threats.*

## DETECTING ICS INTEGRITY ATTACKS IN OPERATIONAL TECHNOLOGY (OT) TO PROTECT THE GRID.

Cyber-facing host control systems (referred to as supervisory control and data acquisition or SCADA) in the grid are constantly attacked to disrupt the integrity of physical devices and industrial processes. Current defenses to protect SCADA are limited because of the semantic gap between software operation and physical behavior. For example, it is difficult to know if SCADA commands have been maliciously altered during their generation at the software execution level. OT-GRITY provides an OT-aware software analysis solution via symbolic execution to address this execution integrity problem, which is informed

by an understanding of the grid’s cyber-physical behaviors to analyze SCADA dynamic execution states. In a matured state, OT-GRITY will provide automated threat assessment and attack detection in a hybrid and de-coupled way, increasing practical applicability in the grid. A successful prototype was developed based on this research, which is especially important since no commercial product exists. OT-GRITY influenced joint proposal collaborations with external industry partners and grid system operators, and a follow-on LDRD project funded. (PI: Moses Ike)





## PROVIDING FULL-PHYSICS DEVICE MODELING OF SATELLITE COMPONENTS.

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Using the Sandia-developed multi-physics and modeling software SIERRA, this LDRD team was able to create a full-physics device model of satellite components. The result provided threat and damage analysis for all materials in a device through physics-based light-matter interactions. Upon further examination, the team was able to identify layers of interest that could be vulnerable to optical damage by using the Beer-Lambert laser absorption law.

(PI: Seth Melgaard)

## GET OFF MY BACK! PROPRIOCEPTION FOR ADVERSARIAL ATTACHMENT DETECTION ON SATELLITES.

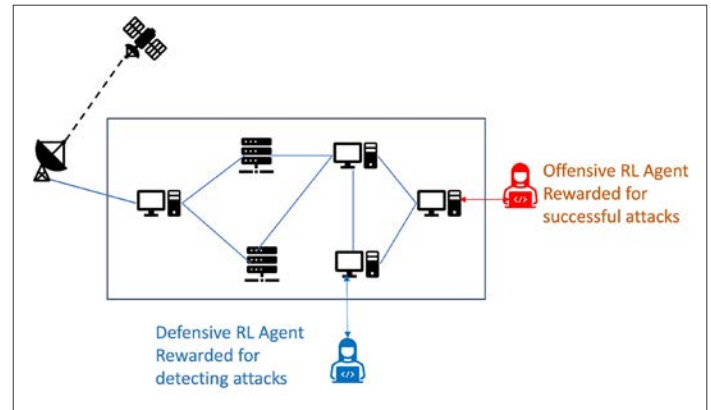
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The success of a satellite mission is reliant on the accuracy of the measurement of its mass. Without proper measurement, the satellite is in jeopardy of having a larger gravitational force. In collaboration with Manoranjan Majji and his team at Alliance partner Texas A&M, this LDRD project discovered ways to detect changes in the mass of satellites. The team's approach leveraged system identification and Bayesian calibration methods to identify unexpected changes in satellite inertia. However, the team was limited to sensors that are typically already available on satellites, and the minimization of disturbances to the nominal mission (i.e., avoid the excitations that are typically used to gather sufficiently rich data for system identification). Through a modular and multi-fidelity simulation framework, the team developed detection algorithms and demonstrated their sensitivity to very small changes in mass. Since the solution relies solely on sensors and data made available on satellites, it can be applied to existing satellites already in space, potentially augmenting their survivability in various scenarios. The LDRD project resulted in the development of three new tools for autogenerating models and corresponding algorithms which lay the foundation for an external follow-on project. (PI: Anup Parikh)

## REINFORCEMENT LEARNING APPROACH FOR CYBER SECURITY IN SPACE (RELACSS).

Several U.S. national security missions rely on satellites and their ground stations for cyber related attacks. However, cyber-attacks on ground stations pose a grave threat to these missions due to potential vulnerabilities. This project focused on developing a reinforcement learning framework to enable an intelligent attacking agent to automatically discover vulnerabilities, as well as the means to exploit them. A defensive agent is incorporated to work against the attacking agent, improving each agent's performance over time. This framework builds a hierarchy of agents that can decompose a complex cyber-task into simpler constituent modules. Modularity allows for flexibility to adapt to various scenarios. This

approach can also be adapted to other types of cyber-physical systems for various national security missions. (PI: Srideep Musuvathy)



Reinforcement learning approach for cyber security in space framework.

## NOVEL TRAINING METHOD FOR NEURAL NETWORKS HELPS TO MITIGATE RADIATION-INDUCED UPSETS.

Algorithms, such as neural networks, cannot reliably operate in high-radiation environments due to the induced upsets in high-performance commercial parts. Currently, this problem is addressed through a combination of radiation hardened parts and voting/redundancy methods. To allow for the use of commercial devices in high-radiation environments, the Sandia LDRD team created a novel training method for neural networks to mitigate radiation-induced

upsets. Using the collected data from radiation environment testing of commercial devices, the team informs the training of the model to take the upsets into account. This results in a higher accuracy of the model, comparatively, to a model that was trained with the standard method. The results from this LDRD project will inform future national security missions and be used in collaborations with other national laboratories and agencies. (PI: Gary Simon)

## DISTRIBUTED ACOUSTIC SENSING FOR ENVIRONMENTAL MONITORING AND STRATEGIC VALUE OF ARCTIC COASTLINE.

The Arctic coastline has high environmental and strategic value, but it isn't monitored due to harsh conditions. Through an LDRD partnership with the University of New Mexico, the University of Washington, and Woods Hole Oceanographic Institute, it was shown that [distributed acoustic sensing](#) can observe a [range of phenomena with spatial and temporal resolution](#). Journal articles include [Geophysical Research Letters](#) and [The Seismic Record](#). (PI: Rob Abbott)



## PROJECT HIGHLIGHTS – TECHNICAL VITALITY

LDRD is essential to maintaining the Labs' scientific vitality and Sandia, as the nation's most diverse national security laboratory, is uniquely equipped to tackle groundbreaking, interdisciplinary research. Researchers collaborate across a broad spectrum of disciplines and achieve research breakthroughs, which enables national security technology to be transferred to industry, commercialized under licensing agreements, and brought to market for the U.S. public good. The LDRD accomplishments in the technical vitality section highlight research outcomes that significantly extend knowledge in the scientific field or have the potential to provide a new capability for Sandia in the future.

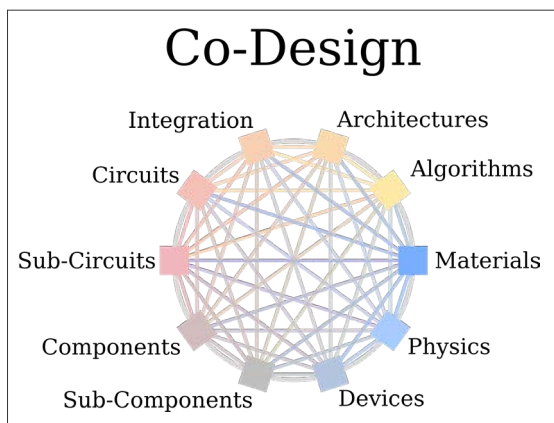
## ARTIFICIAL INTELLIGENCE-ENHANCED, MULTI-LEVEL, MODULAR SYSTEM DESIGN.

The current performance of computers is limited by CMOS scaling. To make computers more energy-efficient, they need to be redesigned at all system levels—from materials to algorithms.

During this project, the Sandia LDRD team developed AI-enhanced tools to automate co-design (simultaneous design across multiple system levels). Using high-fidelity circuit simulations (Xyce), the team trained an AI algorithm known as hierarchical reinforcement learning to build electronic systems that spanned five system levels: circuits, sub-

circuits, components, sub-components, and devices. This is believed to be the first time that AI has been used to co-design electronic systems with this many system levels. This work paves

the way for discovering new paradigms for computing that dramatically improve the speed and energy-efficiency of computers. This work, performed in collaboration with Pennsylvania State University and Sandia Alliance partner Texas A&M, resulted in two conference papers through IEEE and [ACM](#). (PI: Cale Crowder)

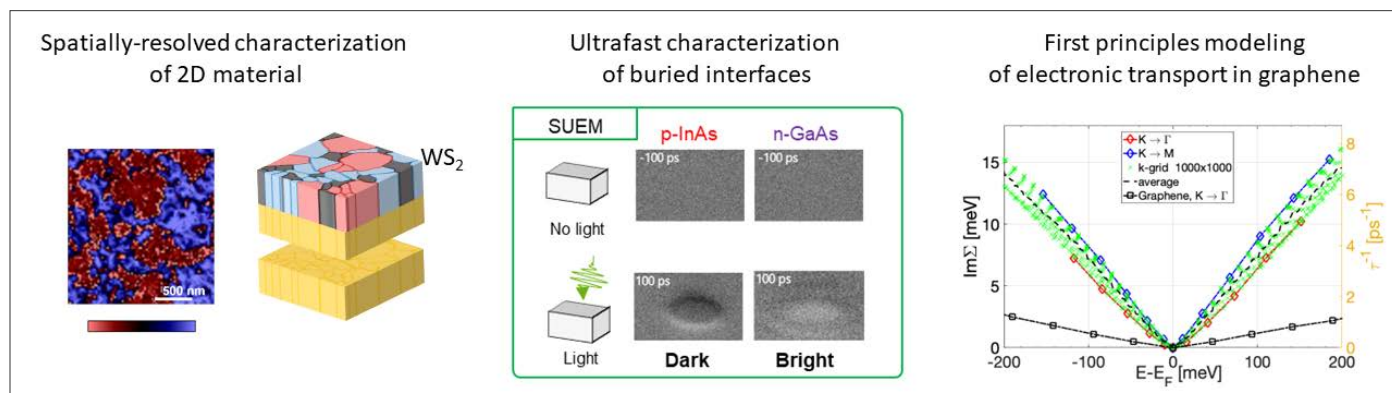


*This project showcases the first time AI has been used to co-design electronic systems with this many system levels.*

## CORRELATING ELECTRONIC STRUCTURE WITH CHARGE TRANSPORT IN 2D TMD HETEROSTRUCTURES.

Two-dimensional materials such as graphene and transition metal dichalcogenides (TMD) have shown promise for applications in electronics, optoelectronics, and chemical sensing. When integrated into devices, interfaces between materials often become the determining factor governing performance. In this work, the Sandia LDRD team developed experimental and theoretical approaches to characterize the properties of these interfaces and discovered that the substrate directly determines the electronic properties of the 2D material, even imprinting

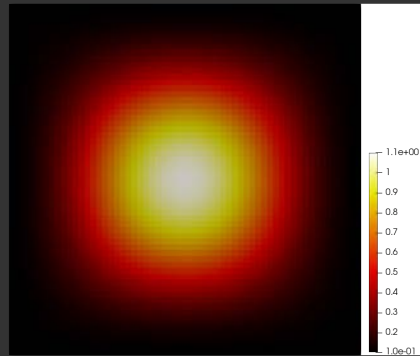
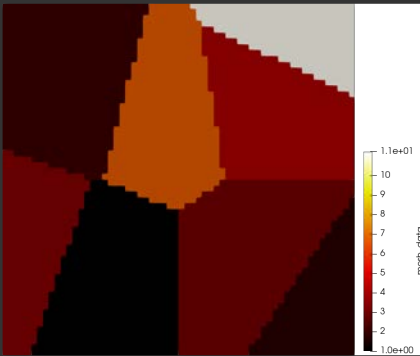
its own mesoscopic structure. The project demonstrated the ability to image the dynamical evolution of buried interfaces at picosecond time scales, and the team was able to calculate the electronic transport properties of bilayer graphene for the first time by developing a new modeling approach. This work, performed in partial collaboration with Sandia Alliance partner UC Berkeley, resulted in two published articles in *ACS Nano* (1) (2) and two invited presentations at Materials Research Society Conferences. (PI: Francois Leonard)



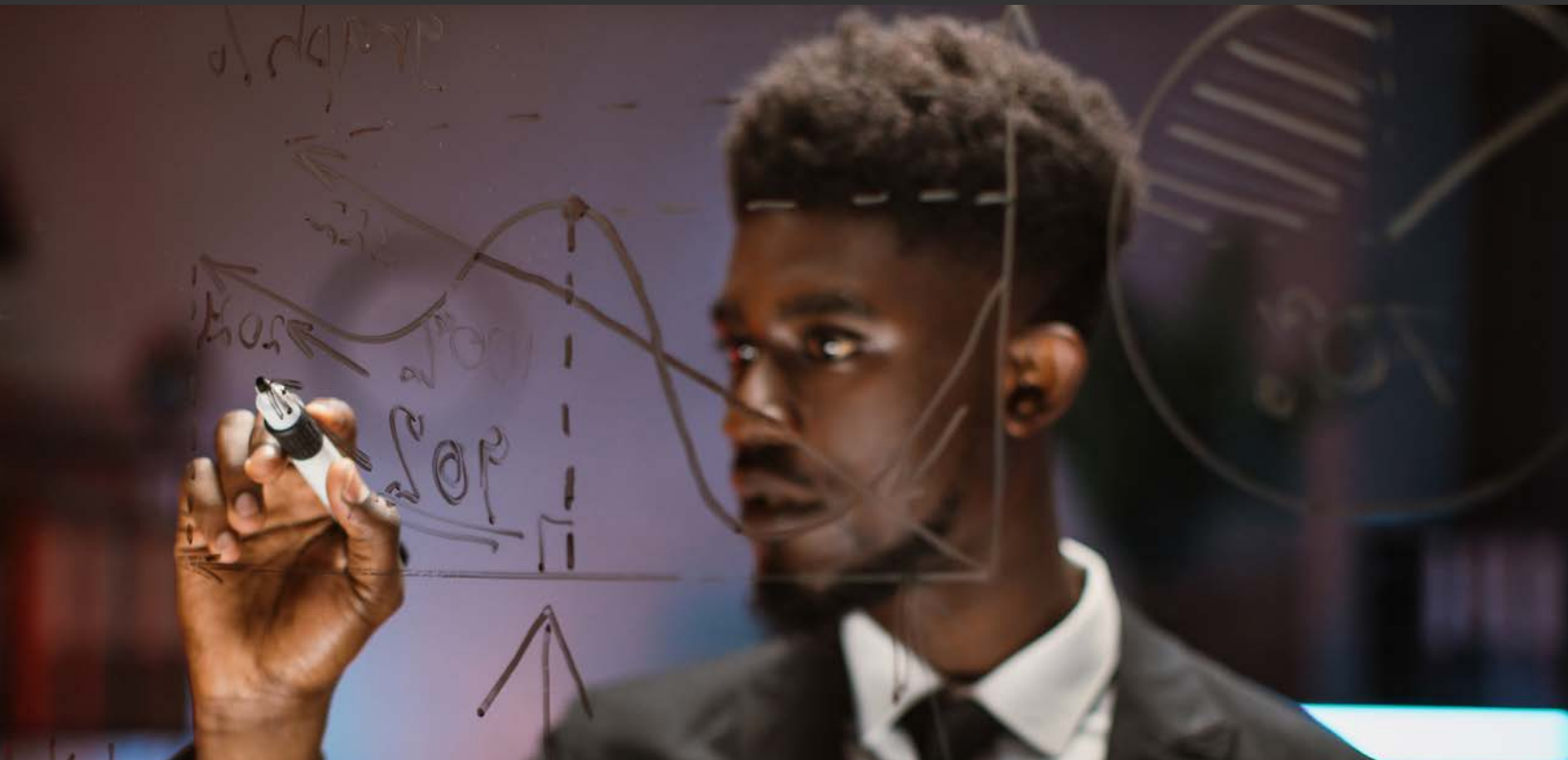
## DATA-DRIVEN SMOOTHERS FOR EXTREME-SCALE COMPUTING.

Many computational simulations require solving a large system of linear equations as one of the core challenges. One common approach for preconditioning and solving such systems is domain decomposition (DD) methods, which involves solving pieces of the original large problem on smaller domains. However, many applications have repeated patterns and material properties, which causes DD approaches to waste computation solving similar small problems. To counteract this, the Sandia LDRD team developed data-driven theory-backed approaches to identify and exploit structure in these DD methods. This project introduced compression techniques on a linear solver to allow for faster and larger

problems on Sandia high performance computing. The structure detection informs the linear solver to avoid re-solving similar small linear systems, therefore reducing the amount of computation and data a simulation requires and speeding up the solver as much as 20%. This project was performed in collaboration with National/Regional partner University of Texas at El Paso, Alliance partner University of Illinois at Urbana-Champaign, Memorial University of Newfoundland, Emory University, and Baylor University. Results were showcased in three invited conference presentations and a university seminar, and the research received follow-on funding. (PI: Graham Harper)



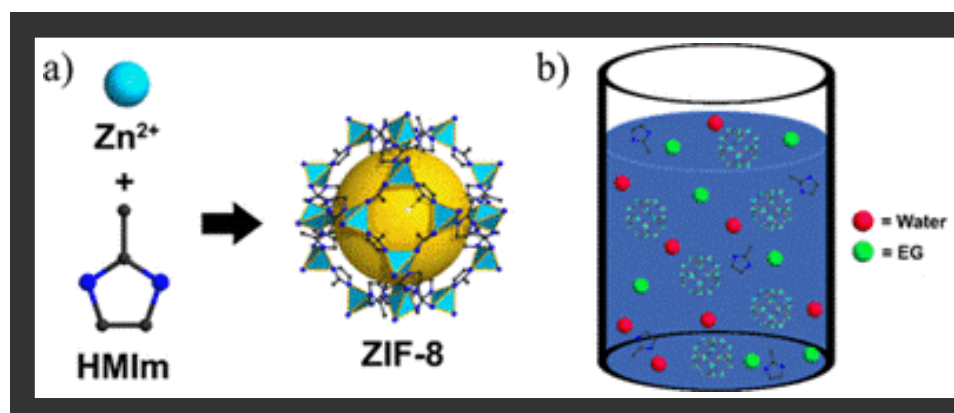
Graphical illustration for a discontinuous case (left) and for a smooth case (right).



## DESIGN OF CO<sub>2</sub> SELECTIVE TYPE 3 POROUS LIQUIDS THROUGH POROUS HOST MORPHOLOGY.

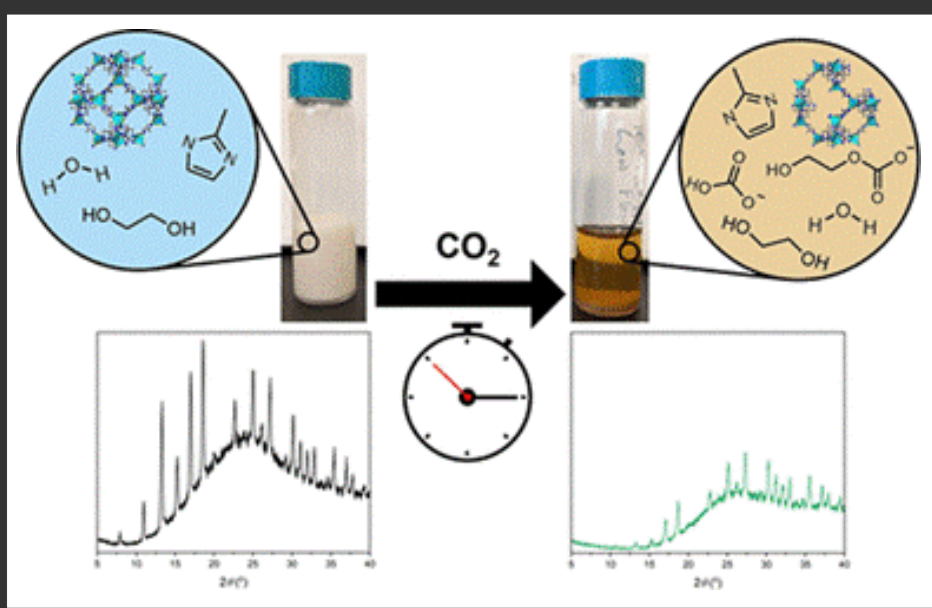
Materials with high-gas adsorption capacity that can be incorporated into existing technologies, such as porous liquids (PL), are required for carbon capture directly from the atmosphere. PLs have permanent porosity from the presence of a porous host dissolved in a solvent. The fundamental properties of PLs are unknown, including gases binding sites, PL stability, and self-assembly mechanisms. PLs were synthesized with different metal-organic frameworks in a multicomponent solvent. The most stable was based on ZIF-8 and exhibited degradation following CO<sub>2</sub> exposure. Molecular simulations identified a three-step carbon capture mechanism, which was experimentally validated through identification of

carbonate phases and decreasing pH during CO<sub>2</sub> exposure. A multistep pathway for PL degradation was identified, along with the critical role of aging of every PL component to assess overall stability. The project was performed in collaboration with Oak Ridge National Laboratory and resulted in two publications, [Journal of Molecular Liquids](#) and [ACS Applied Material Interfaces](#). In addition, Sandia researcher Tina Nenoff and PI Jessica Rimsza hosted a symposium at the 2023 Fall American Chemical Society meeting titled "Structure, Properties, and Applications of Porous Liquids." This is the first ever symposium specifically targeted at understanding the structure and properties of PLs. (PI: Jessica Rimsza)



(a) Description, composition, and structure of ZIF-8 MOF used as a porous host, (b) illustration of a porous liquid (PL) formed from ZIF-8 and a mixed solvent system made of water (red spheres), ethylene glycol (EG, green spheres), and 2-methylimidazole (HMIIm). Hydrogens are omitted for clarity.

Scheme demonstrating color change of a ZIF-8 porous liquid and change in crystallinity of the ZIF-8 structure after carbon exposure.



## INFORMING COMPONENT RESPONSE TO COMBINED ENVIRONMENTAL EXTREMES BY A PLATFORM REDESIGN.

The goal of this project was to address challenges limiting in situ nanoscale electron microscopy analysis of materials subjected to combined environmental extremes. The team investigated electron microscope design modifications for enabling more flexible combinations of stimuli and signals. Advances were made in exploring the concept of additively manufactured graded magnetic materials for application in electromagnetic optics. In parallel with these hardware development activities, the project explored how materials respond to extreme environments in a variety of materials systems, emphasizing new scientific



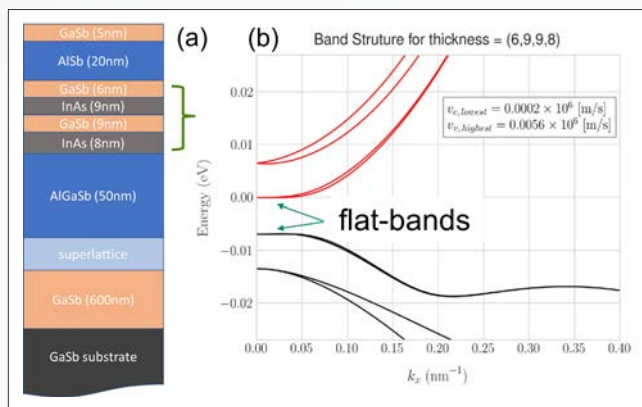
The expertise of Sandia researchers Stephen House (left) and Chris Smyth (right) helped lead to the advancements on this project.

insights resulting from the application and development of advanced in situ microscopy techniques. The Sandia LDRD team included 10 postdocs, student interns, and two early-career staff. The project generated over 17 publications including those in [Acta Materialia](#), [Journal of Materials Research](#), and [Science Advances](#), a provisional patent application, and involved collaborations with several universities, including the University of Tennessee Knoxville and Trinity College Dublin, and industrial partners, including Hummingbird Scientific. (PI: Doug Medlin)

## SEMICONDUCTOR TWISTRONICS.

One of the most exciting discoveries in materials science research is moiré materials. These materials form when two van der Waals materials are stacked with a small twist angle. A nearly dispersion-less flat-band electronic structure is formed, leading to myriad novel quantum phenomena. Moreover, the density of states in these flat bands increases considerably, yielding strong optical response. Through this

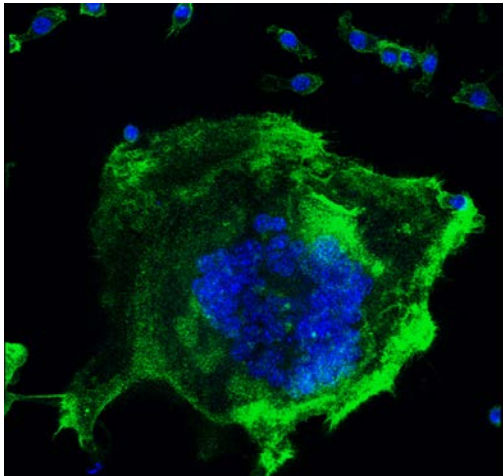
effort, the Sandia LDRD team designed flat-band structures without twisting in semiconductor InAs/GaSb vertical superlattices and published an article on the project in [Nanotechnology](#). Fruitful collaborations were established with the Intelligence Community Postdoc Office, Alliance partners Georgia Tech and University of Illinois at Urbana-Champaign, Securing Top Academic Research & Talent at Historically Black Colleges & University partners Florida A&M University and Norfolk State University, plus the University of Southern California and University of Texas at Dallas. In addition, a strong partnership was forged with the National High Magnetic Field Laboratory. (PI: Wei Pan)



(a) shows one growth structure of such superlattices, consisting of four InAs and GaSb quantum wells (QW). The coupling of these four QWs gives rise to flat bands. (b) Results from magneto-cyclotron resonance and magneto-transport measurements demonstrate the formation of flat bands in these band-engineered InAs/GaSb vertical superlattices.

## USING SYNTHETIC BIOLOGY TO GROW 3D BONES.

Materials with tailored 3D structures that are capable of sensing and repairing damage without human intervention are on the cutting-edge of biodesigned systems. For this LDRD, Sandia and Alliance partner University of New Mexico investigated the properties of bone to answer the question: Can synthetic biology be used to control bone remodeling and 3D structure outside



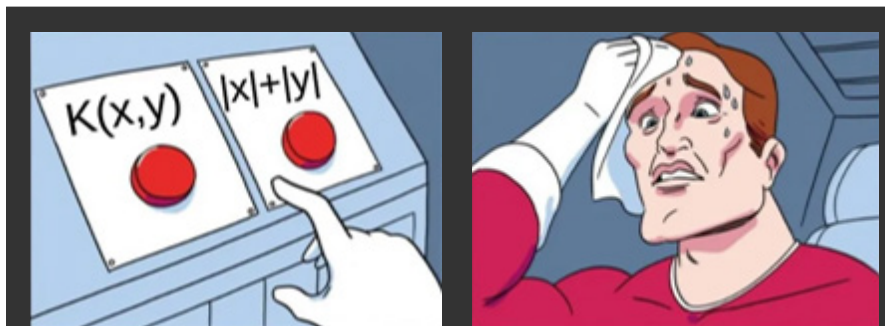
*Osteoclasts are differentiated from macrophage cells and act to resorb bone tissue. They are characterized by containing multiple (3-20) nuclei and a thick actin ring. This image highlights a large multinucleated osteoclast cell surrounded by precursor macrophage cells. The F-actin (green, cytoskeleton) is labeled with Alexa488-conjugated phalloidin, and the nuclei (blue) are labeled with Hoechst 33342.*

of a complete organism? The team leveraged expertise in synthetic biology to modify the cell signaling pathways that control the bone remodeling process in multiple cell types and developed methods for growing bone. The team also combined Raman microscopy and multivariate analysis to formulate a label-free method to identify bone cell types. The results of this interdisciplinary research laid the groundwork for novel, organism-free and shape-controllable synthesis of 3D bone. The team, which included two staff hires, participated in two invited talks, one at the Society of Industrial Microbiology and the other at the Rio Grande Symposium on Advanced Materials. (PI: Jeri Timlin)

## NOVEL UNSUPERVISED AND SEMI-SUPERVISED TECHNIQUES SUITABLE FOR COMPLEX NATIONAL SECURITY-RELATED DATASETS.

Most of today's machine learning techniques require very specific types of data and preprocessing that take a tremendous amount of work. Since the world doesn't already come in the form of vectors, processing data for machine learning requires expensive feature engineering. The pioneering work done by this team in the field of compression analytics (CA) described how to adapt file compression algorithms to allow analysts to analyze raw data directly, eliminating the need for costly and subjective feature engineering. Prior to this LDRD, there was no statistical understanding of CA, which made credible statements of uncertainty in predictions derived from CA methods impossible, and limited research and development in CA techniques. Collaborating with Sandia Alliance partner, University of Illinois at Urbana-Champaign, this

work addressed both limitations by developing a rigorous understanding of CA rooted in foundational statistical results governing optimal decisions in the face of uncertainty. This LDRD resulted in provable optimal classification rules for CA, as well as novel unsupervised and semi-supervised techniques suitable for complex cybersecurity, physical security, and other national security-related datasets. (PI: Alex Foss)



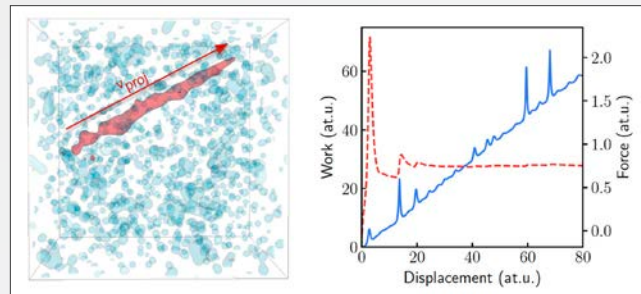
*This project provides information regarding which Normalized Information Distance is optimal.*

## ESTABLISHING A LIBRARY OF QUANTUM SIMULATION PROBLEMS THAT SPAN THE DOE.

Quantum computing might offer profound computational advantages over classical computers. In fact, it is believed that quantum computers will someday solve certain physics simulations problems more accurately than is feasible on any classical computer. Quantum simulations like this are seen as the most promising application of quantum computers for end users in the national labs, academia, and industry. To better understand the prospective impacts of this technology, the Sandia LDRD team identified and studied subroutines in quantum simulation algorithms common to all scientific domains. The researchers created theory to analyze the prospective advantages, benchmarks for assessing progress towards implementation, and resource estimates for problems with scientific value to DOE/NNSA.

The team collaborated with Tameem Albash and his team at Alliance partner University of New Mexico to understand and enhance the limits of

quantum simulation on classical computers. They also worked with research scientists at Google, led by Ryan Babbush and Nick Rubin, to create a complete quantum algorithmic protocol that will outperform classical computers in plasma physics simulations that consume 100M+ CPU hours/year on DOE/NNSA supercomputers. Two postdocs were hired as full-time staff during this project, and follow-on funding was secured from DOE Fusion Energy Sciences. (PI: Andrew David Baczewski)



(Left) proton stopping in deuterium plasma and (right) its stopping power N.C. Rubin, et al., arXiv:2308.12352

## EVENT FORECASTING THROUGH DYNAMIC BAYESIAN NETWORKS AND TOPOLOGICAL DATA ANALYSIS.

The interest in event forecasting capabilities continues to increase. Methods are being tested on mission-relevant data and are approaching usable performance. If performance can be further improved, it can be inserted almost immediately

into a direct mission application. This work has led to the development of several capabilities: (1) extended development for Bayesian Network model building, (2) inference and analysis in Python, (3) fast methods for determining



The Sandia LDRD team accelerated two-mode generalized blockmodeling, which allows identifying network communities frequently involved in events together.

reasonable ordering of classifier chains, and (4) a Python algorithm prototype that will be adapted to the problem of evolving optimal Bayesian Network structures for multilabel classification problems from a given set of seed networks. The Sandia LDRD team collaborated with researchers at National/Regional partner New Mexico Tech and Cornell University on aspects of this work. (PI: Matt Hoffman)

## IMPLEMENTING NEW ML PRACTICES BY EXTENDING PARSIMONIOUS BAYESIAN INFERENCE FOR DATA-EFFICIENT LEARNING IN HIGH-DIMENSIONS.

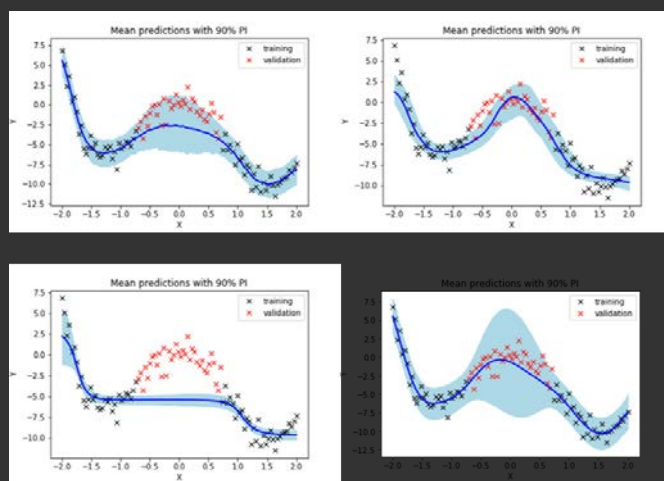
Machine Learning (ML) has made transformative advancements in data science that have now become integral to scientific progress, economic prosperity, and national security interests. Yet, standard ML practices remain challenging to apply in resource-limited domains, such as on devices that are either power-limited or communication-limited. Parsimonious Bayesian inference is a theoretical framework for efficient data assimilation that seeks to balance increased consistency between predictions and training data against corresponding increases in model complexity. Within this framework, over-training is understood as optimization that encodes excessive information within model parameters while only achieving small

improvements between predictions and training data. Aiming to support enhanced sparsification, this project team examined new approaches to high-dimensional variational inference that will allow researchers to calibrate and control parameter uncertainty during optimization. Identifying which parameters can sustain sparsifying perturbations with little impact on prediction quality allows better pruning strategies to be developed by framing them as approximate Bayesian inference. This project included collaborations with faculty at Ghent University in Belgium and Sandia Alliance partner UC Berkeley. (PI: Jed Duersch)

## IMPROVING AND ASSESSING THE QUALITY OF UNCERTAINTY QUANTIFICATION IN DEEP LEARNING.

Deep learning models have powerful predictive capabilities, with the potential to sometimes exceed human level performances. High-quality uncertainty quantification (UQ) is a critical part of developing trustworthy deep learning models in high-consequence applications. This project focused on developing a framework of methods and metrics to enable the principled assessment of UQ produced by deep learning methods. Working with Alliance partner University of Illinois Urbana-Champaign and National/Regional partner New Mexico Tech, the Sandia LDRD team demonstrated that different deep learning methods trained on the same data can produce vastly different UQ, and developed a method that allows for UQ quality assessment for deep learning models trained on real data. It also provided insights into the information captured by UQ metrics as well as guidance for when to use them. To bring the powerful predictive capabilities of deep learning to support high consequence problems encountered at Sandia, a high degree of confidence in the quality of a model's UQ is essential. Therefore, this framework has potential for significant impact across Sandia research and disciplines. The developed software

package implements the methods and metrics of Sandia's framework and provides clear guidance for the principled assessment of the quality of UQ produced by DL models. A presentation on the project was given at the IEEE International Conference on Machine Learning and Applications. Other positive results include the hiring of a postdoc and a full-time staff member. (PI: Jason Adams)



Uncertainty estimates from four different deep learning methods trained on the same data.

## QUANTIFYING THE PERFORMANCE OF CO-DESIGNED FPGA ACCELERATORS FOR COMPUTATIONAL SCIENCE APPLICATIONS.

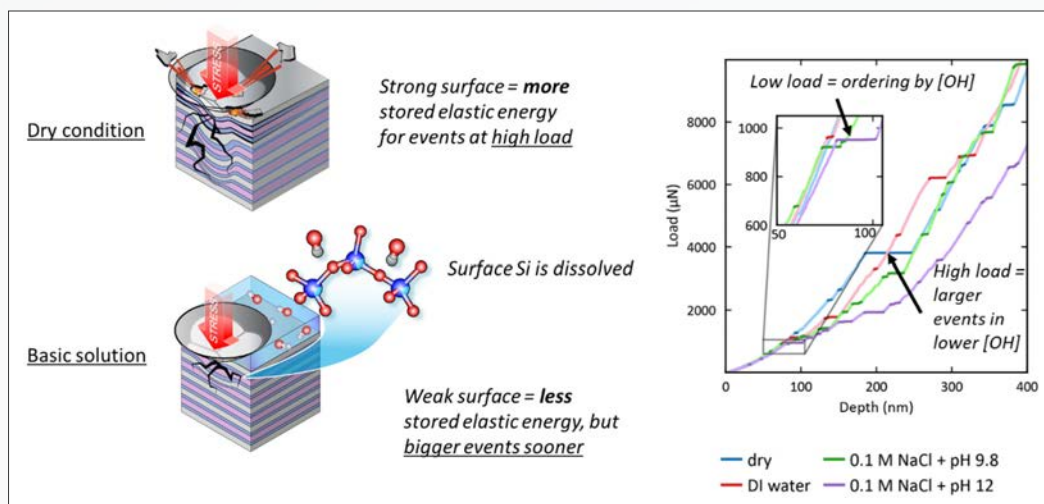
Field Programmable Gate Arrays (FPGA) are software-configurable circuits with common applications in embedded computing, video processing, radar, and cryptography. These application-specific accelerators (ASA) can potentially achieve exceptional performance and energy efficiency for Sandia's high-performance computing (HPC) applications but are unproven at a meaningful scale. To further explore these applications, the Sandia LDRD team studied ASAs to accelerate particle-in-cell methods and multigrid solvers with the goal of quantifying the application impact of ASA hardware and addressing the technical barriers that prevent their adoption in HPC. This included assessing the technical

viability of ASAs from viewpoints such as hardware performance, software development cycle, and application scalability. Sandia researchers successfully developed first-of-a-kind prototypes and conducted experimental studies to create a data-driven foundation for subsequent efforts towards custom hardware in post-exascale NNSA platforms. The needs of this project led to establishing collaborative relationships with Alliance partner Georgia Tech and industry. An ASA preparation roadmap for future at-scale deployments was created and a paper was submitted for the [2022 IEEE International Parallel and Distributed Processing Symposium Workshops](#). (PI: Gwendolyn Renae Voskuilen)

## CHEMICALLY ASSISTED FRACTURE CONTROLS DEFORMATION OF ROCKS AND DEGRADATION OF MANMADE MATERIALS.

Chemical effects on fracture have been recognized for decades, and yet chemical mechanisms involved in fracture are still debated. The interdisciplinary Sandia LDRD team partnered with the Cornell University and Alliance partner University of Illinois Urbana-Champaign to identify the chemical mechanisms and how they affect the molecular- to macroscopic fracture/deformation properties. They utilized molecular dynamics simulations, statistical analysis, in situ liquid nanoindentation (see figure to the right), three-point bending, compaction, and triaxial deformation tests. The analytic relations were developed describing crack growth to highlight the impact

of reactions on the mechanical properties of carbonate and silicate minerals. The tests showed that water and anions define the mechanical response including displacement and fracture. These results were published in four papers and include articles in [Journal of Materials Science](#) and [Journal of Physical Chemistry](#). (PI: Anastasia Ilgen)

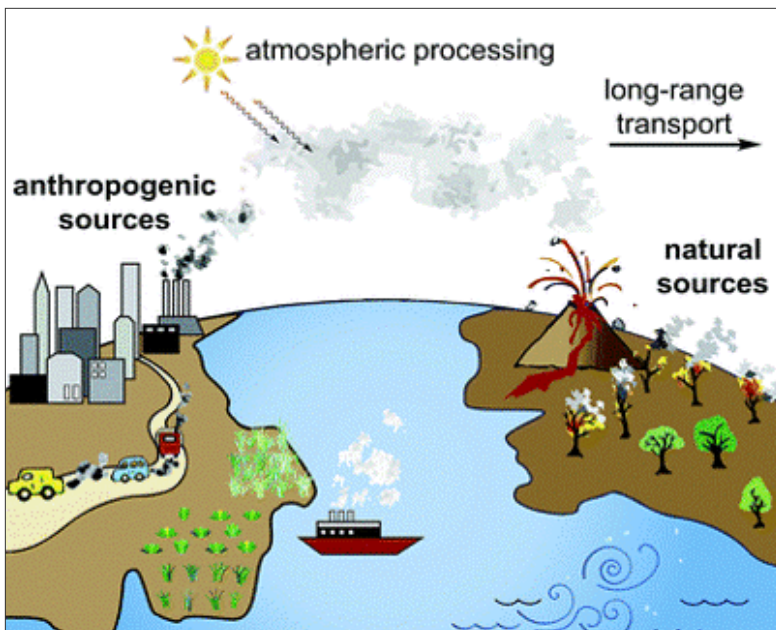


The image on the left shows molecular mechanisms that affect fracture and how the molecular-scale processes affect the fracture/deformation properties and observables at the laboratory scales. The image on the right shows how cracking identified can be interpreted within an avalanche—while the field model describes how earthquakes happen.

## PLUMINATE: CLIMATE CONTROL INTERVENTION THROUGH SCI INTERJECTIONS IN CLOUDS AND OTHER ENVIRONMENTS.

While solar climate intervention (SCI) strategies use aerosol injections to increase rain droplets, solar radiation remains the largest source of uncertainty in climate models. To enhance scientific understanding, this LDRD project with National/Regional partner University of Washington has developed novel injection parametrizations at varying spatio-temporal scales. Because of the significance of the results which demonstrate injections in cloud-like environments with Sandia's MiniFog chamber and the impact of scale on interactions and the significance of turbulence, this project was featured on the front cover of the [Journal of Applied Optics](#). Continuing on with

this project, satellite imagery of injections was leveraged, and a pipeline built to study these interactions. When combined with a subgrid scale parameterization, an understanding of conditions most suitable for SCI can be learned. These results were published in [news releases](#), and in seven journal articles. Five articles are currently under review and approval and two other articles have been published in the journal of [Environmental Data Science](#), and the Journal of [AAAI 2023 Fall Symposium on Artificial Intelligence and Climate: The Role of AI in a Climate-Smart Sustainable Future](#). This work was also presented at the SPIE Defense + Commercial Sensing Conference. (PI: Lekha Patel)

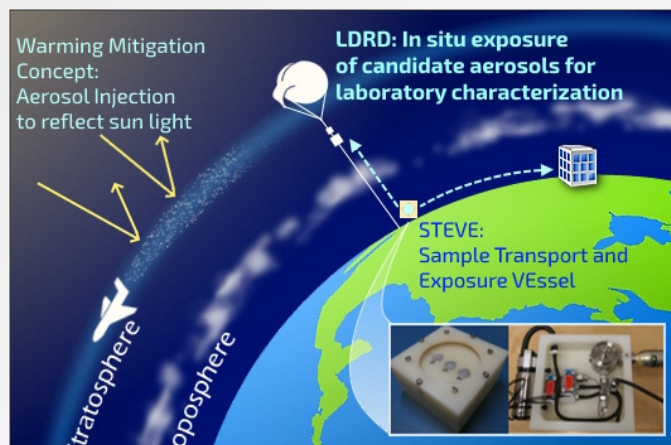


*Ship tracks are shown—clouds that reflect sunlight and are formed by moving ships (very similar to contrails from planes)—to help people understand the benefits and risks of this technology to help slow down climate change.*



## REDUCING GLOBAL MEAN TEMPERATURES THROUGH AEROSOL INJECTIONS.

Aerosol injection is a proposed strategy to reduce global temperatures and avoid extreme consequences of climate change. However, the atmosphere presents conditions that may alter the injected aerosol's impact on climate, the environment, and health. In this LDRD, Sandia



developed a unique capability to study aerosol samples exposed to Earth's upper atmosphere. Sample vessels were programmatically controlled so that specimens were only exposed at the altitude of interest; this preserved the integrity of specimens between the lab and stratospheric balloon flights. Through a partnership with material science company Sceye, prototype vessels were carried by a solar-powered airship up to 65,000 feet and returned for analysis. This new capability, accomplished through a larger project team, has enabled ongoing efforts to understand aerosol-atmospheric chemistry and microphysics. (PI: Raymond Friddle)

*The Sandia LDRD team accelerated two-mode generalized blockmodeling, which allows identifying network communities frequently involved in events together.*

## USE OF ENVIRONMENTALLY FRIENDLY LEACHING SOLUTIONS TO EXTRACT AND SEPARATE DOMESTIC RESOURCES.

A secure, reliable, and sustainable domestic supply of critical minerals is essential to national security. The goal of this three-year LDRD was to develop an environmentally benign method of extracting and separating critical metals and materials known to be enriched with them. The team's model utilized environmentally friendly leaching solutions (modified supercritical CO<sub>2</sub> fluids) to extract and separate rare earth elements (REE) and other

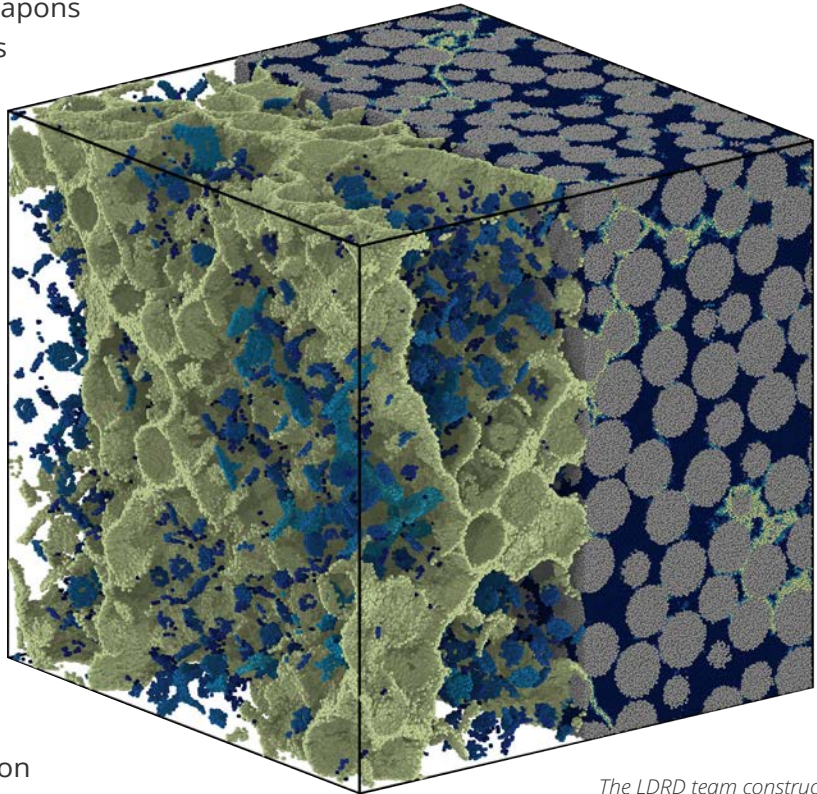
critical metals from coal ash, coal, and shale. This work can be used to further design and optimize a chemical process for REE recovery from ore concentrates, recycled materials, and acid mine drainage. This will help ensure the supply chain security and improve economic competitiveness for the U.S. These results were published in the [Journal of Solution Chemistry](#). (PI: Guangping Xu)



## A MESHFREE METHOD FOR DISCOVERING MECHANISMS IN ENERGETIC AND OTHER WEAKLY BONDED GRANULAR MATERIALS.

Many accidental explosions have been caused by low-speed impacts. In this LDRD project, which included lab collaborations with Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and the Atomic Weapons Establishment, Sandia used experiments and innovative meshfree models to advance knowledge of the mechanical damage mechanisms that drive such events. In collaboration with Alliance partner Texas A&M, the team experimentally studied damage evolution for a range of strain rates, cyclic compression, and impact conditions. Sandia researchers also measured heating due to frictional processes in explosives. Mesoscale models at Sandia and Alliance partner Purdue were used to further study emergent damage mechanisms under multi-axial stress states. The models and experiments both showed that pressure dependent yielding and plastic strain accumulation were key deformation behaviors. Leveraging these discoveries, thermal-chemical-mechanical reproducing kernel meshfree macroscale models with extreme numerical robustness were developed that have potential to significantly advance model-based explosives

safety assessments. The project was featured on the cover of *Mechanics of Materials* and published in *Applied Composite Materials*. (PI: Judith Brown)



*The LDRD team constructed four mesoscale models focused on identifying key trends in the global mechanical response and mesostructural changes in energetic materials, such as the crack network shown here.*



## A NEW PARADIGM FOR FAILURE PREDICTION USING 4D MATERIALS SCIENCE AND DEEP LEARNING.

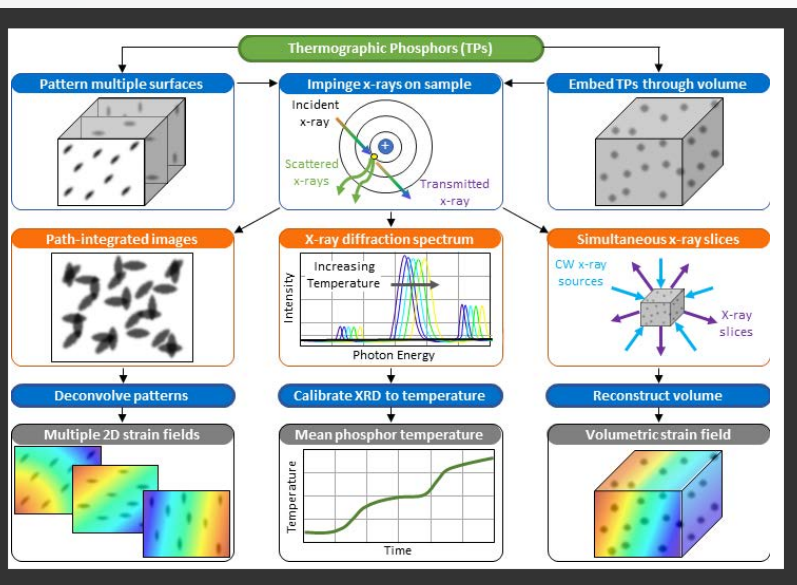
Accurate prediction of ductile failure is critical to Sandia’s nuclear weapons mission; however, including the salient physics and mechanics is too computationally expensive. This project developed modern data-driven methods that add important microstructural information, capturing the important physics “for free.” The tool uses stress and strain fields from a structural model and overlays information from a machine-learned model to output time-history of structural response and failure. The team performed innovative three-dimensional experiments to elucidate mechanisms of void nucleation and evolution. Crystal-plasticity finite-element models from the experimental observations were

developed to compute fields not readily measured. The team also developed engineering length-scale simulations to understand how the engineering fields evolve in the presence of fine-scale defects. Finally, deep learning neural networks were developed to predict failure and then extended using graph-based neural networks to encode the findings of the experiments and simulations and efficiently make forward predictions. The project included collaborations with external faculty at Purdue University, a Sandia Alliance partner, and Florida A&M, through the Securing Top Academic Research & Talent at Historically Black Colleges and Universities Program. (PI: Kyle Johnson)

## VIEWING WITH X-RAYS: 4D STRAIN AND THERMOMETRY MEASUREMENTS FOR THERMAL-MECHANICAL TESTING.

Understanding temperature-dependent material decomposition and structural deformation induced by combined thermal-mechanical environments is critical for safety qualification of hardware in accident scenarios. This LDRD elucidated the physics necessary to develop X-ray strain and thermometry diagnostics for use in

optically opaque environments by combining experiments, simulation, and analysis. The team demonstrated X-ray thermometry using X-ray diffraction of inorganic doped ceramics (i.e., thermographic phosphors) and multi-surface strain measurements with Path-Integrated Digital Image Correlation (DIC) and Frequency Multiplexed

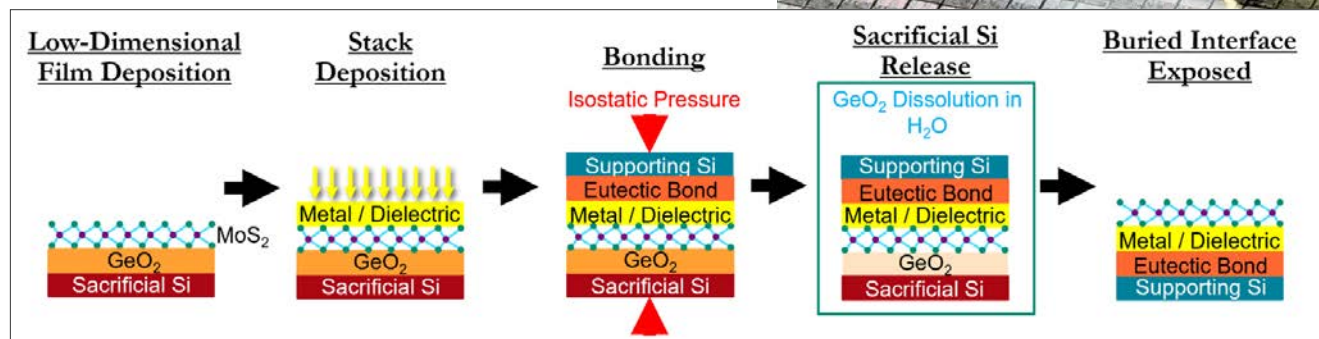
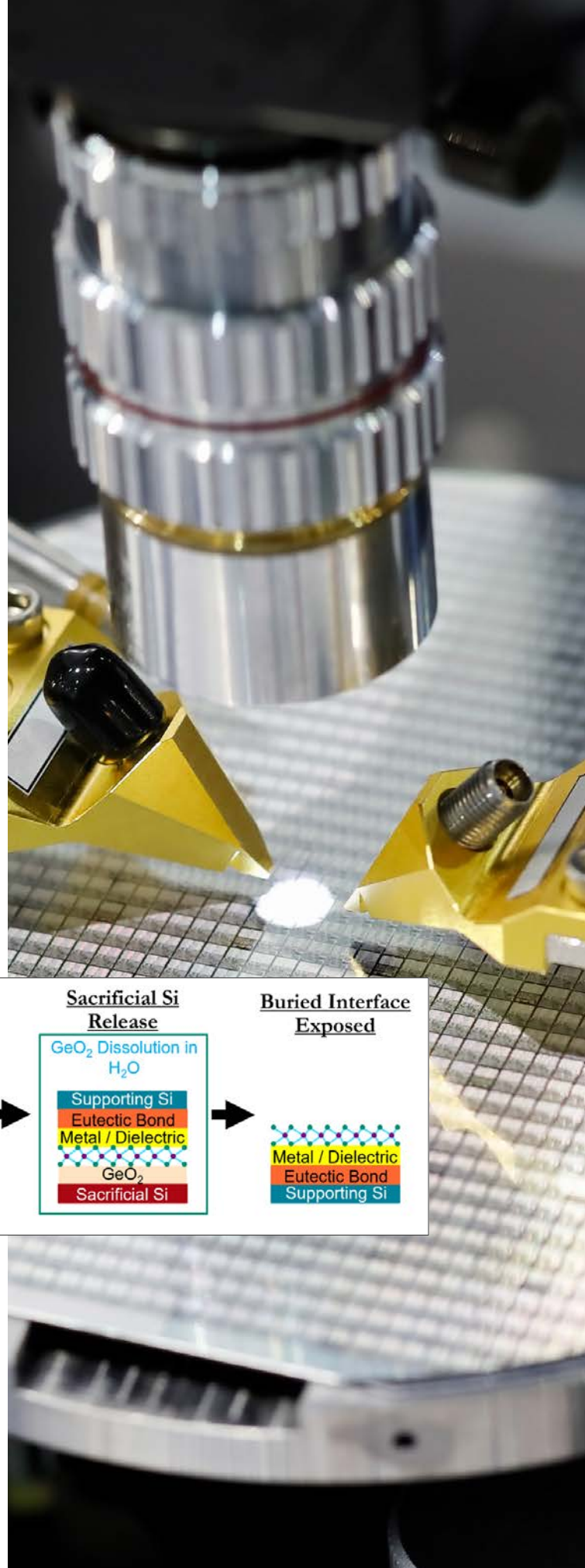


DIC. Preliminary demonstration of Time-resolved Digital Volume Correlation leveraged limited view reconstruction techniques. This work was furthered through collaboration with Alliance partner Purdue University and Argonne National Laboratory. To date, three Technical Advances, leading to two patent applications, four journal publications including articles in *Journal of Applied Physics*, *Experimental Mechanics*, and *Optical Materials*, and twelve conference papers were produced. (PI: Caroline Winters)

This LDRD elucidated the physics necessary to develop X-ray strain and thermometry diagnostics for use in optically opaque environments by combining experiments, simulation, and analysis.

## INTEGRATING LOW-DIMENSIONAL MATERIALS INTO COMMERCIAL ELECTRONICS APPLICATIONS.

Novel computing technologies have recently been enabled by the development of low-dimensional materials. However, a dedicated integration process is needed to integrate low-dimensional materials into commercial electronics applications. In this LDRD, Sandia demonstrated a technique that enables the transfer of low-dimensional films and devices onto any substrate and is compatible with many materials. The new process is enabled by a water-soluble  $\text{GeO}_2$  substrate, and the technique was utilized to fabricate and transfer a working  $\text{MoS}_2$  transistor, which demonstrates the potential to integrate low-dimensional materials into mature electronics. This research clarified how to transfer low-dimensional materials onto the  $\text{GeO}_2$  substrate, how to transfer low-dimensional materials from the  $\text{GeO}_2$  substrate onto a conventional materials platform, and how to maintain high quality contact metal and gate oxide interfaces within the device throughout the device fabrication and transfer processes. A follow-up LDRD will pursue sample fabrication, and a Technical Advance describing the transfer process was selected to be filed for a provisional patent (PI: Chris Smyth)



Device-relevant 2D material-based heterostructures are fabricated on a  $\text{GeO}_2$  substrate by depositing any combination of materials onto the low-dimensional material,  $\text{MoS}_2$ . A supporting substrate (supporting Si) is then wafer bonded to the deposited heterostructure. The buried interface is exposed to enable direct characterization by dissolving the  $\text{GeO}_2$  substrate in deionized  $\text{H}_2\text{O}$ .

## CHARACTERIZING DEFECT-DERIVED BEHAVIOR IN WIDE-BAND-GAP-BASED MICROELECTRONIC MATERIALS.

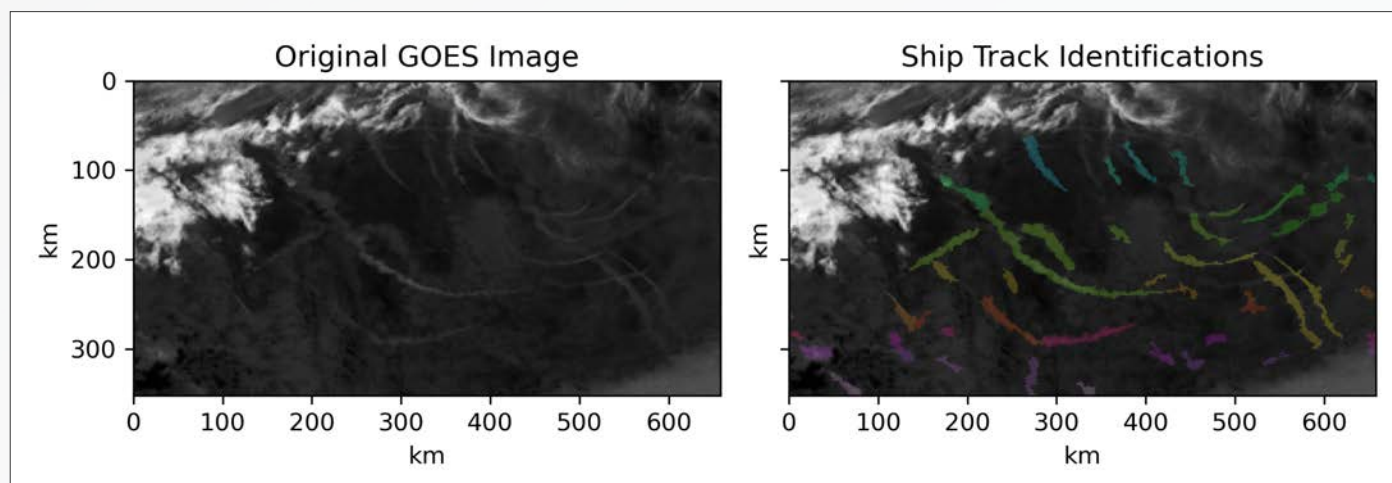
Wide-band-gap (WBG) semiconductors, such as gallium nitride (GaN), revolutionized solid state lighting, have immense potential—greater temperature tolerance, faster switching, larger breakdown voltages—to advance power electronics, optoelectronics, and quantum applications. Limiting this potential is ignorant of atomic effects, either unintentional, damaging defects or dopants engineered for desired functionality, e.g., quantum color centers. Experiments in WBG are mostly chemically

undifferentiating optical probes of excited states. State-of-the-art chemically differentiating density functional theory (DFT) is a ground state theory. This project discovered that a simple extension to DFT to compute excited states yielded predictions sufficiently accurate to chemically fingerprint optical experimental data. For GaN doped with 3D transition metals, this novel analysis reinterpreted years of experiments and predicted new functional defect candidates (quantum color centers) in GaN. (PI: Peter Schultz)

## DEVELOPING AUTOMATED METHODS TO IDENTIFY SHIP EMISSIONS IN SATELLITE IMAGERY.

Fuel-burning ships crossing the ocean sometimes produce long, curvilinear cloud features, called ship tracks, visible in satellite imagery; however, there has been little exploitation of satellite imagery for global monitoring of ship emissions or their impacts on climate models due to the difficulty of automated ship track detection. This project developed a detect-then-classify pipeline based around a statistical anomaly detection technique to identify and isolate ship tracks from surrounding clouds in National Oceanic and Atmospheric Administration (NOAA) Geostationary

Operational Environmental Satellites (GOES) satellite data. Using a novel, annotated dataset, the team investigated cloud properties which are sensitive to ship aerosol emissions, showed the high variability of day-to-day satellite measurements of those properties, and quantified the performance of the proposed identification method. This new process takes a step toward using satellite images of ship tracks to monitor emissions and improving climate models. (PI: Kelsie Larson-Vos)



(Left) An original NOAA GOES satellite image containing ship tracks. (Right) Automatic ship track identifications. Though not perfect, this automated identification process takes a step toward enabling use of satellite image observations of ship tracks for emissions monitoring and improvement of climate models.

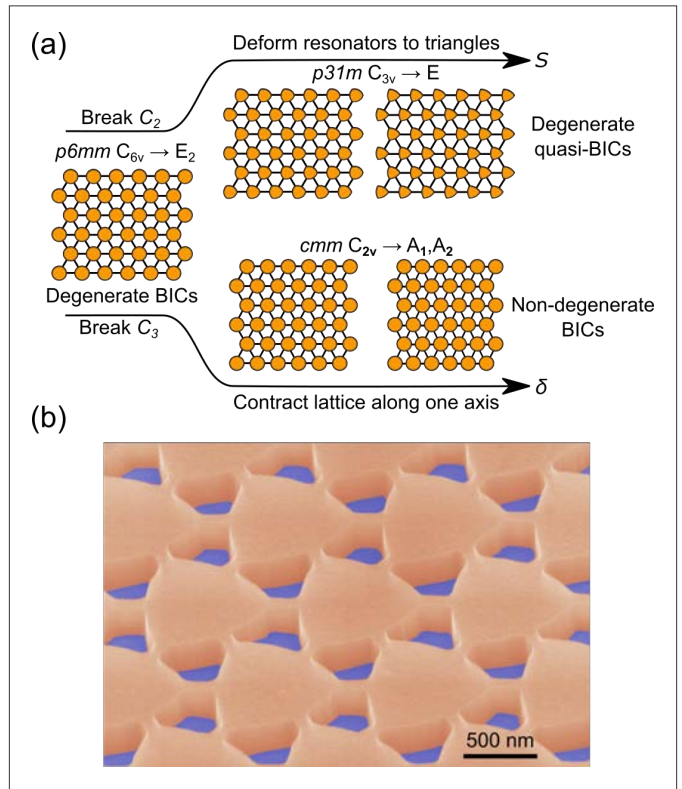
## ENHANCING PHOTONIC SYSTEMS USING TOPOLOGY AND NON-HERMITICITY.

A feature of photonic systems is that their geometry and constituent materials can be tailored during fabrication, allowing for control over their symmetries, and enabling these systems to exhibit phenomena protected by these symmetries. In particular, spatial symmetries can be used to perfectly confine light within a photonic device, while judicious breaking of time-reversal symmetry can yield photonic topological insulators. The goal of this LDRD project was to leverage control over a photonic system's symmetries to discover new device designs for enhancing light-matter interactions and protecting photonic transport. In pursuit of this goal, the team realized symmetry-guaranteed pairs of bound states in metasurfaces, with tailorable frequency splitting and outcoupling. In collaboration with faculty at Alliance partner University of New Mexico and the New Jersey Institute of Technology, the team also discovered and observed the first topological metal in an acoustic metamaterial platform.

This work yielded 10 journal publications, including two in *Nature Communications* (1) (2), and government collaboration with Naval Research Laboratory, and other collaborations with Pennsylvania State, TU Kaiserslautern, Alliance partner Texas A&M, and National/Regional partner University of CA, Davis. In addition, the PI was selected as an American Physical Society [Outstanding Referee](#) in 2023 (a lifetime award) and received an [Outstanding Reviewer](#) recognition from *Light: Science & Applications*, a top journal in

the field of optics and photonics. Support from this LDRD directly contributed to the ideas that were submitted for a DOE Early Career award.

(PI: Alex Cerjan)



(a) By deforming the circular resonators into triangles,  $C_2$  symmetry can be broken (an operation that preserves  $C_3$ ). Correspondingly,  $C_3$  symmetry can be broken by contracting the lattice along one axis (an operation that preserves  $C_2$ ). From these two deformations, we define symmetry-breaking parameters  $S$  and  $\delta$  to denote the strength of  $C_2$  and  $C_3$  symmetry breaking, respectively. (b) False-color scanning electron micrograph of a fabricated silicon metasurface on a fused silica substrate. (Graphic by Chloe Doiron)

## FROM ATOMS TO DEVICES: ADVANCING NANO-ELECTRONICS THROUGH ATOMIC SCALE ELECTRON ENERGY-LOSS SPECTROSCOPY CHARACTERIZATION.

Power electronics, ultra high-density memory storage, and probabilistic computing need device efficiency improvements, and this LDRD project sought to do that by bridging a gap between nanoscale electronic properties and bulk electronic properties in functional materials through the knowledge of valence electron energy-loss spectroscopy (EELS). Low-loss electron EELS in a scanning transmission electron microscope (STEM) were used to map spatial electronic, chemical, and structural information to understand nanoscale device performance origins. Major findings in AlGaIn regrown devices used for power electronics were that chemical nonuniformities at the interface (increased Al content) and structural

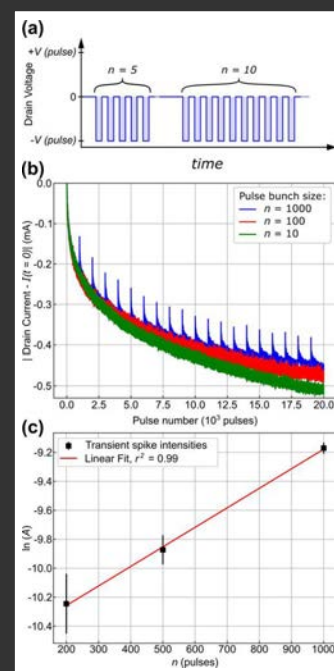
defects (dislocations) did not provide a pathway for current leakage. Eliminating these as potential sources of leakage will help enable AlGaIn-based vertical switching transistors and remove a critical barrier to next generation power circuits. Low-loss EELS were employed for magnetic tunnel junction characterization to analyze magnetic anisotropy spatially through plasmon mapping. This work resulted in seven peer-reviewed publications including [Materials Horizons](#), [Nano Research](#), and [Nanoscale](#), six conference presentations including one invited, and two invited seminars for Alliance partner Purdue and National/Regional partner New Mexico State University. (PI: Julia Deitz)

## DISCOVERING NEW ELECTRONIC MATERIAL FOR NEXT-GENERATION MICROELECTRONICS.

Transition metal dichalcogenides, which have diverse properties, have been identified as an important class of electronic material for next-generation microelectronics. Their 2D ultra-thin body implies mechanical flexibility as well radiation hardness. Gateable non-volatile current-voltage behaviors were observed in polycrystalline MoS<sub>2</sub> transistors, opening up possibilities of radiation-hard, non-volatile memory in this material family. This LDRD project team discovered the impact of surface adsorbates on the memory behavior, which may result in new knobs for controlling these 2D devices. The team, which included three Sandia postdocs hired to support the project, assessed the impact of irradiation on the materials and the correlation with electrical properties and invented processes for processing and transferring 2D devices for investigation of interfacial properties and device integration. The results paved the way toward integrated 2D non-volatile memory with silicon. The project involved faculty collaborations with Northwestern University, Kansas State University, Alliance

partners University of Texas at Austin and Texas A&M, and resulted in publication in [Journal of Materials Research](#) and [Applied Physics Letters](#), with another article accepted for ACS Applied Materials & Interfaces. (PI: Tzu-Ming Lu)

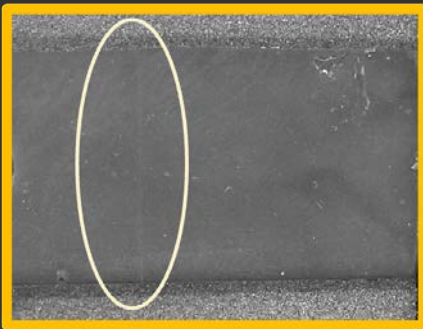
*Controlling trap occupancy through variable pulse bunch size. (a) Diagram depicting how grouping the pulses into smaller bunches introduces more frequent breaks and a lower pulsing duty cycle overall. (b) The effect of the pulse bunch size,  $n$ , on the kinetics of the persistent switching process. Smaller bunches that fill the traps to a lesser degree result in faster resistive switching. The traces shown here have been shifted vertically to more clearly illustrate the difference in switching rate. (c) Transient spike amplitude plotted on a semilog plot against pulse bunch size,  $n$ . Since the detrapping is exponential in trap occupancy, the squared correlation coefficient ( $r^2$ ) near unity is evidence for a linear relationship between  $n$  and trap occupancy.*



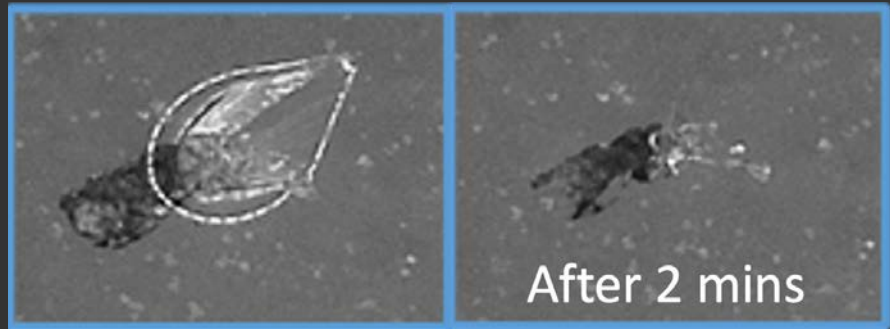
## DESIGNING SELF-HEALING POLYMERS WITH TARGETED PROPERTIES.

Self-healing polymeric materials could significantly impact Sandia's missions by enabling the ability of components to self-repair, particularly in applications where the ability to access or quickly swap out a damaged material is not feasible or cost-efficient, e.g., conformal or dielectric coatings. The first project objective was to create the toolkit necessary to intelligently design a range of intrinsically self-healing polymers with targeted properties, using Van der Waals interactions. Ultimately, the team developed a simple bulk

chemistry approach to self-healing polymers over a range of temperatures (-22 to 24 °C) which require no external stimuli for repair. In these systems, full modulus recovery can be achieved and, in some cases, near invisible repairs. Molecular dynamics simulations were able to help elucidate a mechanism for the self-healing based on a combination of hydrogen bonding, crosslinking, and chain entanglements. Results were published in *Macromolecules* (1) (2). (PI: Erica Redline)



*Some formulations create a nearly invisible seam and almost full tensile property recovery after being cut completely in half; these polymers could be used for seamless joints.*



*Material exhibits autonomous self-healing that could eliminate voids in dielectric coatings.*

## A WORLD-FIRST CHARACTERIZATION OF OVONIC THRESHOLD SELECTOR DEVICES IN RADIATION ENVIRONMENTS.

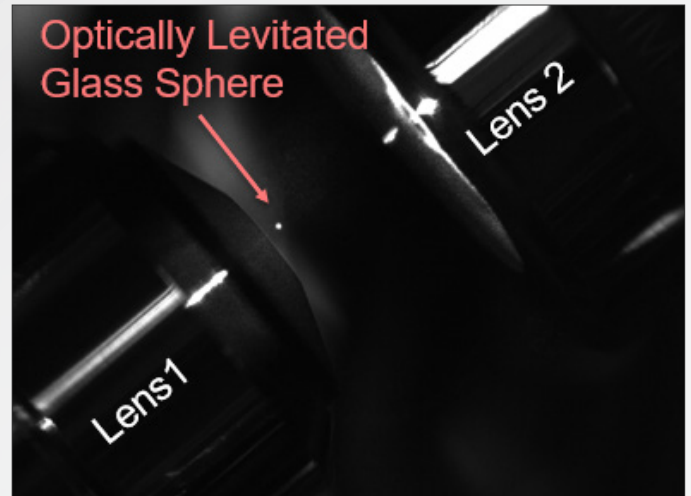
Downscaling of CMOS technology has yielded tremendous performance benefits in the commercial space, but current methods for creating radiation-hardened SRAM in smaller spaces is unlikely to scale beyond the 180 nm node, so new materials and techniques are in development. Through this LDRD project, the team collaborated with National/Regional partners Arizona State University and University of Florida to investigate active switching materials known as ovonic threshold switching (OTS) devices which

may be able to protect scaled SRAM. It must still be able to enable fast access times, potentially, to improve the performance of the rad-hard CMOS by three to four times, and to bridge the gap with advanced node commercial technology. This partnership focused on the OTS device fabrication, thermal and electrical characterization, and a world-first study of the OTS switching mechanism in radiation environments. Follow-on funding was secured for further development. (PI: Robin Jacobs-Gedrim)

## LASER LEVITATION OF MICROFABRICATED PROOF-MASSSES FOR DISRUPTIVE INERTIAL SENSORS.

Optical levitation is an exciting field, but typical setups are not portable due to large, power-hungry optics and manual proof-mass loading. In this LDRD project, Sandia explored optical levitation of microfabricated proof-masses for highly isolated exquisite sensors. The team constructed a testbed that successfully laser levitated glass spheres for several weeks and customized for an optically levitated gyroscope. Microfabricated, untethered micro-scale glass disks designed for levitating were also created. In partnership with Alliance partner Purdue, the team achieved a hybrid levitation of a diamond particle by using electromagnetic fields for levitation and optical fields for readout. This work yielded new

infrastructure, new staff development, university partnership, and four journal publications, with the most recent appearing in [Arxiv](#) in September 2023. (PI: Alejandro Grine)

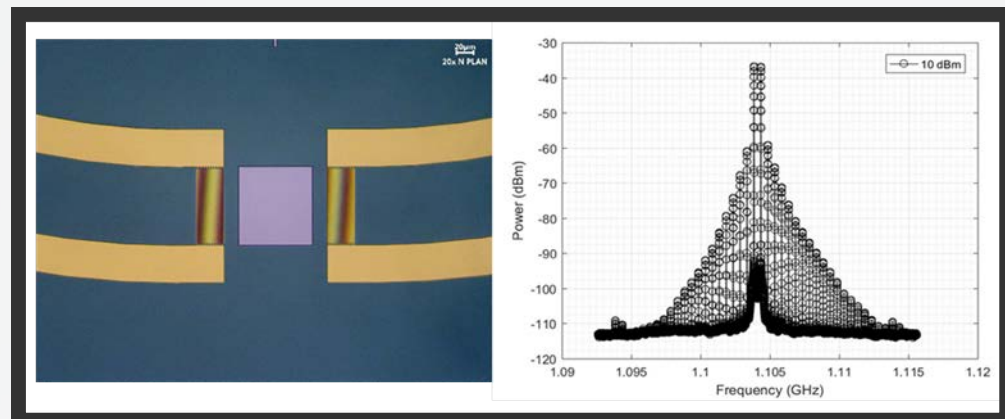


*An optically levitated glass sphere scatters laser light.*

## BRINGING A NEW CAPABILITY TO THE FIELD OF QUANTUM PHONONICS THROUGH A SEMICONDUCTOR-PIEZOELECTRIC HETEROSTRUCTURE.

This LDRD team developed a semiconductor-piezoelectric heterostructure that enabled study of electron-phonon coupling at cryogenic temperatures with unprecedented interaction strengths. While previous efforts were limited to weak coupling, unique physics emerge in the strong coupling regime. The material platform combines an ultra-high mobility, two-dimensional, electron-gas semiconductor with a piezoelectric. As a result, the hybridization between the semiconductor charge and piezoelectric phonons allows electronic nonlinearities to mediate nonlinear interactions between phonons. Exceptionally large, phononic, nonlinear coefficients were demonstrated through four-wave mixing studies, bringing a new capability

to the emerging field of quantum phononics. Two new projects leveraging the developed material platform were funded. A technical advance was also submitted and expertise in heterogenous integration has been extended to new materials and applications. This project, which included a faculty collaboration with University of Arizona, resulted in two follow-on LDRDs and one publication in [Nature Electronics](#). (PI: Lisa Hackett)



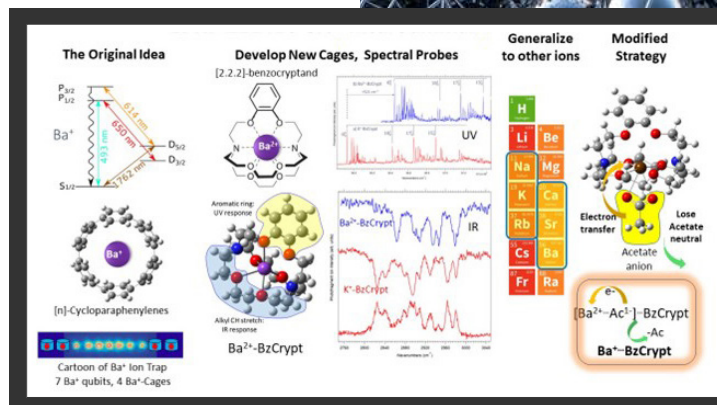
*Fabricated device to study nonlinear mixing (left) and measured phononic frequency comb (right).*

## NANOSCALE IMAGING OF NANO-OPTICS AND PHOTONICS.

Nanophotonics emerged as a way to control the flow of light using nanostructures to mold light-matter interactions at nanoscale. To further capability in this arena, this team sought to develop a tool based on photoelectron imaging that sees electromagnetic fields at length scales below the optical wavelength. Photoelectron imaging probes electric fields created by light-matter interaction, but measures these fields by sensing photoemitted electrons, delivering spatial resolution below 10 nm. This project exploits this spatial resolution to investigate electromagnetic field profiles of quasi-bound states in the continuum, supported by silicon resonator arrays and cavity modes in the suspended transition metal chalcogenides layers. EM field profiling based on photoelectron imaging revealed significant merit for scientific inquiries of light-matter interactions and for nanophotonics device metrology toward national security applications. The unique capability developed through this project led to numerous new projects/programs including two spin-off LDRD projects and a DOE Office of Science Basic Energy Sciences core program and resulted in a journal article published in [Review of Scientific Instruments](#). The project included faculty collaboration with Alliance partner Purdue University. (PI: Taisuke Ohta)

## A NEW STRATEGY FOR INCORPORATING MOLECULAR QUANTUM STATES INTO QUANTUM INFORMATION.

This project pursued a novel strategy for incorporating multiple qubits per ion into ion-trap-based quantum computing (ITQC) involving  $\text{Ca}^+$  and  $\text{Ba}^+$ . By forming molecular complexes of these cations with molecular-scale cages, the team hypothesized that molecular energy levels could be incorporated into quantum computing, while retaining key properties of the atomic ions intact. The project experimented with a variety of molecular cages and found that  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  could be captured and brought into the gas phase efficiently by imbedding them inside [2.2.2]-benzocryptand. IR and UV spectra of these cage complexes are sensitive to the size and charge state of the ion, reporting on the structures and binding properties of the cage complexes. UV photofragmentation of the  $\text{Ba}^{2+}$ -Acetate-1-BzCrypt complex produces  $\text{Ba}^+$ -BzCrypt, the complex targeted for exploration in the original hypothesis. The electronic states of  $\text{Ba}^+$ -BzCrypt have not yet been explored as a platform for molecular ITQC. This LDRD, which was supported by two postdocs and one graduate student from Alliance Partner University of Texas at Austin, resulted in publications in [Physical Chemistry Chemical Physics](#) and the [Journal of Physical Chemistry A](#). Follow-on funding was received to continue the investigation into cryptand molecular cavities. (PI: Timothy Zwier)



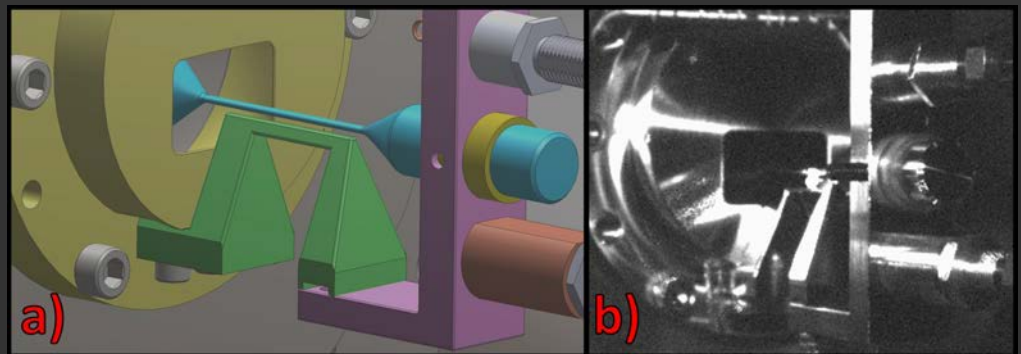
Project work from origination to completion.

## ENABLING DIRECT MEASUREMENT OF LOW-DENSITY ELECTRODE PLASMAS TO CONSTRAIN POWERFLOW SIMULATIONS.

Terawatt-class accelerators, such as the Sandia Z machine, experience a reduction in power delivery via current losses in their inner Magnetically Insulated Transmission Lines (MITL). The primary source of these losses are plasmas, ranging from  $1 \times 10^{13}$ – $1 \times 10^{18}$   $\text{cm}^{-3}$ , shunting current across the anode-cathode gap. A collinear Second-Harmonic Orthogonally Polarized interferometer (SHOPi) diagnostic to measure this plasma's density was developed at Alliance partner University of New Mexico, which led to a [Review of Scientific](#)

[Instruments](#) publication. The interferometer was then successfully fielded at Sandia's Mykonos pulsed power facility using an existing parallel plate platform electrode geometry that imitates the Z machine's inner MITL. This new capability has enabled the first direct measurement of low-density plasma formation in high field power flow gaps, enables an extension of power flow physics development, and will provide constraining data for modeling codes. (PI: Nathan Hines)

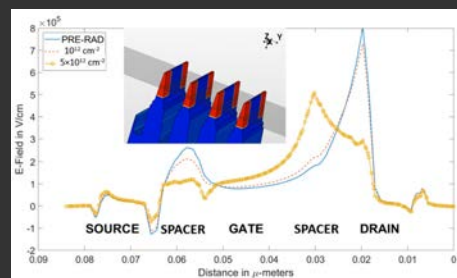
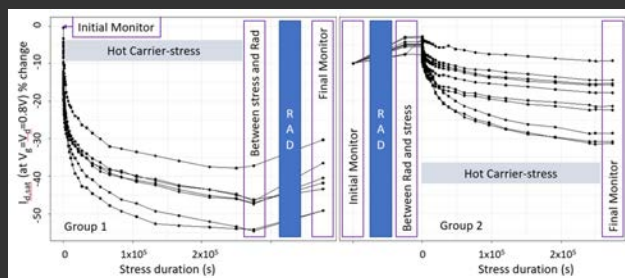
These graphics show (a) the 3D rendering of the parallel plate hardware, and (b) an infrared image of the parallel plate hardware on Mykonos with the bright reflection of the SHOPi laser located in the middle of the anode-cathode rods.



## INTERPLAY OF RADIATION AND ELECTRICAL STRESS EFFECTS ON ADVANCED CMOS RELIABILITY.

The radiation response of devices and integrated circuits can interact with other stresses (e.g., thermal and electrical) to produce degradation profiles that are not a linear combination of stresses. These synergistic interactions are well documented in devices with planar geometry. As transistor geometry has changed, basic degradation mechanisms have evolved, requiring further study on combined stress effects in advanced nodes. In a rapid one-year project, the Sandia LDRD team demonstrated a synergistic interaction between total ionizing dose and electrical hot carrier stress

in 12 nm fin field-effect transistors (FinFET). The team worked with students from National/Regional partner Arizona State University to explain the mechanisms using 3D TCAD simulations, which showed how a trapped charge in the spacer can alter the electric field at the interface near the drain; this study is currently in review for publication in *Transactions on Nuclear Science*. The team also developed a prototype system to rapidly evaluate synergistic interactions of electrical stress and radiation in advanced node test structures. (PI: David Hughart)

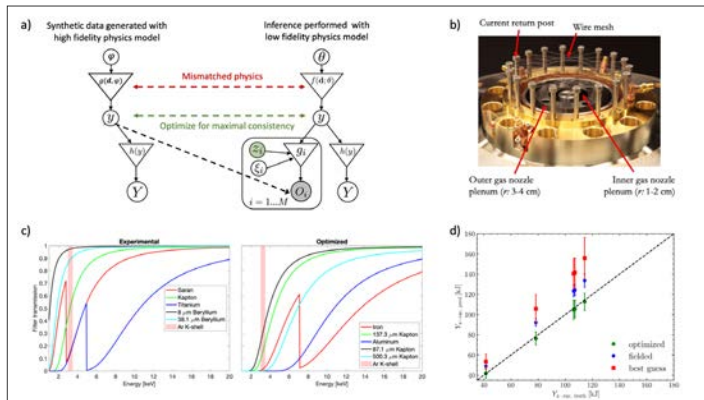


(Left) the drive current degradation of the FET. (Right) the FET electric field simulation.

## DEVELOPING AND APPLYING QUANTIFIABLE METRICS FOR DIAGNOSTIC AND EXPERIMENT DESIGN ON Z.

Z experiments provide access to incomparable conditions for studying questions of high importance for national security. Complex design tools and experimental constraints, however, have traditionally limited designs and diagnostic configurations for selection through expert intuition rather than modern statistical and machine learning based approaches. This LDRD study applied optimal experiment design methods to automate this task in collaboration with Roshan Joseph at Alliance partner Georgia Tech and graduate student Gina Vasey at Michigan State University. The Sandia LDRD team published a proof-of-concept ability to design experiments

incorporating instrument effects, uncertainties, and model bias in a special issue of the [Journal of Plasma Physics](#) on Machine Learning for Plasma Physics and Fusion Energy. Additional work on X-ray synthetic diagnostics that were key components of this study and performed under this LDRD was also published in [Review of Scientific Instruments](#). Finally, the team discovered a diagnostic configuration that could be fielded on an upcoming experiment to improve confidence in the approach and reduce bias in X-ray yield inferences used in stockpile stewardship work. (PI: William Lewis)



(a) Diagram showing optimization framework in the presence of instrument uncertainty and model bias, (b) Gas puff experiment platform, (c) Plot of the PCD X-ray filter response for experimental as-fielded and optimized configurations, and (d) Results on inference of out-of-sample data, showing Sandia's method results in reduced bias while improving or maintaining uncertainty in inferred X-ray yield on the Argon gas puff platform. The team hopes to field the optimized and experimental filter configurations simultaneously on a future experiment to demonstrate the impact on experimental data versus synthetic data.

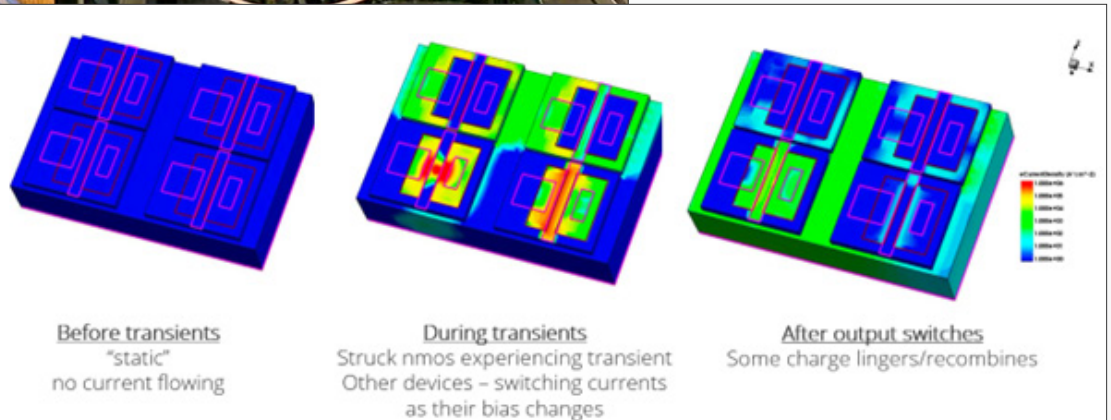
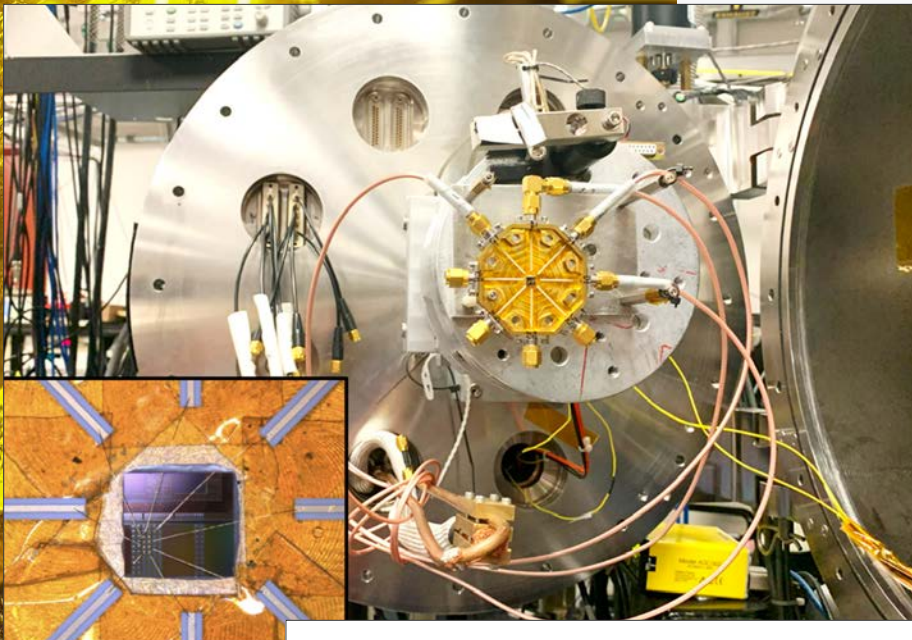
## A UNIFIED FULL-FEATURED TO LOW-COST-MODEL DEVELOPMENT FOR ACCELERATED DESIGN OF ELECTRICAL NUCLEAR DETERRENCE SYSTEMS IN COMBINED RADIATION ENVIRONMENTS.

Scalable, radiation-aware modeling capabilities can dramatically reduce design and qualification cycles for nuclear deterrence electrical systems. Circuits and component models are frequently built bottom-up from many complex device models and do not scale across the ND hierarchy levels. This LDRD project investigated application of reduced order models (ROM) and system identification methods for development of scalable, rad-aware hierarchy of data-driven models operating at multiple system integration levels. The team developed an innovative nonlinear compact photocurrent ROM that remains accurate over a wide range of dose rates. A behavioral model

for CMOS amplifiers and comparators based on first-of-its kind "greedy" Hammerstein and Wiener architectures captures the behavior of the circuits and scale favorably. In collaboration with Alliance partner University of New Mexico hardware security experts, ROMs are being extended towards assessment of physical sources of entropy for strong unclonable functions. The team also collaborated with Alliance partner University of Illinois Urbana-Champaign. Accomplishments include publication in [IEEE Transactions on Nuclear Science](#) and [Journal of Hardware and Systems Security](#). (PI: Biliana Paskaleva)

## UNIQUE SIMULTANEOUS DOSE RATE AND SINGLE-EVENT RADIATION-RESPONSE PHYSICS IN INTEGRATED CIRCUITS.

Many Sandia-developed systems must withstand harsh radiation environments. An environment of particular concern contains combined high dose rates and neutron fluxes that can produce single event effects (SEE). These two stresses are routinely examined in isolation but not simultaneously. The Sandia LDRD team used the Ion Beam Laboratory's combined electron and ion beam platform to subject integrated circuits manufactured at MESA to high ionizing dose rates and particle fluxes that produced SEEs. With the team's partners at Vanderbilt's Institute for Space and Defense Electronics, 3D TCAD device physics modeling was used to mimic experimental conditions and identify driving response mechanisms. The team observed first-of-a-kind sub-nanosecond current transients in individual MOSFETs and a new non-linear combined response in SRAM circuits in this simultaneous combined environment. Further work is needed to investigate combined radiation effects and the newly proposed Combined Radiation Environments for Survivability Testing (CREST) facility will significantly expand the capability. (PI: Andrew Tonigan)

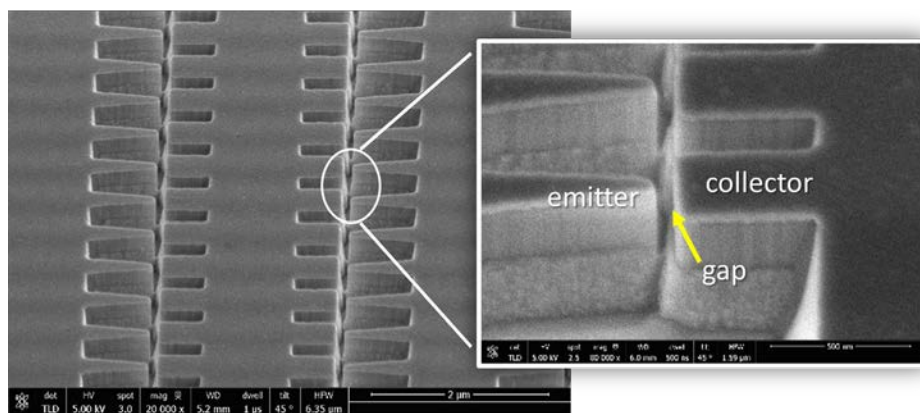


(Top) MOSFET experiment. (Bottom) SRAM strike.

## SCALE-UP OF GAN NANOSCALE VACUUM ELECTRON DIODES ENABLES A NEW PATH TO ELECTRONICS FOR HARSH ENVIRONMENTS.

Operability and survivability in high radiation environments such as space is a significant challenge for modern semiconductor devices. In contrast, vacuum electron devices such as vacuum tubes are typically more robust to harsh environments but are bulky and power-hungry. In this project, the Sandia LDRD team investigated radiation effects in a new class of Sandia-developed, gallium nitride (GaN) based, solid-state nanoscale vacuum electron devices to determine their potential for radiation-hard electronics.

These hybrid, miniaturized on-chip devices have shown in-air operability and low turn-on voltages comparable to modern semiconductor devices. GaN vacuum electron nanodiodes were tested to exposures to proton, electron, and neutron irradiation and were found to exhibit extreme radiation hardness. The team posit this is due to their unique architecture, which has an air or vacuum channel that cannot be damaged. Results were published in [IEEE Transactions on Electron Devices](#), and funding was received for a follow-on LDRD (PI: George Wang)



Scanning electron micrograph of a 1000 parallel GaN vacuum electron nanodiode array. Inset shows close-up view of device.

## DEVELOPING INNOVATIVE NANOSTRUCTURAL GRANULAR METALS FOR IMPROVED EMP PROTECTION.

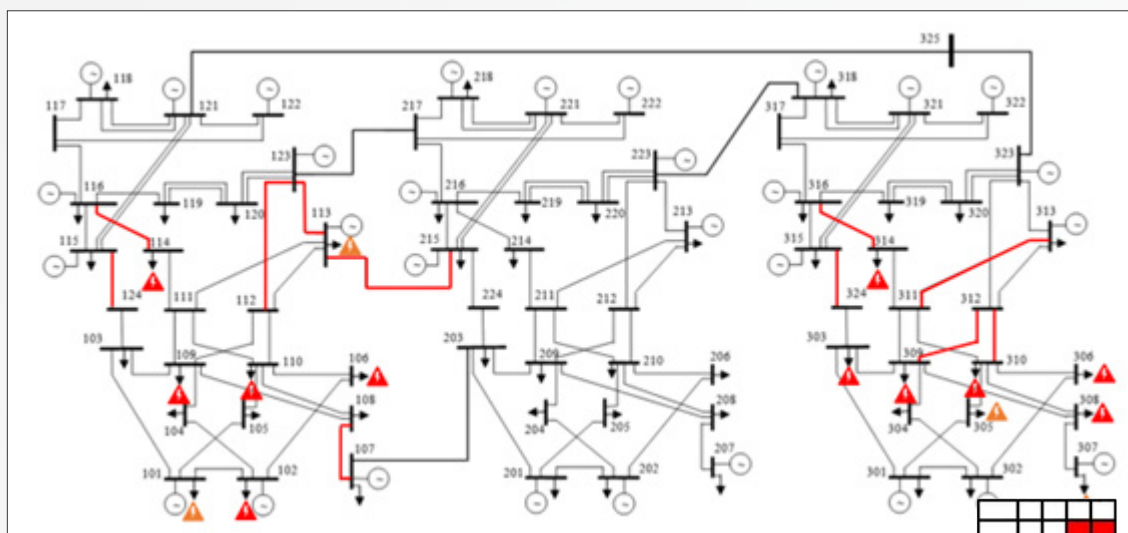
While the probability of a high-altitude nuclear detonation is low, the risk with ensuing nanosecond electromagnetic pulse events posed to the electrical grid is high. New ultrafast grid-scale protection devices are needed to protect against resulting dangerous high-voltage, high-current transients that couple to grid transmission lines. The Sandia LDRD team developed innovative high voltage-strength granular metals to be the active material in future grid protection devices. Granular metals, consisting of metal nanoparticles within an insulating matrix, have complementary tunneling and capacitive conduction paths to safely shunt harmful nanosecond transients to ground. The team discovered that, through optimization of the granular metal material family, growth conditions, and post-growth thermal

annealing, they could create high-voltage strength granular metals that demonstrate the robust filter performance necessary for protection devices. This project supported two postdocs and one undergraduate intern who contributed to four publications. Postdoc Simeon Gilbert, who later converted to staff, led one of the research thrusts. Gilbert received two presentation awards—first place at Sandia’s 15th Annual Postdoctoral Technical Showcase and third place at the 2022 Rio Grande Research SLAM—presenting on the topic of this project. Research accomplishments, which were highlighted in [Nanotechnology](#) and [Journal of Physics: Condensed Matter](#), led to the receipt of follow-on funding from [ARPA-E](#) and Sandia’s Resilient Energy Systems Mission Campaign. (PI: Laura Biedermann)

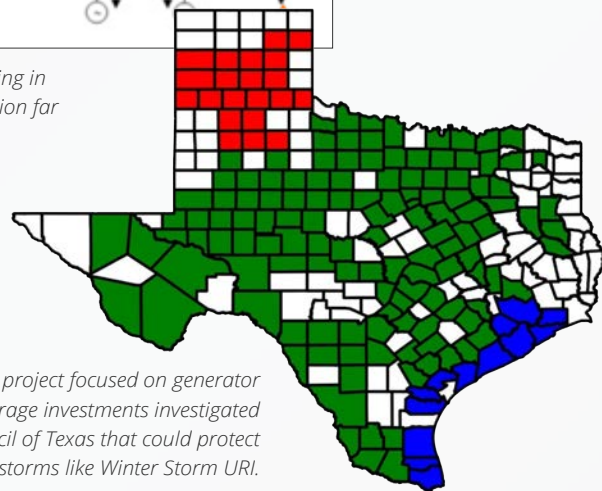
## IDENTIFYING VULNERABLE COMPONENTS OF AN ELECTRIC POWER GRID THROUGH CRITICAL NODE IDENTIFICATION, VULNERABILITY MODELING, AND TOPOLOGY OPTIMIZATION.

The Critical Nodes LDRD project formulated mathematical programming and machine learning techniques to help determine the most vulnerable components of an electric power grid that is subjected to known natural threats and intentional attacks. A secondary objective was developing methodologies to help select the most effective mitigation investments to protect against these threats. Through the course of the Sandia LDRD team's research, the team discovered several simplification strategies to make the models easier to solve without losing important details. This research laid the groundwork for future researchers to scale the team's approaches and

provide grid stakeholders and regulators tools for finding extreme grid vulnerabilities along with investment decision methodologies. The team partnered with Erhan Kutanoglu and Surya Santoso along with their graduate students at Alliance partner University of Texas at Austin. Their research was instrumental in developing Sandia's multistage investment models. Results include three publications, including two at the IEEE/PES Transmission and Distribution Conference and Exposition: (1) (2), and one at the [International Conference on Probabilistic Methods Applied to Power Systems](#). (PI: Bryan Arguello)



Finding the worst outages in a power grid involves exploring all subsets of outages, resulting in a combinatorial explosion. Sampling these outages will result in a power outage distribution far away from the worst. Shown is the worst N-12 outage.



The case study used in the project focused on generator protection and mobile energy storage investments investigated by the Electricity Reliability Council of Texas that could protect Texas against storms like Winter Storm URI.

## DISCOVERY OF NEW HIGH FREQUENCY MAGNETIC MATERIALS FOR THE GRID ENABLED THROUGH AI.

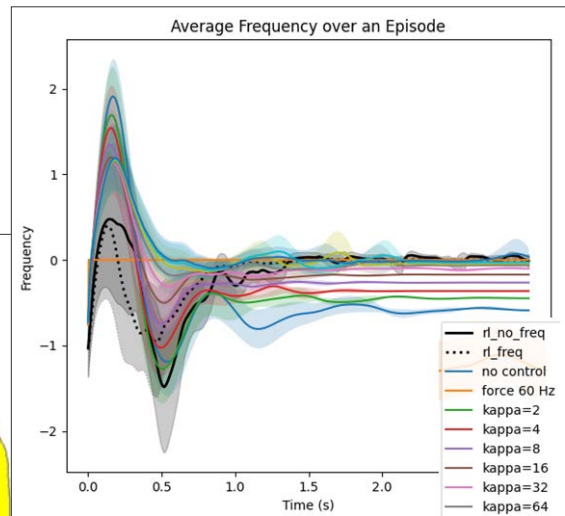
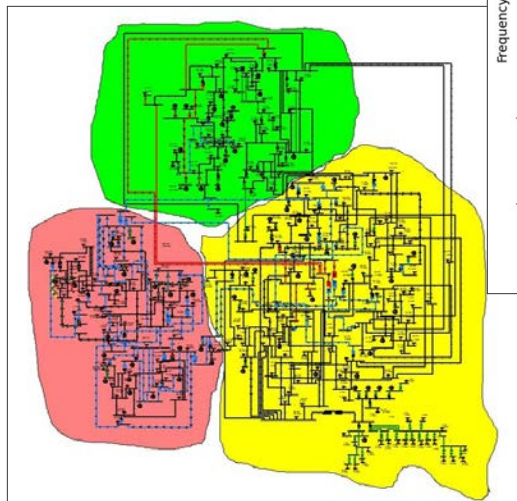
Solid state transformers can make the grid more stable and resilient, however new high frequency magnetic materials are needed to achieve their potential. Electromagnetic and optical metamaterials can be designed having assured real-world performance using MIRaGE. Density Functional Theory (DFT) calculations train AI to find candidate materials with enhanced properties. These are validated by DFT, and then candidate materials are synthesized using an automated reaction system under AI control. The AI system uses reinforcement learning to continuously improve the reaction conditions to yield the

desired phase. Rapid prototyping methods are then utilized to generate parts for immediate testing in real systems. New magnetic materials have been discovered, synthesized, and tested using these approaches, and the results published in [Nanoscale Advances](#) and [Advanced Materials](#). The general approach has been applied to other systems, including the development of new catalysts. The LDRD team collaborated with faculty at Alliance partner Purdue, Clemson University, and the University of Southern California. (PI: Dale Huber)

## ADVERSARIAL POWER SYSTEM VULNERABILITY IDENTIFICATION AND DEFENSE THROUGH DEEP REINFORCEMENT LEARNING.

Recent power systems failures underscore the need for dynamic response capabilities. In this project, the Sandia LDRD team applied Deep Reinforcement Learning (DRL) to train controllers for both power distribution and transmission systems. A lower-order Kuramoto model of power transmission systems was developed that mirrors real-world dynamics for rapid model development and testing. The team demonstrated that their approach can be used to train agents using the high-fidelity simulators OpenDSS and PowerWorld, which allows the

trained defensive agents to respond to these events. Through this effort, it was discovered that defensive agents can prevent grid failure conditions, and furthermore, agents trained on non-adversarial scenarios are also effective at protecting from adversarial effects. This work, which was supported by a collaboration with Alliance partner Georgia Tech, provides a path toward a DRL-trained controller for complex infrastructure networks. (PI: Drew Levin)



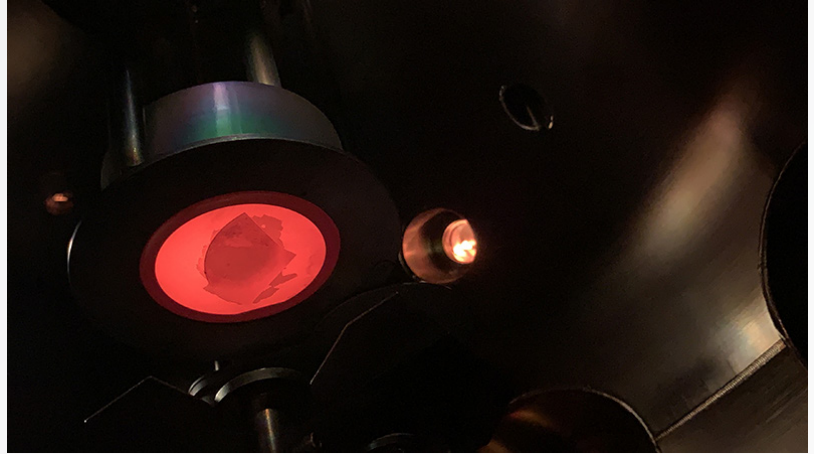
The modeling environment was integrated with the [PowerWorld](#) simulator for high-fidelity control.

The Deep Reinforcement Learning for Power System Defense LDRD project has successfully applied continuous-space deep reinforcement learning methods to manage voltage stability on a 701-bus (neighborhood-sized) power distribution system.

## RECONFIGURING UNPATTERNED METASURFACES THROUGH ACOUSTOELECTRIC GATING OF GRAPHENE.

Reconfigurable optoelectronics implemented in graphene metasurfaces can benefit applications ranging from sensing to communication, but previously were insufficient in their ability to “tune” at levels compelling for national security applications. By merging the advantages of surface acoustic waves and 2D materials, this LDRD project realized a solution with compelling performance in reconfigurable architecture that can enable multi-parameter tuning of the graphene plasmonic. The result is new classes of reconfigurable classical and quantum devices. Sandia’s collaborations with Alliance partners Purdue and the University of New Mexico helped lead to the project’s success, and the results

were included in seven journal articles, including [Advanced Photonics Research](#). (PI: Aleem Siddiqui)

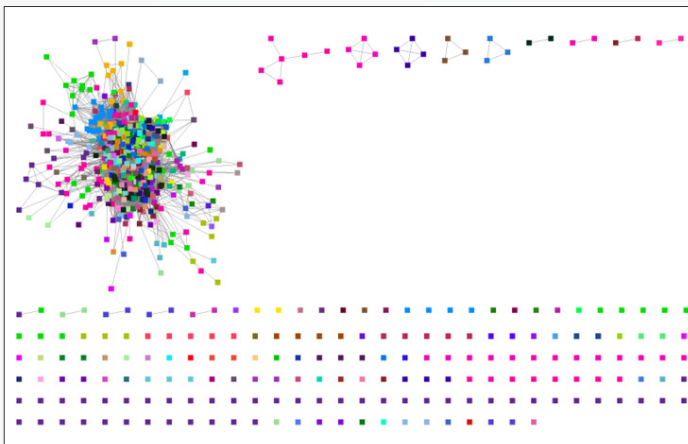


*Sandia in collaboration with Alliance partners Purdue and the University of New Mexico developed a new approach to creating popular thin films used for devices. This image shows work on a sample of that innovation while it was heating up.*

## MALGEN: MALWARE GENERATION WITH SPECIFIC BEHAVIORS IMPROVES MACHINE LEARNING-BASED DETECTORS.

As malware infections grow at exponential rates, ML techniques are used to identify malware at mission speeds in a myriad of data. Despite reported classification accuracy greater than 99%, ML-based malware detection lags far behind in deployed settings. To improve this, the Sandia MalGen LDRD team, in collaboration with Sandia National/Regional partner New

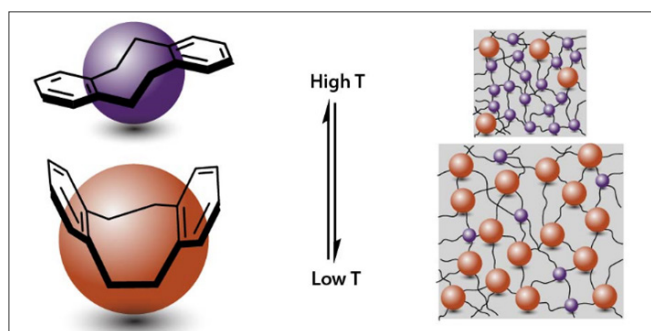
Mexico Tech, proposed to identify commonly exhibited behaviors such as dynamic link library injection and process hollowing. Novel malware is presented to end-users annotated with behaviors, reducing the burden on cyber analysts. To enable the methodology, New Mexico Tech developed a method to automate labeling malware with behaviors for training an ML model. The methods developed through this three-year project lay a foundation for improved integration of ML that have been highlighted in two journals, with one just accepted into [ACM Digital Threats: Research and Practice](#), as well as four conferences and workshops. (PI: Michael R. Smith)



*Visualization of how data points are linked together when using Sandia’s genomics distance measure for a Malpedia data set. Many of the data points are connected, but without any noticeable structure. There are many that do not link with any other data point and are singletons. This indicates possibly a sparse coverage of the input space.*

## RESOLVING THERMAL EXPANSION MISMATCH IN EPOXY COMPONENTS.

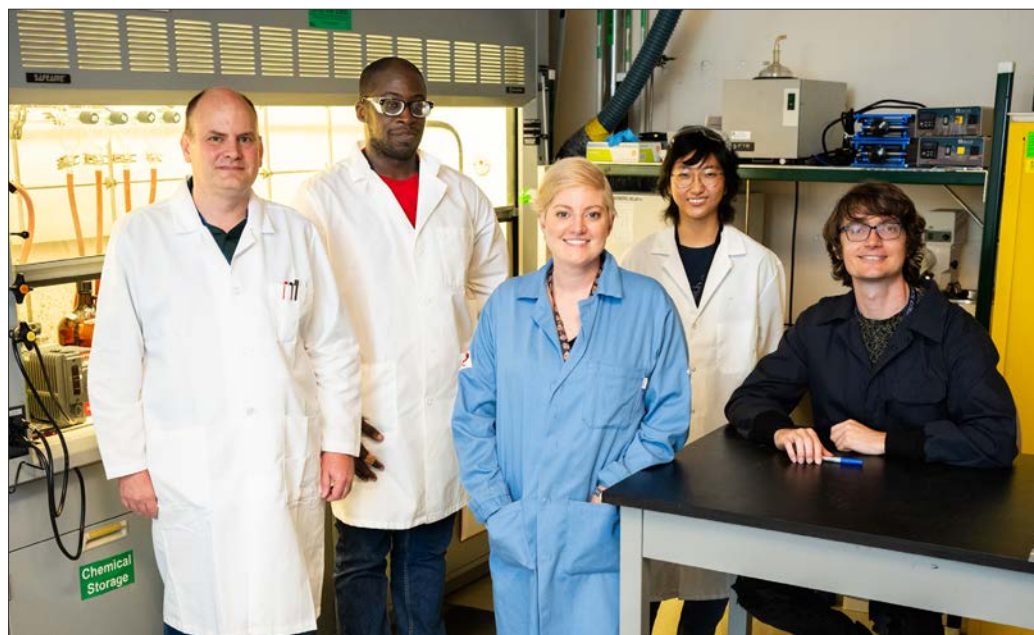
Harsh, dynamic environments can wreak havoc on applications, especially when multiple types of materials are bonded together. One specific problem is a thermal expansion mismatch between encapsulant and components, which rely on encapsulation for protection against thermal, mechanical, and/or electrical insult. However, coefficient of thermal expansion (CTE) mismatch has been attributed to failures prior to part fielding and during testing activities. Currently, fillers are added to reduce this mismatch; however, fillers create additional issues while only moderately addressing the problem.



(Right) Incorporation of contractile units into thermoset materials influences their thermal expansion and contraction behavior. (Left) DBCO undergoes thermally controlled isomerization between twist-boat and chair conformers. The orange circles in A represent the twist-boat conformer and the purple circles the chair conformer.

The Sandia LDRD team partnered with Alliance partner University of Texas at Austin (UT Austin) to design a [novel solution that incorporates CTE tunability directly into the epoxy network chemistry](#) that delivers unprecedented CTE-matching ability and eliminates the need for fillers. Multiple provisional patents have been filed, and one covering a divinyl variant of DBCO molecule made by [UT Center for Dynamics and Control of Materials](#). Collaborators from UT Austin include Zachariah Page in the McKetta Department of Chemical Engineering, Meghan Kiker, a UT Austin graduate research assistant, and Sandia technologist Alana Yoon (formerly an intern supporting the project). This project resulted in publications in [ACS Macro Letters](#) and multiple presentations including the Materials Research Society Spring Meeting and ACS PacifiChem.

PI Erica Redline's proposal was one of only two across all DOE labs funded for NNSA's Energy I-Corps program, an 8-week DOE-led training where researchers define technology value propositions, conduct customer discovery interviews, and identify viable pathways for their technologies. Follow-on funding based on this work is being pursued. (PI: Erica Redline)



From left to right, Sandia chemist Chad Staiger, technologist Kenneth Lyons, materials scientist Erica Redline, technologist Alana Yoon, and postdoc Eric Nagel are part of a research team helping make materials more durable. (Photo by Craig Fritz)

## PROJECT HIGHLIGHTS - WORKFORCE DEVELOPMENT

Sandia's LDRD program enables principal investigators and research teams to collaborate with other national laboratories, academic institutions, and industry partners to revolutionize what is possible in science and engineering. This not only develops Sandia's workforce, but it also grows the nation's technical research capabilities overall, and even contributes to the economy. The highlights in this section are only a small subset of the impacts that have been made in 2023 through LDRD, but they give a glimpse of how significant the program is to the country and to the world.

## PRESTIGIOUS FELLOWSHIPS, APPOINTMENTS AND MEMBERSHIPS

### SOCIETY OF INDUSTRIAL AND APPLIED MATHEMATICS FELLOW



**Ali Pinar** was selected by the Society of Industrial and Applied Mathematics (SIAM) as a 2023 Fellow. Pinar's career at Sandia has focused on studying network science, from power network to cyber

networks. He applies graph theory to model complexities and understand vulnerabilities. His SIAM recognition is "for theoretical, algorithmic, and application impacts, and community leadership in combinatorial scientific

computing and network science." He has led three LDRD projects (machine learning, cyber simulations, and cybersecurity) and been a team member on 17 LDRDs.



*"The LDRD program is Sandia's window to the research world. We learn from others, but we have a lot to offer as well. The great work and the great researchers at Sandia would not have received the recognition from scientific community without the LDRD program. Being fellow was a dream for me since my graduate student days, and I am grateful to the LDRD program for helping me realize this dream."*

### AMERICAN CHEMICAL SOCIETY FELLOW

Materials scientist and researcher **Hongyou Fan** was named Fellow of the American Chemical Society (ACS) in 2023. Fan has been an active LDRD participant, leading eight projects and serving as a team member for ten. He is the recipient of six R&D 100 Awards, was selected as the Asian American Engineer of the Year in 2012, elected as a Fellow for both the Materials Research Society and American Physical Society

in 2016, and won the Society of Asian Scientists and Engineers Career Achievement Award in 2022. His work has applications in electronics, energy, materials separation and more. The society recognized Fan "for outstanding contributions to the novel design, synthesis, functionalization, and integration of



*nanoscale colloids leading to innovative applications in nanoelectronics, clean energy, sensor development, and photocatalysis."*

*"LDRDs are great funding resources to foster innovative science ideas that play as the foundation for tomorrow's big technologies."*



### DEPARTMENT OF THE AIR FORCE SCIENTIFIC ADVISORY BOARD MEMBER



Mechanical engineer **Bo Song** was appointed to the Department of the Air Force Scientific Advisory Board. The board gives the Air Force independent technical advice and is the principal external advisory body to the Secretary of the Air

Force and senior leaders in the various commands. Song has supported five LDRD projects as a team member.

## IEEE FELLOW



Senior Scientist **Stan Atcitty** was named a Fellow of the Institute of Electrical and Electronics Engineers (IEEE), one of the world's largest technical professional organizations. Atcitty has been involved with multiple LDRD projects focused on integrating energy storage

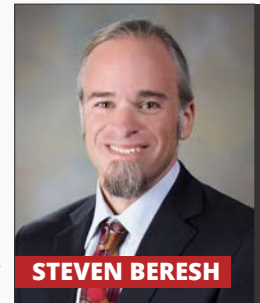
and distributed generation with the electric utility grid. Six of his projects have won R&D 100 awards and one Gold Green Energy award from *Research & Development Magazine*. Atcitty, a member of the Navajo Nation, leads the power

electronics subprogram as part of the DOE Office of Electricity's Energy Storage Program within the Nuclear Fuel Cycle and Grid Modernization Center at Sandia. Atcitty also leads the Tribal Energy Storage Program and the NNSA's Minority Serving Institute Partnership Program, working with tribal colleges and universities. In 2012, President Barack Obama presented Atcitty with the Presidential Early Career Award for Scientists and Engineers, the highest honor bestowed by the federal government for outstanding scientists and engineers who show exceptional leadership at the frontiers of scientific knowledge during the 21st century.

## AMERICAN INSTITUTE OF AERONAUTICS AND ASTRONAUTICS FELLOW

**Steven Beresh**, 2023 Fellow of the American Institute for Aeronautics and Astronautics (AIAA), emphasizes the use of optical diagnostics for compressible aerodynamics, particularly particle image velocimetry, in his research studies. He is currently focused on maturing instrumentation techniques for hypersonics and is also responsible for a wide range of high-speed wind tunnel testing and operation of that facility. Baresh served as

Chair for the AIAA Aerodynamic Measurement Technology Technical Committee, is a past President of the Supersonic Tunnel Association International, and is now a Deputy Director of the Aerospace Sciences group for AIAA. Baresh has led two LDRD projects and been a team member on six more.



*"LDRD projects were integral to me building the physical understanding and lab capabilities needed to launch and sustain my early career. Now that I am later in my career and I am involved in the larger programmatic picture, I see much more clearly how important LDRD projects are to establishing the technologies that eventually will become key components of the lab mission."*



## AMERICAN INSTITUTE OF AERONAUTICS AND ASTRONAUTICS FELLOW



American Institute of Aeronautics and Astronautics Associate Fellow **Dan Guildenbecher**, a researcher in thermal/fluid experimental sciences, was appointed as a 2023 Fellow of the American Institute for Aeronautics and Astronautics (AIAA). Guildenbecher became interested in the field as a

doctoral student when he ran into limitations in commercial diagnostics for studying multiphase flows. He joined Sandia in 2011 and teamed with researchers working in digital imaging. Guildenbecher has led five LDRD projects and been a team member on another five LDRD efforts, including the Light Speed Grand Challenge. Guildenbecher is now an associate professor in the School of Mechanical Engineering at Purdue, a Sandia Alliance partner.

## AMERICAN PHYSICAL SOCIETY FELLOW

Dan Dolan, 2023 American Physical Society (APS) Fellow, has worked extensively on designing and improving the photonic Doppler velocimetry diagnostic which can measure electron densities on Sandia's Z machine, and has extensive

knowledge on interferometry measurements. His APS citation reads: "For scientific contributions to understanding phase transitions under dynamic compression,



DAN DOLAN

specifically, freezing in water, and for broadly impactful contributions to the field of dynamic compression science in the area of diagnostics and analysis tool development." Dolan has served as PI on three LDRD projects and been a team member on six others.

*"The LDRD program helped me take a longer view, thinking about problems that need to be solved but don't fit within immediate deliverables. I appreciate the fail-fast mentality—if every LDRD project worked \*exactly\* as predicted, we are not taking enough risks."*



## AMERICAN PHYSICAL SOCIETY FELLOW



AIDAN THOMPSON

**Aidan Thompson** develops predictive atomistic materials modeling capabilities enabled by extreme scale computing platforms. His American Physical Society citation

recognizes him "for advancing large-scale atomistic simulations of materials by devising quantum-accurate machine learning interatomic potentials and developing LAMMPS, the leading open-source molecular dynamics package." Thompson leads the development of FitSNAP software, which was an outgrowth of LDRD.

He has served as PI on three LDRD projects and as a team member on 11 additional LDRD projects.

*"Good LDRD projects allow staff to pursue promising but risky new ideas. This type of risk-taking keeps Sandia at the forefront of innovation, instead of merely following behind. The FitSNAP machine learning software for generating high-accuracy interatomic potentials for atomistic simulation of materials emerged from a FY2012 LDRD project. It gave Sandia a worldwide leadership position in the transformation of molecular dynamics from a qualitative/descriptive to quantitative/predictive materials modeling method that is still continuing. I am very grateful to the LDRD program for giving us an early start in this exciting and impactful field."*



## LDRD IMPACT STORY

### SANDIA ACADEMIC COLLABORATIONS AND WORKFORCE DEVELOPMENT CONTINUE EVEN AFTER A4H MISSION CAMPAIGN ENDS

Academic partnerships across the nation have been key to the success of the Autonomy for Hypersonics (A4H) Mission Campaign. These engagements were intentionally cultivated and stimulated through the strategic outreach of Sandia.

Over the last six years (FY18-FY24), Sandia teams supporting the \$38M A4H Mission Campaign have collaborated with researchers from more than 15 universities through nearly 30 research efforts. The outcomes from those research partnerships alone make the A4H Mission Campaign a success, however, these connections are continuing to pay significant dividends through the support of external sponsors. The Air Force Research Lab and the Navy are just two of the sponsors who are leveraging the outcomes of these hypersonics-focused research partnerships and springboarding toward possible application.

The Joint Hypersonics Transition Office recently stood up the University Consortium for Applied Hypersonics (UCAH) to develop the nation's hypersonics workforce. Several A4H university scientists have successfully proposed new research under UCAH and are proceeding with Sandians as co-principal investigators on these university-led projects—a bit of role-reversal from A4H!

A few examples of ongoing work include:

#### FAST: Full Airframe Sensing Technology for Hypersonic Aerodynamics Measurements

This 3-year, \$3.3M University Leadership Initiative (ULI) award performed at UT Austin will enable high-fidelity aerothermal simulations of hypersonic vehicles. Work done on Sandia's A4H LDRD Mission Campaign led UT to focus on creating a new paradigm in sensing for hypersonic vehicles that could also be applied to lower-speed craft. Sandia will collaborate on this work by providing expertise in hypersonic vehicle air flow simulations.

#### Emission & Absorption Spectroscopy Sensors for Hypersonic Flight Control

This 3-year, \$3.5M ULI award to Purdue resulted from their collaboration on Sandia's A4H LDRD Mission Campaign. The project will focus on the development of novel in-flight and ground measurement techniques for hypersonic flight. The optical and laser sensor capabilities developed through the A4H project will be used to examine the surfaces and flow of hypersonic vehicles.

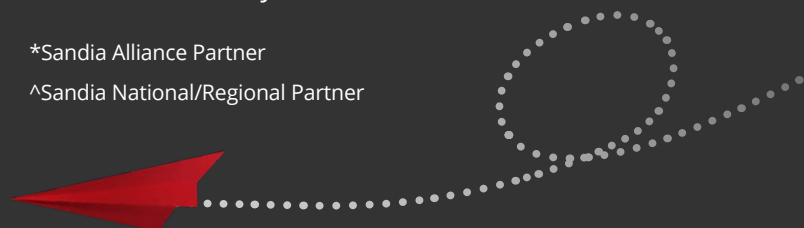
Through these UCAH and ULI projects and other government-sponsored research, A4H efforts will continue beyond FY24 as part of a national team largely built through the Sandia Mission Campaign.

#### Hypersonic research partners

1. Arizona State<sup>^</sup>
2. Georgia Tech<sup>\*</sup>
3. George Mason University
4. Kansas State University
5. Ohio State University
6. Pennsylvania State
7. Purdue University<sup>\*</sup>
8. Texas A&M<sup>\*</sup>
9. University of Arizona<sup>^</sup>
10. University of Illinois Urbana-Champaign<sup>\*</sup>
11. University of Maryland
12. University of New Mexico<sup>\*</sup>
13. University of Southern California
14. University of Texas, Austin<sup>\*</sup>
15. University of Texas, Dallas

<sup>\*</sup>Sandia Alliance Partner

<sup>^</sup>Sandia National/Regional Partner





*Joint Flight Campaign 1 for the Navy's conventional prompt strike and Army's long-range hypersonic weapons program.*

## A4H COLLABORATIONS LEAD TO JOINT APPOINTEE



**ANIRBAN MAZUMDAR**

assistant professor in the mechanical engineering

A4H collaborations also facilitated a Faculty Loan joint appointee between Sandia and partner university Georgia Tech.

Anirban Mazumdar,

department, is the first inbound Joint Appointee with Georgia Tech and is being hosted by Sandia's Autonomy for Hypersonics Department. Mazumdar said of the appointment, "The faculty loan appointment allows me to work closely with Sandia's hypersonics experts and programs onsite in Albuquerque, NM... Our overall goal is to ensure that collaborative Georgia Tech-Sandia research has long-term relevance and impact."

## FY23 TRUMAN POSTDOCTORAL FELLOWSHIPS

### HARRY S. TRUMAN POSTDOCTORAL FELLOWSHIP

Sandia established the three-year fellowship, funded by LDRD, to attract the nationally recognized PhD scientists and engineers. Truman Fellows conduct independent groundbreaking research that supports Sandia's national security mission.

#### JOSEPH CUOZZO – TRUMAN FELLOW

Joseph Cuozzo will use his Truman Fellowship to develop quantum-scale innovations for high-speed computing. Joseph is investigating if it is possible to craft topological features in a structure that allows superconductivity that becomes the basis for quantum computing. He hopes his work can help reduce errors in quantum calculations. He graduated from the University of South Florida in 2017 with degrees in math



**JOSEPH CUOZZO**

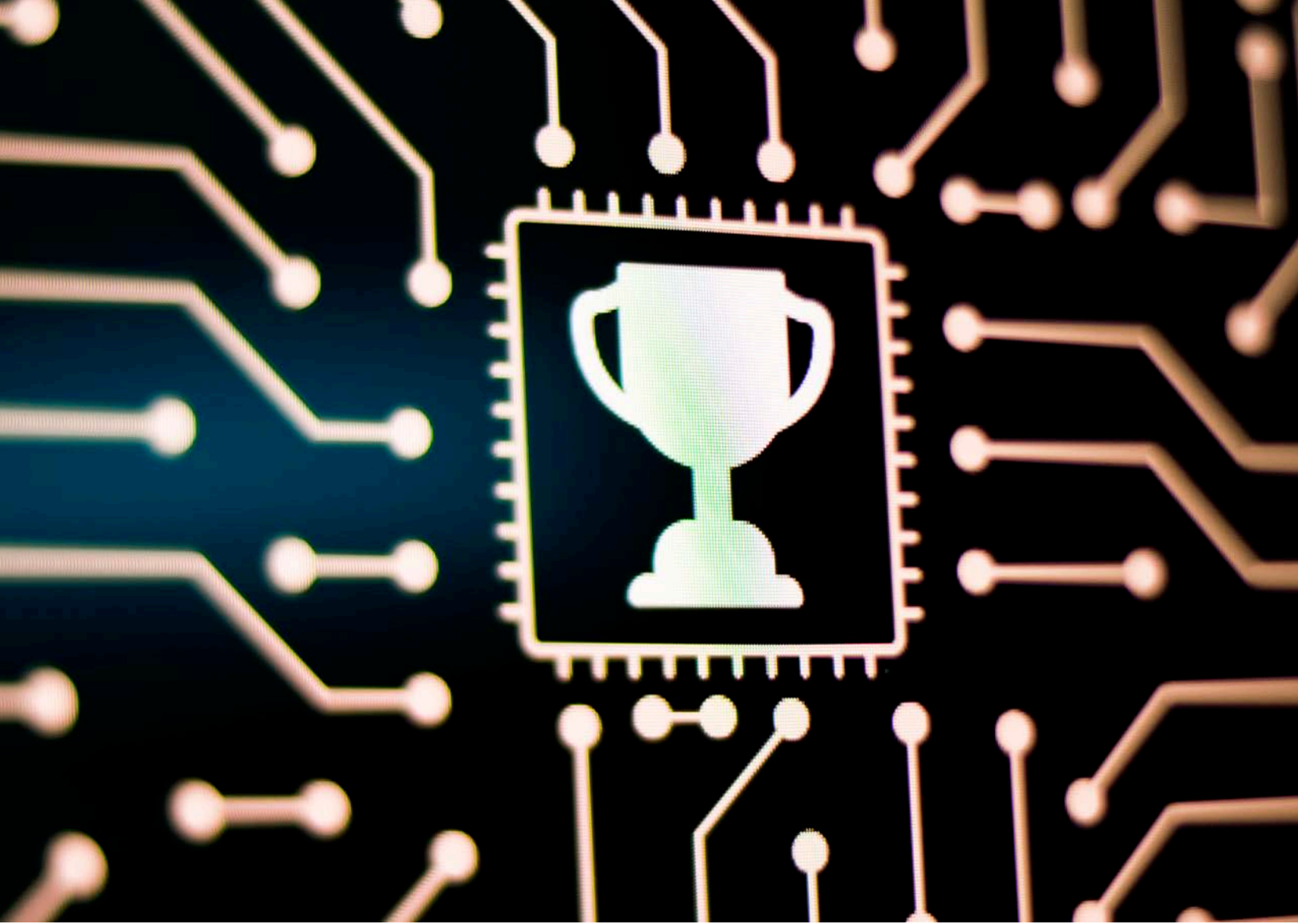
and physics and completed his doctorate at the College of William & Mary in 2022, authoring his dissertation, "Electronic transport in topological superconducting heterostructures."

#### JOSEFINE MCBRAYER – TRUMAN FELLOW

Josefine McBrayer will use her Truman Fellowship to improve performance in rechargeable lithium metal batteries. She received her doctorate in chemical engineering at the University of Utah. Her stopover at the University of New Mexico for a bachelor's in chemical engineering and a master's in nanoscience and microsystems engineering also met with academic success. As a master's student studying energy storage, she sought to improve the longevity of lithium-sulfur batteries. For her doctoral research, Josey developed techniques to determine how long a lithium-ion battery with a silicon anode maintains a charge while sitting idle. Determining how long a battery will work once it's off its charger and deployed in the field is critical to national defense.



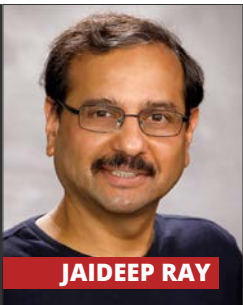
**JOSEFINE MCBRAYER**



## EARLY CAREER AWARDS AND HONORS

### DOE SC ADVANCED SCIENTIFIC COMPUTING RESEARCH AWARD

Sandia researcher **Jaideep Ray** leads one of only three DOE Office of Science Advanced Scientific Computing Research awards to support collaborative research to advance epidemiology frameworks and computational modeling. The three projects were selected by competitive peer review under the DOE Laboratory Announcement for “Advancing Computer Modeling and Epidemiology for Bio-preparedness and Response,” for an award totaling \$5M. Ray has been the lead PI on eight LDRDs.



**JAIDEEP RAY**

### ELSEVIER JOURNAL NUCLEAR MATERIALS AND ENERGY EARLY CAREER EDITORIAL BOARD

**Mary Alice Cusentino** joins the early career editorial board for the Elsevier Journal Nuclear Materials and Energy for a three-year term. Cusentino led two LDRDs in FY23 focused on modeling of materials in extreme environments.



**MARY ALICE CUSENTINO**

## PROFESSIONAL SCIENCE AND CONFERENCE AWARDS

### 2023 ASIAN AMERICAN ENGINEER OF THE YEAR



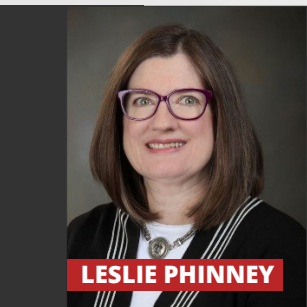
**Tian Ma**, a distinguished computer engineer in research and development at Sandia, has been honored as a 2023 Asian American Engineer of the Year (AAEOY) by the Chinese Institute of Engineers-USA. Each year, CIE recognizes exceptional

Asian American engineers who demonstrate strong technical skills, leadership abilities and a commitment to public service. Previous

recipients of this award include Nobel laureates and astronauts. His journey began in 2003 when he joined a Sandia Labs university fellowship program, ultimately earning engineering master's and doctorate degrees. The AAEOY award acknowledges Ma's significant contributions to remote-sensing systems, including related LDRDs, where his pioneering data processing algorithms play a pivotal role in detecting and tracking objects of interest critical to national security missions.

## SOCIETY OF WOMEN ENGINEERS AWARDS

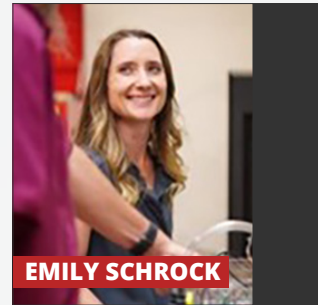
Sandia engineers [won 12 awards](#) at Society of Women Engineers (SWE) WE23 Conference.



**Leslie Phinney**, manager of Sandia's thermal sciences and engineering department, was awarded a 2023 Advocating Women in Engineering by the Society of Women Engineers (SWE). Phinney has served as a team member on numerous

engineering-science focused LDRDs. She arrived at Sandia in 2003 as an experimentalist qualitatively examining laser interactions and the heating of polycrystalline silicon microdevices and then worked on developing modeling and computations for improved diagnostic techniques to quantify the temperatures of the materials.

**Emily Schrock** was named a 2023 Distinguished New Engineer by SWE. Schrock is an electrical engineer conducting experimental lab work with various pulse-power systems. She performs modeling designs and diagnostics for both the systems and their components. Starting her career with Sandia in 2017, Emily has been the PI on two LDRDs.



**Laura Biederman, Suma Cardwell, Gabriella Dalton, Katharine Harrison, Nadine Miner, Stacy Nelson, Karla Reyes, Dorina Sava Gallis, Heidi Smartt, and Erika Vreeland** all received patent recognitions from SWE. Each of these women have led LDRDs or been part of an LDRD team.

## HENAAC SCIENTIST OF THE YEAR



Hispanic Engineer National Achievement Awards Conference (HENAAC) honored Sandia's [Sal Rodriguez](#) as Scientist of the Year at their national conference, one of the two highest awards. It's reserved for individuals who model excellence and leadership, making profound contributions to industries, STEM fields, communities, and the nation. Rodriguez's expertise spans computational fluid dynamics, advanced high-temperature refractory high-entropy alloys,

turbulence, aerodynamic drag reduction through surface modification, advanced manufacturing, swirl and heat transfer. Rodriguez has led and supported LDRD projects utilizing his expertise in design, safety and analysis of nuclear, non-nuclear and aerodynamic systems.

## SOCIETY OF ASIAN SCIENTISTS AND ENGINEERS

Sandia scientists **Patrick Feng** and **Thushara Gunda** recently were honored with national achievement awards by the Society of Asian Scientists and Engineers. The awards recognize recipients' leadership and accomplishments in STEM.

**Patrick Feng**, a materials scientist and a PI for five LDRD projects, received a Professional Achievement Award, 10-plus years, for his leadership in developing radiation-detection materials.



Systems research analyst **Thushara Gunda** has been PI on two LDRD projects, and she earned a Promising Professional Achievement Award, 2-10 years, for her advances in water security, energy resilience, and anticipatory science.



## HONORS AND DISTINCTIONS

**Weng Chow** was recognized in [Optics and Photonics News](#) for his work in 2022 towards understanding the fundamental quantum mechanical limits of semiconductor lasers. The article described a six-institute collaboration formed to investigate cavity quantum electrodynamics effects on the fundamental limits on intensity and frequency stability in semiconductor lasers. Sandia's work on this effort was funded by CINT user proposals and through an LDRD proposal led by PI Michael Gehl.

**Alexander Cerjan** was invited to serve on the [Physical Review A Editorial Board](#) and on the CLEO 2023 subcommittee: "[FS 5: Nonlinear Optics and Novel Phenomena](#)." Each term is three years and includes handling and reviewing abstract submissions, scheduling, and chairing the conference sessions. Cerjan also received the [APS Outstanding Referee Award](#), a lifetime award. He is currently leading two LDRDs.

**Frank DelRio** received the [2023 G. A. Brewer Award](#) from the Society for Experimental Mechanics in "recognition of outstanding achievements as a practicing experimentalist in the fields of nanomechanics and nanotribology." DelRio led an LDRD in 2021-2022.

**John Dallyn** received the [U.S. DOE Office of Science Graduate Student Research award](#) for his proposal that is synergistic with the Mesh-Oriented datABase (MOAB) program. Dallyn is currently a team member on an LDRD focused on the modulation of optomechanical interactions through acoustoelectrically enhanced Brillouin physics.

**Andy Castillo** won a Laboratory Residency Graduate Fellowship. Castillo is involved with an LDRD investigating SF6 Alternatives in spark gap switches for global warming potential reduction.

**Jason Larsen**, a Sandia intern, was awarded the [DOE Computational Science Graduate Fellowship](#). He is currently a team member on an LDRD focused on a quantum information science toolkit for the characterization and control of chemical dynamics.

**Sivasankaran Rajamanickam** received Outstanding Technical Paper Award for TenSQL: An SQL Database Built on GraphBLAS at the [IEEE High Performance Extreme Computing Virtual Conference](#). The award was given to five papers out of approximately 100 papers accepted to the conference. Rajamanickam has led two LDRD projects and been a team member on nine more.

**Umakant Mishra** was awarded the [JEJU Award 2022](#) by the International Union of Soil Science (IUSS). This is the mid-career award that IUSS gives once every four years. Mishra has led three LDRD projects and supported two others.

The "**Radio-Imaging Diagnostic for Critical Component Defect Detection**" LDRD team demonstrated a radio-imaging analysis method to image and detect discharge/breakdown in commercial capacitors and was awarded the NNSA's prestigious Defense Programs Award of Excellence for Technology Transfer.



*The DPAE winning team developed a radio-imaging analysis method to image and detect discharge/breakdown in commercial capacitors. From left, Julie Tilles and Ray Martinez. Not pictured, Paul G. Clem, Kirk Slenes, and Hap Stroller.*

## JOURNAL COVERS AND EDITOR'S PICKS

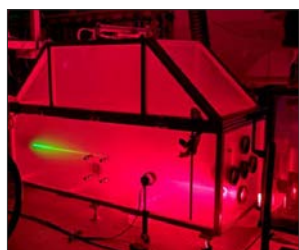


PI **Scott Bobbitt** and LDRD team members were recognized on the cover of



[Journal of Chemical & Engineering Data](#) for their article, “MOFX-DB: An online database of computational adsorption data for nanoporous materials.” Bobbitt

and another LDRD team were also featured on the cover of [Molecular Systems Design & Engineering](#) for their article, “Machine learning predictions of diffusion in bulk and confined ionic liquids using simple descriptors.”

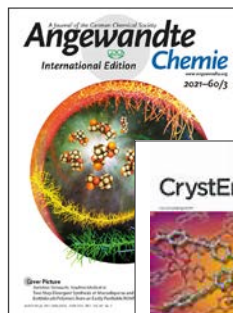


PI **Lekha Patel** and other LDRD team members, were recognized for their journal cover on “Influence of Sodium Chloride concentration on the optical scattering

properties of water-based aerosols” in [Applied Optics](#). Shown on the cover is Sandia’s tabletop fog chamber that acts as an optical test-bed capable of concurrent aerosol generation and characterization.



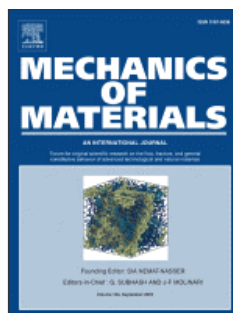
LDRD PI **Dorina F. Sava Gallis** and other team members had their article on “Encoding Multilayer Complexity in Anti-Counterfeiting Heterometallic MOF-Based Optical Tags” featured on the cover of [Angewandte Chemie](#).



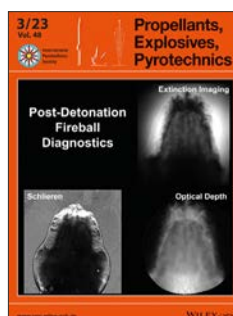
LDRD PI **Dorina F. Sava Gallis** and different team members also made the cover of [CrystEngComm](#) for their article on “Improved quantum yield in geometrically constrained tetraphenylethylene-based metal-organic frameworks.”



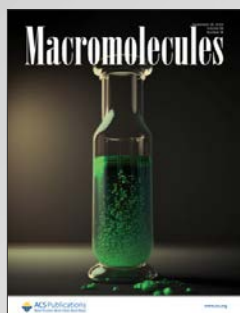
PI **Kevin Long** and the other LDRD team members published “Development of a Bench-Top Intermediate-Strain-Rate (ISR) Test Apparatus for Soft Materials,” and it was highlighted on the cover of the [Journal of Dynamic Behavior of Materials](#).



LDRD PI **Judith Brown** and other team members had their journal article on “Exploring pressure-dependent inelastic deformation and failure in bonded granular composites: An energetic materials perspective,” featured on the cover of [Mechanics of Materials](#).



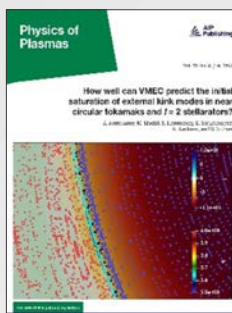
[Propellants, Explosives, Pyrotechnics](#) journal featured PI **Ashley J. Saltzman** and other team’s LDRD article on “Extinction imaging diagnostics for in situ quantification of soot within explosively generated fireballs.”



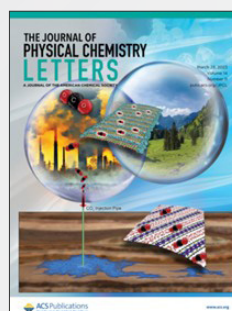
The article “Encapsulated Transition Metal Catalysts Enable Long-term Stability in Frontal Polymerization Resins” by current PI **Brad Jones**, previous PI **Samuel C. Leguizamon** and other LDRD team members was published on the cover of [Macromolecules](#).



PI **Philip James Noell** and other LDRD team members had their article “[Interlocking metasurfaces](#)” featured on the cover of [Journal of Materials Science](#).



The article “Improving Dynamic Collision Frequencies: Impacts on Dynamic Structure Factors and Stopping Powers in Warm Dense Matter” by PI **Stephanie B. Hansen** and other research team members was recognized as Editor’s Pick in [Physics of Plasmas](#). The work is partially funded out of LDRD.



LDRD PI **Tuan Anh Ho** and team members had their article, “Exploitation of Nanoconfinement-Enhanced Solubility and Fast Water Flow for Direct Air Capture of CO<sub>2</sub>” featured on the cover of [The Journal of Physical Chemistry Letters](#).

# ACKNOWLEDGMENTS

Thank you to the LDRD principal investigators and Investment Area leaders who contributed to this report.

## ANNUAL REPORT PRODUCTION

Amy Treece,  
*Report Project Manager*

Victoria Aranda, *Designer*

Jon Sanchez, *Designer*

Becky Cox, *Editor*

Vonceil Daniels, *Editor*

Stan Mathews, *Editor*

Sophia Horowitz, *Editor*

Laura Sowko, *Editor*

Krystal Romero-Martinez, *Editor*

Shelby Owens, *Editor*

## LDRD PROGRAM OFFICE

Wahid Hermina

Marie Arrowsmith

Dorean Chaleunphonh

Ladonna Martin

Jenni Pandazis

Nicole Seay

Amy Treece

Karla Weaver

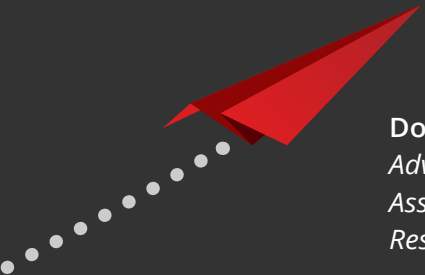
Nedra Bonal

Michael Hast

Ty DeGroff

Andy Nelson

## CHIEF RESEARCH OFFICE



Doug Kothe,  
*Advanced Science & Technology  
Associate Labs Director & Chief  
Research Officer*

Basil Hassan,  
*Deputy Chief  
Research Officer*

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