RESEARCH

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

FY22 ANNUAL REPORT

LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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.

SAND2023-00990R

FROM THE CHIEF RESEARCH OFFICER

The Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories is transformative. Every mission application of the future relies on the science and engineering teams of today for the innovative processes, technologies, and capabilities it will need to be actualized.

At its core, the LDRD Program is high risk, high reward. High risk means that researchers who didn't find the answer they were expecting still learned valuable insight that can guide upcoming discoveries. High reward indicates these experts found new ways to meet strategic priorities and help realize initiatives.

LDRD is also strategic. Much of the research aligns with the high-level problems covered on the news every day. It combats climate change, creates new supercomputing systems, fuels bioscience research, protects the country from terrorism, and discovers more efficient energy sources. For decades, scientists have tried to make reliable, high-performing lithium-metal batteries. The Customized Lithium Batteries for Mission Applications Grand Challenge LDRD project has made remarkable strides toward this goal. They identified a system electrolyte that achieves high energy density, designed printable separators that enable much better performance, and used additive manufacturing to print electrodes on complex geometries. These achievements, which grew from smaller experiments and scientific inquiries, will one day contribute to the construction of custom-form batteries for mission applications.

In 2022, LDRD helped to fuel other accomplishments from the identification of Arctic microbes that contribute to the rapidly melting permafrost, to a prototype of a cold-atom interferometer that helps vehicles stay on course where GPS is not available, to a new type of rotary electrical contact for next-generation large-scale wind turbines. Sandia is even investigating tiny ultra-porous crystals that could transform cancer treatments. It's the questions of today asked by scientists and engineers that lead to the answers our nation needs.

Sandia's LDRD program is also motivational. It encourages highly talented team members to innovate and grow as experts by coordinating with others on multi-disciplinary projects. It also is a proven technical talent pipeline recruitment tool as it allows bright minds at academic institutions to partner with national laboratories like Sandia on leading-edge research projects. This step into our laboratories encourages many other steps toward permanent employment or other collaborative endeavors.

It has been my honor to be the Chief Research Officer at Sandia. I am not only proud of Sandia's LDRD Program, but I am continuously inspired by what is achieved through it. It takes a spark of an idea to help achieve a long-term impact, and we see them every day.

Susan J. Seestrom, Ph. D.
Associate Laboratories Director & Chief Research Officer
Advanced Science and Technology

CONTENTS

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.

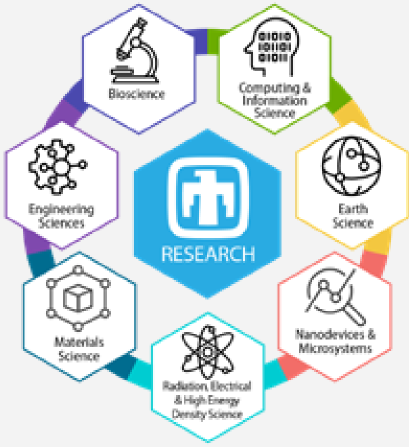
LDRD PROGRAM OBJECTIVES

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 (IA). 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.

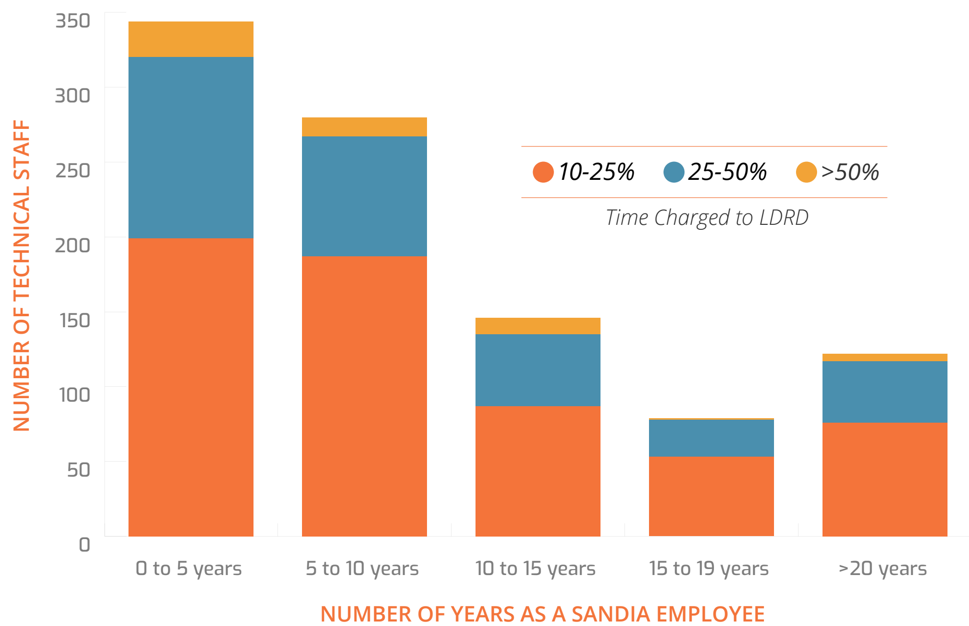
SI include Grand Challenge projects to solve major research challenges that require large multidisciplinary teams; Mission Campaign IAs to move ST&E intentionally from idea to mission impact; Exploratory Express to execute short-term projects of strategic importance; and New Ideas to pioneer fundamental R&D to discover game-changing breakthroughs. These initiatives also support strategic academic collaborations (120 in FY2022) and both the Harry S. Truman and Jill Hruby Postdoctoral Distinguished Fellowships.

LDRD PROGRAM VALUE

PERFORMANCE INDICATORS

While the FY22 LDRD program represented only about 5.1% 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 engaged in the LDRD program, thus validating LDRD's important role in attracting, developing, and retaining a world-class workforce to meet the most challenging national security needs.

$214.7M	$375K	522	290
Total Program Cost	Median Project Size	Total LDRD Projects	New Projects in 2022



46% OF SANDIA TOTAL	45% OF SANDIA TOTAL	26% OF SANDIA TOTAL	42% OF SANDIA TOTAL	43% OF SANDIA TOTAL	18% OF SANDIA TOTAL	50% OF SANDIA TOTAL
209	42	380	117	40	26	3
LDRD-Supported Postdocs	LDRD-Supported Postdoc to Staff Conversions	Refereed Publications	Technical Advances	Patents Issued	Copyrights	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 years) 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 five 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. In FY20, 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 KPIs 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 FY22, 13 out of the 15 staff promoted to Senior Scientist/Engineer were involved in the LDRD program as a PI or team member during their careers. Since FY11, 75% of Sandia's Top 2% have LDRD roots.

Sandia also reserves a special recognition for an elite group of individuals—Sandia Fellows—recognized for careers of significant technical accomplishment for the Labs and for the nation. In Sandia's history, only 15 individuals have held this title. In FY22, six of these Fellows were on staff, and all six had 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. The following Fellows' projects are featured in this year's report:

- Active Learning for Language Model Improvement (ALLM)—PI Emily Kemp
- Biomimetic calcification for carbon sequestration from seawater—PI Todd Lane
- Development and utilization of quantitative secondary electron imaging for the study of quantum computing materials—PI Suhas Kumar
- Experimental Quantum-Enabled Super-Resolution Imaging—PI Daniel Soh

LDRD AND TOP 2% TECHNICAL STAFF AT SANDIA NATIONAL LABORATORIES

	SINGLE YEARS			FIVE YEARS		TO DATE*
	FY20	FY21	FY22	FY11-15	FY16-20	FY11-22
TOTAL AWARDS	16	8	15	26	53	102
AWARDS WITH LDRD ROOTS	15	5	13	15	44	77
PERCENTAGE WITH LDRD ROOTS	93%	62%	86%	57%	83%	75%
AVERAGE YEARS FROM FIRST LDRD EXPERIENCE	18.8	15.2	19.5	9.9	17.8	16.2

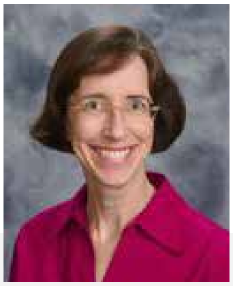
**Initial year to date: Each laboratory has chosen the appropriate lookback period that will ensure data integrity.*

NEWLY PROMOTED SENIOR SCIENTIST HIGHLIGHTS

DAVID P. ADAMS

David P. Adams joined Sandia as a postdoc in 1994, and is currently a member of Sandia's Material, Chemical, and Physical Sciences Center. He leads several teams involved with the research of thin film deposition processes, process-structure-property relationships and microfabrication, and has over 130 publications in these areas. In FY22, he was elected as Fellow of AVS Science & Technology of Materials, Interfaces and Processing (formerly referred to as the American Vacuum Society), and will serve as President of AVS in 2024. He has contributed to LDRD projects as a PI, team member, and mentor since 1998.

LAURA SWILER



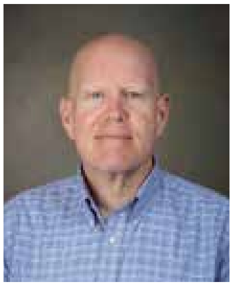
Laura Swiler has had a distinguished career at Sandia focused on developing and deploying uncertainty quantification (UQ) methods across many mission areas. Her research interests include uncertainty and sensitivity analysis of computational models, design of computer experiments, parameter calibration, adaptive sampling algorithms, Bayesian inference, and surrogate models. She has applied UQ methods to nuclear reactors, nuclear waste disposal, cyber, additive manufacturing, and climate. She led five LDRD projects and is currently a co-lead for the CLDERA Grand Challenge (CLimate impact: Determining Etiology thRough pAthways).

"I had an LDRD early in my career that resulted in two of my most cited publications, a patent, a lasting collaboration with another center, and follow-up funding from external sponsors. This LDRD had a profound influence on my career. Overall, LDRDs are essential to the Laboratories, allowing us to investigate and develop innovative, foundational capabilities that will support Sandia's technical expertise in the future. LDRDs allow one to collaborate broadly across Sandia mission areas and multiple centers and are an important vehicle for early career staff to explore and prove out new ideas."

TRAVIS BAUER

Travis Bauer has a PhD in computer science and cognitive science. He has extensive experience with text analysis algorithms. Additionally, Bauer founded and developed three text analysis frameworks at Sandia for applying text analysis algorithms to national security problems. He was the PI on six LDRD projects, and a key contributor on numerous others. Read more about Travis' work applying algorithms and compression data techniques early in the coronavirus pandemic to identify, arrange, and code relevant studies to help researchers ascertain key trends.

TODD JONES



Todd Jones is a longtime computer science researcher with experience in adversarial software risk, system assessment, modeling and simulation, data analysis, and security and intelligence policy. His research focuses on computing and security in adversarial environments. From 2011 to 2013, he served as a science and technology advisor to the Permanent Select Committee on Intelligence in the U.S. House of Representatives. He has led two LDRD projects and contributed as a key team member to nine others. He is currently PI of the RAMSeS portfolio of projects.

ERIC VUGRIN

Eric Vugrin is a mathematician, specializing in optimal control, and recognized as one of Sandia's leading experts in the development of resilience analysis and design methods. He has led the research and development of formal resilience analysis techniques for more than a decade. He was the PI for five resilience-related LDRD projects, led numerous projects for the Department of Defense (DOD), Department of Homeland Security (DHS), and DOE resilience programs, and co-authored the book *Critical Infrastructure System Security and Resilience*.

"From a technical perspective, the LDRD program has broadened my mindset to be more forward-thinking, to take more risks, and to get in the habit of continuously developing new research ideas. It has also helped expand my professional network."

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 each site 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 140 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, 54% of Sandia's R&D 100 winning contributions have been rooted in LDRD; over the past 17 years, over 68% 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*
	FY20	FY21	FY22	FY11-15	FY16-20	FY06-22
TOTAL AWARDS	7	9	6	20	32	88
AWARDS WITH LDRD ROOTS	4	5	3	15	22	60
PERCENTAGE WITH LDRD ROOTS	57%	56%	50%	75%	69%	68%
AVERAGE YEARS FROM FIRST LDRD EXPERIENCE	8	4.6	4.3	5	5.6	5

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

R&D 100 HIGHLIGHT: CATEGORY MECHANICAL/MATERIALS

Ultra-Stable Thermally Excellent Advancements in Material Strength (USTEAMS)

Guangping Xu, right, with his team of Sandia researchers, from left, Hongyou Fan, Haley Davis, Chad McCoy, Jens Schwarz, and Melissa Mills, won an R&D 100 award for Ultra-Stable Thermally Excellent Advancements in Material Strength. (Photo courtesy of Guangping Xu)

Originating out of a three-year LDRD project that started in 2021, as part of the Assured Survivability and Agility with Pulsed Power (ASAP) Mission Campaign, Guanping Xu and his team developed a technique to synthesize composite coatings using a combination of silica and sugar. When common confectioners' sugar is burned to a state called carbon black, interspersed between layers of silica, and baked, the resulting material coating can protect materials in hostile environments, exhibiting high thermal stability up to 1650°C. The coatings, which resemble the structural layering of a seashell, also have strong mechanical properties (hardness of more than 11 GPa), making them ideal as shielding in the form of mechanical barriers, body armor, and space debris shields.

Described in a recent article in *MRS Advances*, the work was done in anticipation of the increased shielding that will be needed to protect test objects, diagnostics, and drivers inside the more powerful pulsed power machines of the future. Sandia's pulsed-power Z machine—currently the most powerful producer of X-rays on Earth—and its successors will certainly require still greater debris protection against forces that could compare to numerous sticks of dynamite exploding at close range.

The new shielding should favorably impact our nuclear survivability mission," said paper co-author and Sandia physicist Chad McCoy. "Z is the brightest X-ray source in the world, but the amount of X-rays is only a couple percent of the total energy released. The rest is shock and debris. When we try to understand how matter—such as metals and polymers—interacts with X-rays, we want to know if debris is damaging our samples, has changed its microstructure. Right now, we're at the limit where we can protect sample materials from unwanted insults, but more powerful testing machines will require better shielding, and this new technology may enable appropriate protection."

Physicist Chad McCoy at Sandia's Z machine loads sample coatings into holders. When Z fires, researchers will observe how well particular coatings protect objects stacked behind them. (Photo by Bret Latter)

According to Xu, the material cost to fabricate a 2-inch diameter coating of the new protective material, 45 millionths of a meter and microns thick, is only 25 cents. In contrast, a beryllium wafer—the closest match to the thermal and mechanical properties of the new coating, and in use at Sandia's Z machine and other fusion locations as protective shields—costs $700 at recent market prices for a 1-inch square, 23-micron-thick wafer, which is 3,800 times more expensive than the new film of same area and thickness.

Read more about this unique bio-inspired research here.

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

Since 2011, 82 individuals have been elected fellow to at least one professional society (seven individuals hold appointments from multiple societies), and 82% of fellows had LDRD experience during their Sandia careers.

2022 Awardee Highlights

DAVID P. ADAMS

LDRD PI and newly promoted Senior Scientist David Adams was elected as a Fellow of AVS: Science & Technology of Materials, Interfaces and Processing. Additionally, Adams was elected to be President of AVS, serving as President-elect in 2023 and President in 2024. Adams has served as PI on 47 LDRD projects during his career at Sandia and is internationally known for his technical creativity and contributions to fundamental material science. In FY22, he led three LDRD projects: Reduction/Oxidation Switch Enablement Technology (Nuclear Deterrence), Understanding the Effects of Radiation on Reconfigurable, Phase Change Materials (Materials Science with Purdue University and University of Florida), and Novel Energy Sensor (National Security Programs).

DAVID G. MOORE

David G. Moore was nominated and accepted into the Academia Nondestructive Testing (NDT) International Society during its 13th General Assembly Meeting. The society, with 72 worldwide full members, is focused on promoting science, conducting research, developing new diagnostic tools, and encouraging the application of findings in the field of NDT. Moore has been a key team member on numerous LDRD projects since 2017, focusing on developing technologies to optimize gas transfer system designs, identifying hard-to-find flaws in additively manufactured components, and developing new approaches to the design of damage tolerant structures.

"I have found that working on LDRDs during my career has allowed me to think bigger picture and study problems at a deeper level. It has also given me the skills to present at conferences and write journal papers with staff members and students."

BO SONG

Bo Song, recently recognized as a 2020 Asian American Engineer of the Year by the DiscoverE Engineering Program, has been designated a Society for Experimental Mechanics Fellow as recognition "for his cutting-edge research in Dynamic Behavior of Materials...[who] has established himself as a well-recognized leader of the Experimental Mechanics community." Song has contributed to numerous LDRD projects since 2014, focusing on characterizing additively manufactured materials under loading conditions, developing novel barrier coatings, and designing next generation physical protection systems for asset transportation.

(Photo by Lonnie Anderson)

"LDRD has helped me build multidisciplinary knowledge and connections. I like to see "crazy" LDRD ideas because I believe they will become real and a foundation in the future. The LDRD program is a great investment for tomorrow."

American Physical Society

The NNSA laboratories consider American Physical Society (APS) Fellowships as the exemplar award because physicists naturally link with NNSA's core stockpile stewardship mission, and APS Fellowship is awarded based on scientific merit and impact over an extended period of time.

SHORT-TERM METRICS

Intellectual Property

PATENTS

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

	FY18	FY19	FY20	FY21	FY22
SANDIA PATENTS	148	159	131	120	92
LDRD SUPPORTED	76	76	67	63	40
% DUE TO LDRD	51%	48%	51%	53%	43%

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.

	FY18	FY19	FY20	FY21	FY22
SANDIA COPYRIGHTS	98	97	151	170	146
LDRD SUPPORTED	13	18	40	34	26
% DUE TO LDRD	13%	19%	26%	20%	18%

Corrections to FY18-FY21 based on revised attribution methodology. Minor changes to percentage of LDRD contribution.

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).

	FY18	FY19	FY20	FY21	FY22
SANDIA DISCLOSURES	260	252	299	295	280
LDRD SUPPORTED	112	102	111	128	117
% DUE TO LDRD	13%	40%	37%	40%	42%

Corrections to FY20 and FY21 based on revised attribution methodology. Did not change percentage of LDRD contribution.

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

As a premier engineering and science laboratory, Sandia produces relatively fewer APS fellows when compared to the NNSA physics laboratories. Since 2011, over 81% of Sandia's 22 APS fellows have had LDRD experience.

Peer-reviewed Publications

PUBLICATIONS

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

	FY18	FY19	FY20	FY21	FY22
SANDIA PUBLICATIONS	1170	1399	1299	1493	1456
LDRD SUPPORTED	363	366	343	379	380
% DUE TO LDRD	31%	26%	26%	25%	26%

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.

	FY18	FY19	FY20	FY21	FY22
GRAD STUDENTS	82	106	127	139	147
UNDERGRAD STUDENTS	104	115	100	84	110
SANDIA R&D STUDENTS	614	733	722	711	841
% DUE TO LDRD	30%	30%	31%	31%	31%

POSTDOCTORAL RESEARCHER SUPPORT

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

	FY18	FY19	FY20	FY21	FY22
SANDIA POSTDOCS	302	388	350	428	459
LDRD SUPPORTED >10%	133	148	163	196	209
% DUE TO LDRD	44%	38%	46%	46%	46%

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.

	FY18	FY19	FY20	FY21	FY22
SANDIA CONVERSIONS	53	68	47	61	94
LDRD SUPPORTED >10%	25	34	25	32	42
% DUE TO LDRD	47%	50%	53%	52%	45%

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

LDRD IMPACT STORY

LDRD-DEVELOPED CRITICAL SYSTEM CYBERSECURITY TECHNOLOGIES HELP GOVERNMENT AGENCIES ENSURE THEY ARE BETTER PROTECTED.

Protecting systems, from a personal computer to the power grid, relies on developing and deploying robust cybersecurity technologies that can respond in the event of an attack. Since the early 2000s, Sandia's LDRD program has invested in developing such technologies for national security applications, grid security, and homeland security; 10% of Sandia's R&D 100 awards in the past ten years went to innovative cyber technologies stemming from LDRD. The investments also enhanced Sandia's reputation as a trusted partner in helping government agencies improve their cyber protections. Three examples of LDRD-enabled cyber capabilities are described below.

WeaselBoard enables cyber-physical security for DOD assets. The nation's critical infrastructures (i.e., electrical power plants and oil refineries) use control systems that are vulnerable to targeted attacks that can injure people and cost millions in equipment damage and lost operations. The WeaselBoard, the result of a two-year LDRD project ending in 2013, is a small card that connects into the backplane of an industrial controller, referred to as a Programmable Logic Controller (PLC), that captures traffic between modules and alerts operators to unusual PLC behavior before damage occurs.

In 2021, the team completed production readiness reviews for multiple hardware security devices destined for DOD assets. Through a collaborative effort with Kansas City National Security Campus, the team was able to successfully transition this LDRD-funded work, enabling enhanced trust of cyber-physical security devices that will eventually be installed on DOD assets. Read more about how WeaselBoard works.

National Cyber Range leverages Emulytics expertise. A portmanteau of emulation and analytics, Emulytics (28 LDRD projects over 15 years) focuses on the science of modeling, simulating, instrumenting, and analyzing variable-scale networks with dependencies on networked systems. Sandia's Emulytics™ program is focused on understanding the behavior of complex, distributed cyber systems. Sandia has developed and deployed a suite of cyber emulation, modeling, and analysis tools that support predictive simulation, training, test and evaluation, resilient system design, and more. The tools and expertise developed at Sandia have helped improve the National Cyber Range, delivering prototypes that make cyber-range environments more realistic. A component of the Emulytics package, minimega, is now available for faculty and students of Purdue (part of Sandia's University Partnerships Network) to advance cybersecurity research in discovering security threats in a variety of systems and developing new safeguards.

SECURE Grand Challenge facilitates risk metrics for Chemical Facility Anti-Terrorism Facilities. The Science and Engineering of Cybersecurity by Uncertainty Quantification and Rigorous Experimentation (SECURE) Grand Challenge LDRD (2019-2021) developed a foundation for cyber modeling and experimentation that catalyzes the use of quantitative metrics and analytical evidence to inform high-consequence national security decisions. Tools developed from the Grand Challenge are being leveraged to develop aggregated risk metrics across the population of Chemical Facility Anti-Terrorism Standards (CFATS) regulated facilities (DHS), which will help assess the impact of the CFATS program. The Sandia Cyber Institute for Rigorous Experimentation (SCIRE) is an outgrowth of the SECURE Grand Challenge, aiming to transform how the national security community approaches cybersecurity. Read more about SCIRE here.

Recent R&D 100 awards associated with LDRD investments in cybersecurity

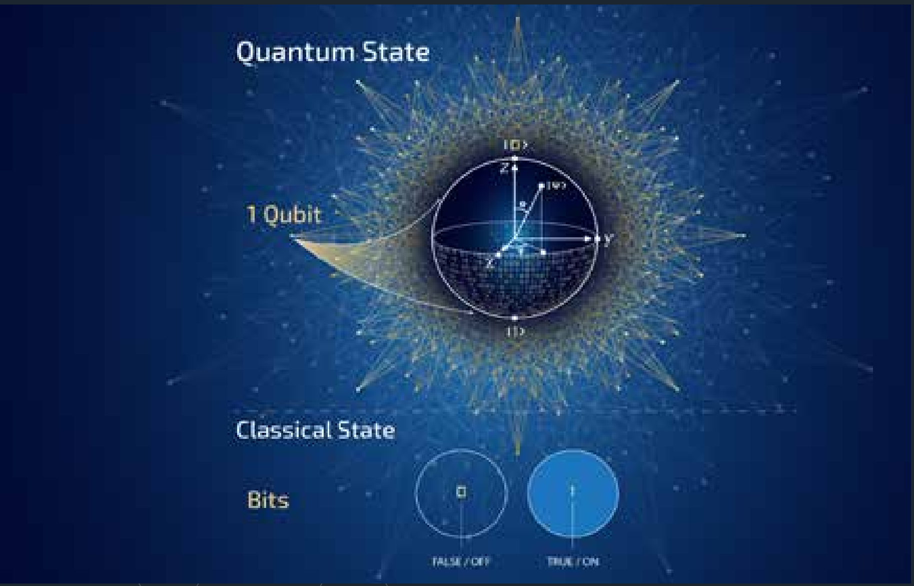
- **2015** — INTEGRATED CIRCUIT IDENTIFICATION
- **2016** — T-QUAKE (TRANSCEIVER FOR QUANTUM KEYS AND ENCRYPTION)
- **2017** — HADES: THE HIGH-FIDELITY ADAPTIVE DECEPTION & EMULATION SYSTEM
- **2019** — CHIRP: CLOUD HYPERVISOR-FORENSICS AND INCIDENT RESPONSE PLATFORM
- **2020** — HECATE: THE HIGH-ENERGY DENSITY EVALUATOR OF COTS APPLICATIONS FOR TRUST & EFFICACY
- **2022** — AUTOMATED THREAT ESTIMATOR FOR NETWORKS AND APPLICATIONS

A team member puts the WeaselBoard through its paces on a test apparatus.

LDRD IMPACT STORY

LDRD-ENABLED QUANTUM RESEARCH PUSHING S&T FRONTIERS, BENEFITTING MULTIPLE MISSIONS.

Sandia built a world-leading program in quantum information science (QIS) with aggressive and targeted LDRD investments. The current program supports many different applications (computing, sensing, communications, and networking), platforms (silicon, trapped ions, trapped atoms, diamond defects), and is supported by the DOE Office of Science, NNSA, Intelligence Advanced Research Projects Activity (IARPA), Defense Advanced Research Projects Agency, and other government agencies.



Quantum bits of information, or qubits, have the potential to make powerful calculations that classical bits can't make. (Image by Michael Vittitow)

Four Grand Challenge LDRD investments were pivotal in enabling existing quantum information science capabilities: **Quantum Information Science and Technology** (2008-2010) focused on developing silicon quantum dots and architectures; **Adiabatic Quantum Architectures** in Ultracold Systems (2011-2013) developed adiabatic architectures, advanced lithography, and neutral atom computing; **Sandia Enabled Communications and Authentication Network using Quantum Key Distribution** (2014-2016) focused on quantum key distribution on a chip; and **Strategic Inertial Guidance with Matterwaves** (2018-2020) advanced capabilities in quantum positional sensing.

This work has been augmented by investments made by other government agencies, most notably IARPA, which funded the Ion Trap Foundry that uses Sandia's Microsystems Engineering, Science and Applications (MESA) facilities to fabricate ion traps for quantum computing applications that are distributed worldwide.

Smaller LDRD investments have also made big impacts in pushing the frontiers of what is possible. For example, the **Quantum Optimization and Approximation Algorithms** project (funded by the Computing and Information Systems Investment Area, 2016-2018) developed some of the first rigorous quantum advantages for approximating discrete optimization problems, producing new quantum approximation algorithms for the well-known Maximum Cut problem. The work has resulted in external investments through high-exposure multi-institutional projects and gone on to revitalize the field of quantum approximation algorithms, resulting in several high-profile Sandia-led publications. **A New Approach to Entangling Neutral Atoms** (Nanodevices and Microsystems Investment Area, 2014-2016) demonstrated advanced neutral-atom quantum computing/

Quantum physicist Tim Proctor is a recent recipient of a DOE Early Career Research Award. Read more about him here.

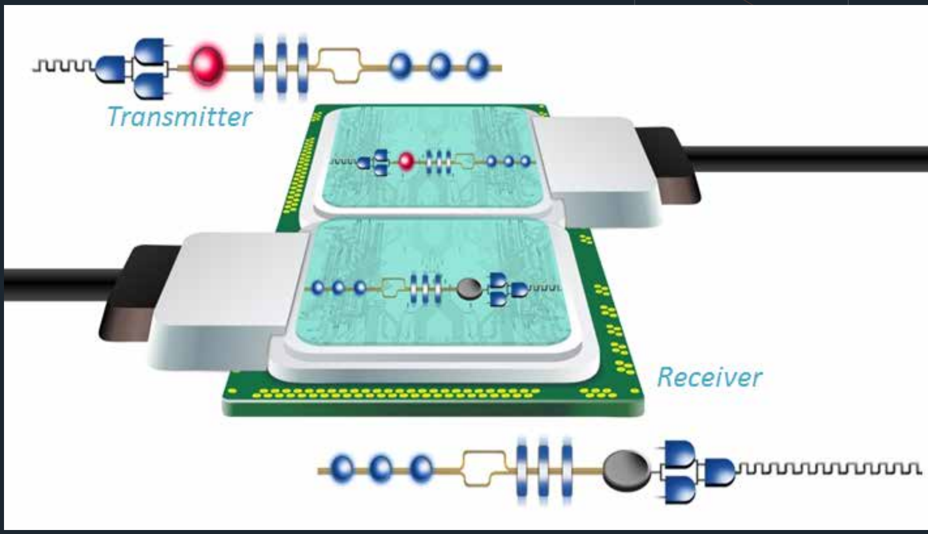
Andy Mounce makes microscopic sensors to try to understand quantum materials. He is also a recent recipient of a DOE Early Career Research Award. Read more about him here.

quantum sensing results based on Rydberg-dressed interaction and initiated a new neutral-atom research area. The LDRD contributed to seven new research projects at Sandia, and partnership in the NSF Quantum Leap Challenge Institute program (Q-SEnSe). The project demonstrated the highest fidelity of two-qubit entangling until the new record was published in 2019 by Harvard University.

While historical LDRD investments helped shape Sandia's quantum landscape, current LDRD research promises to keep Sandia at the forefront of the discipline. Two LDRD PIs were recently awarded DOE's Early Career Research Award. Tim Proctor, a quantum physicist at Sandia, is currently leading an LDRD project to create the scientific foundations for scalable testing of quantum computers, by applying sophisticated and efficient data science techniques to quantum computing data. Since joining Sandia six years ago, Proctor has worked in the Quantum Performance Lab, a research group that develops and deploys cutting-edge techniques for assessing quantum computers. The Early Career Research Award will allow him to build his own team, and he's excited to onboard and mentor other early career scientists. Andy Mounce, another recipient of a DOE Early Career Research Award, specializes in making microscopic sensors to try to understand the nature of quantum materials and their electrons' behavior. He recently completed an LDRD project focused on establishing the technological foundation for a new class of solid-state, quantum light emitters in III-nitride semiconductors. With his DOE Early Career Award, Mounce hopes to understand the topological phase transitions of quantum materials

"With these new capabilities and discoveries, the sky is the limit."

by leveraging diamond quantum sensors. "After the project is over, we're going to have new techniques to make quantum sensors and new capabilities to use quantum sensors," he said. "We're also going to have new discoveries of how quantum materials work as seen by those quantum sensors. With these new capabilities and discoveries, the sky is the limit."



Chip-scale transceiver concept demonstrated in the Sandia Enabled Communications and Authentication Network using Quantum Key Distribution Grand Challenge.

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 the accomplishments below have a higher TRL and could impact Sandia's mission work more quickly.

Unless otherwise noted, these highlights are for projects that ended in FY22.

ADDITIVE MANUFACTURING OF MAGNETICALLY INSULATED TRANSMISSION LINES.

A novel hybrid metalized polymer core (HMPC) concept was investigated for its limitations/ capabilities and efficacy. A notional process was developed, and up/down stream (with respect to the experimental region) hardware was designed, manufactured, and tested. Ultimately, four unique pieces of power flow hardware were manufactured with this technique with skin thicknesses between 200 µm to 1 mm. Results indicate no obvious power flow differences given an apples-to-apples comparison to like-kind shot conditions and hardware topology. Further, the team's HMPC hardware has propagated > 400 kV at > 600 kA, all while maintaining an ~ 3X reduction in overall mass. The Sandia team's HMPC shot hardware works as intended and, with further development, is believed to be a viable candidate for next-generation pulsed-power debris mitigation among other applications. (PI: Charles Edgar Rose)

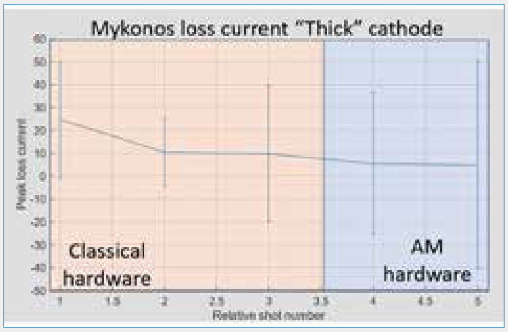


Figure 1: Series 3 shot loss data showing little to no obvious current perturbation. This data is for the thick Laser Powder Bed Fusion (LPBF) variant.

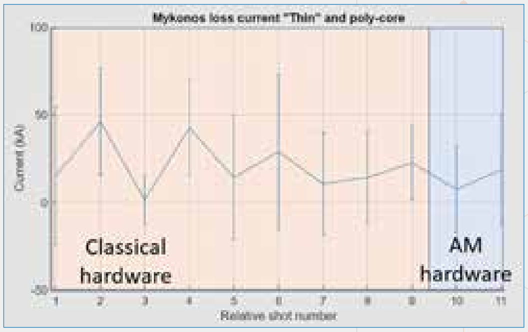


Figure 2: Series D shot loss data showing little to no obvious perturbation. Note: Shot 10 was the thin LPBF variant (no internal polymer) and 11 was the HMPC variant.

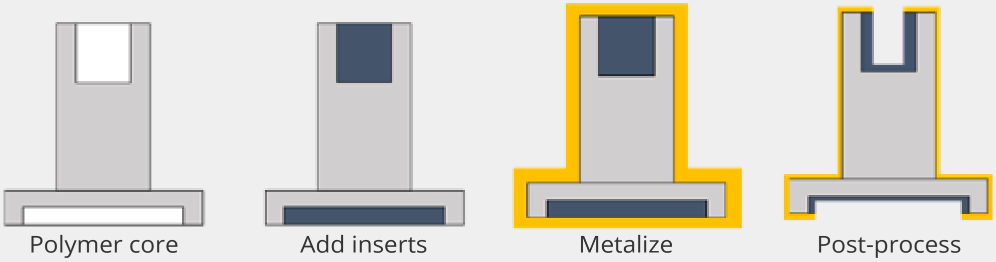


Figure 3: Notional HMPC manufacturing process.

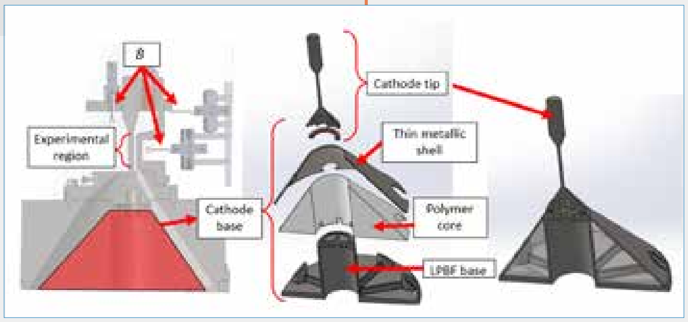


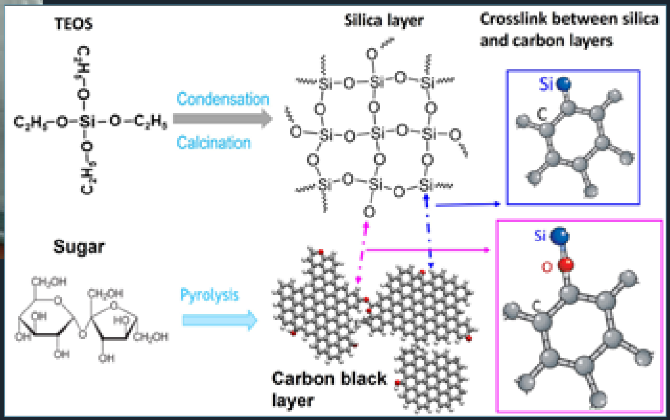
Figure 4: Notational design highlights of up-stream cathode base.

DOE SIMULATORS BENEFIT FROM DEVELOPMENT OF SELF-BREAK, HIGH-PRESSURE AIR

One of the highest priorities for DOE simulators is to upgrade their reliability and repeatability. This requires accurate and predictive models of high-energy and high-density environments. To create these environments, a new paradigm of power flow equipment and manufacture is necessary. Sandia researchers are investigating ways additive manufacturing can create designs that are quicker to load, less expensive to fabricate, and optimized to reduce post shot debris and damage. To that end, PEEK and ULTEM advanced commercial polymer materials were evaluated concurrently for possible use with the high-pressure housings, and computer numerical controlled machining techniques were investigated to help fabricate reliable multimegavolt switches. This operation,

SELF-ASSEMBLED SEASHELL-LIKE COATINGS CAN ACT AS LARGE AREA ROBUST DEBRIS SHIELDS FOR NEXT-GENERATION PULSED POWER DRIVERS.

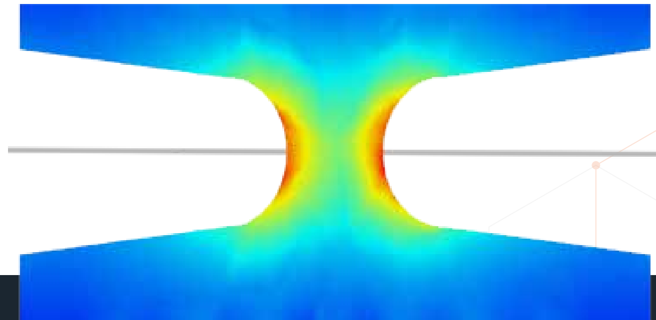
New shield materials with exceptional mechanical properties are needed for next-generation pulsed power capability but are not readily available. Current shield materials involve the use of lithium and beryllium, which cause major concerns for post-recovery cleaning and environmental, safety, and health practices. A coating technology was developed to synthesize composite coatings using silica and sugar-derived carbon, which mimic the natural seashell laminate structures. These coatings exhibited high thermal stability up to 1,650°C and exceeded the hardness of Spectra® by ~44%. The initial tests on the Z machine ride-along showed promising results with coatings outperforming uncoated substrate. This composite material can be used in numerous applications in mechanical and thermal protections. For example, it can be used in the pulse power facility to protect diagnostic equipment and to protect satellites from micro-meteoroid and orbital debris impact. This technology won a 2022 R&D 100 Award in the Mechanical/Materials category (for the Ultra-Stable Thermally Excellent Advancement in Material Strength technique) and was published in *MRS Advances* in 2022. (PI: Guangping Xu)



(Above) Sandia researcher Guangping Xu uses a digital optical microscope to examine the synthesized composite coating, and (right) the coating technology used to synthesize composite coatings using silica and sugar-derived carbon. (Photo by Bret Latter)

R-INSULATED 3 MV SWITCHES.

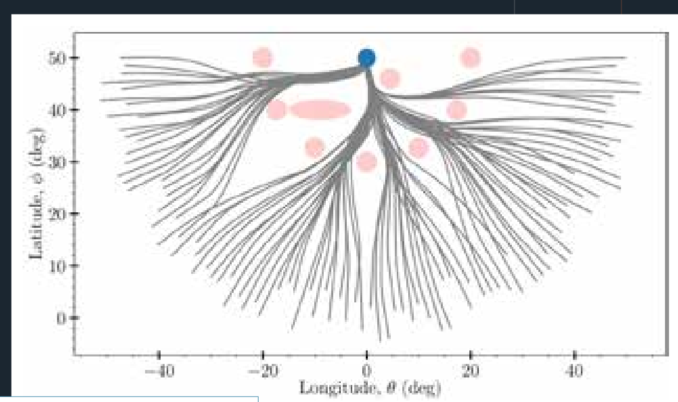
done in subscale with 800 kV switches using high-pressure air, has generated data for a 3 MV switch. This advance in materials and an understanding of the high-pressure physics has led to the potential for building compact 3 MV or greater switches. (PI: Randy Curry)

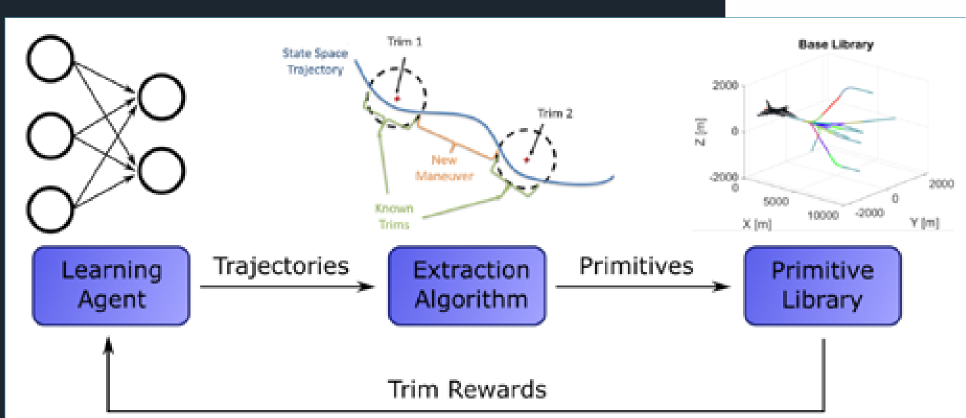


Electromagnetic field plot of enhanced electrodes used to evaluate the Paschen Curve of a subscale high- pressure switch operating at over 30 atmospheres of air.

REAL-TIME EVASIVE MANEUVERS IN CONTESTED, UNCERTAIN ENVIRONMENTS.

This research is concerned with real-time evasive maneuvering in contested, uncertain environments. New algorithms for real-time guidance were developed by leveraging recent advances in Deep Reinforcement Learning. Central thrusts involved: (1) developing high-level action spaces, and (2) concatenating high-level actions (e.g., motion primitives) into feasible, evasive trajectories with Deep Reinforcement Learning and robotics planning algorithms. The methods developed in this project produce trajectories which are feasible, that is, trajectories which do not violate vehicle capabilities and other physical system limits (e.g., heating), and can execute on board the vehicle in real-time. This approach significantly deviates from existing approaches of tracking a trajectory generated offline. Several academic collaborations were instrumental in this effort, including professors and graduate students from Sandia Alliance partners Georgia Tech and Purdue, and George Mason University. This work led to two journal publications, one in the *IEEE Transactions on Aerospace and Electronic Systems Journal* and the other in the *Journal of Aerospace Information Systems* in 2022. (PI: Kyle Williams)





(Top) Real-time evasive maneuvering, and (left) the new algorithm pipeline for real-time guidance.

HYPERSONIC WIND TUNNEL TEST BED FOR FAULT-TOLERANT AND ADAPTIVE CONTROL.

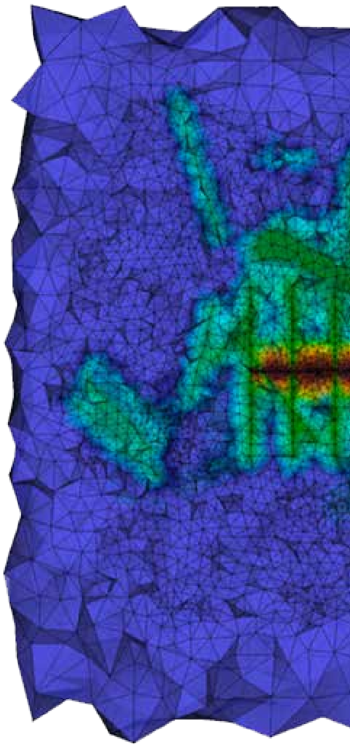
Current hypersonic ground aerodynamics testing is conducted in a static manner. This does not enable study of control system performance or determination of dynamic vehicle behaviors and requires numerous static runs to model the vehicle aerodynamics. To better quantify a dynamic vehicle's performance, a dynamic control testbed was developed in Sandia's Hypersonic Wind Tunnel at Mach 8. Models are flown in the tunnel for 30 seconds using different aerodynamic control algorithms. These models have 360 degrees of roll freedom and +/- 5 degrees of pitch and yaw freedom. Trajectories can be simulated by varying the dynamic pressure and by supplementing the total angle of attack with the wind-tunnel static pitching hardware.

Critical to this effort was an academic collaboration with Professor Anirban Mazumdar and his three graduate students from Sandia Alliance partner Georgia Tech. This work has resulted in a Technical Advance and a filed patent. Follow-on funding is being sought to transition the dynamic test capability to other ground test facilities. To date, four invited presentations have been given demonstrating the applicability of this work, including meetings of the National Hypersonic Stakeholders and the American Institute of Aeronautics and Astronautics Defense Conference. A publication documenting this capability is published in the *Journal of DOD Research and Engineering*. (PI: Katya Casper)

PHYSICALLY RIGOROUS REDUCED-ORDER FLOW MODELS OF FRACTURED SUBSURFACE ENVIRONMENTS WITHOUT EXPLOSIVE COMPUTATIONAL COST

Simulations in fractured media with high geologic realism are needed for both predictions of future geophysical and hydrogeological behaviors, and uncertainty quantifications in many energy and national security-related engineering problems. This Sandia LDRD team developed six new computational capabilities to model multiple physics, including diffusion, transport, and induced polarization in large-scale geologic environments that possess geometrically complex fractures and man-made infrastructure without computational burden, by utilizing the recent developments in the finite element analysis of electromagnetics that allow for the representation of material properties on a hierarchical geometry (Hi-FEM). The team also developed a capability for wellbore integrity monitoring with geo-electric measurements by using the concept of hierarchical material properties. These individual capabilities form a multi-physics simulation tool for complex geologic and engineered environments that can model different physical behaviors by employing a single 3D computational mesh.

Fast, high-fidelity multi-physics Hi-FEM modeling uncovers future opportunities for real-time analysis, inverse problems, uncertainty quantification, and the creation of massive, richly textured training sets for machine learning (ML) applications. This project has generated three publications, including being featured on the cover of *The Leading Edge*. (PI: G. Didem Beskardes)



Simulation of flow diffusion in a fractured porous medium with embedded complex fractures.

PREDICTING INDIVIDUAL DIFFERENCES IN COGNITION USING ADVANCED STATISTICS.

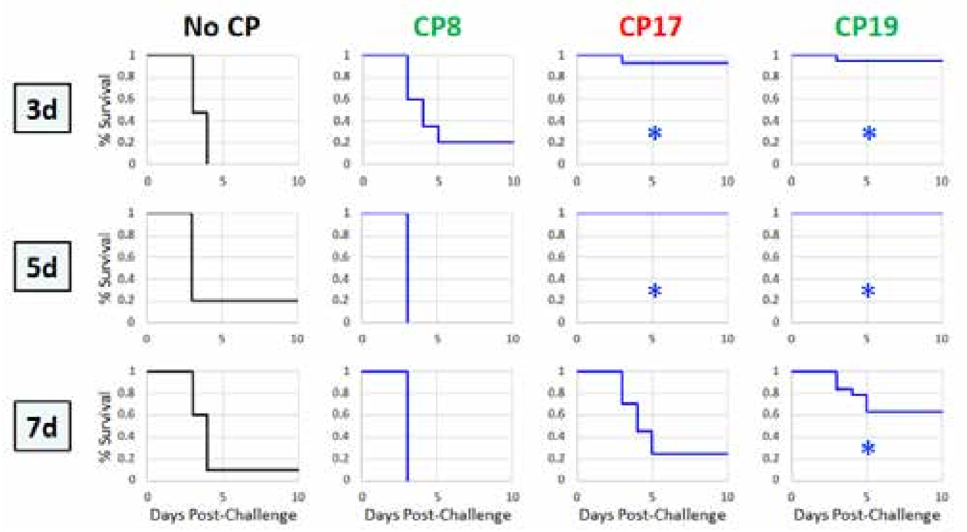
The interdisciplinary research in the MIDAS: Modeling Individual Differences using Advanced Statistics project explored novel methods for extracting relevant information from EEG data to characterize individual differences in cognitive processing. By using cognitive science expertise to interpret results and inform algorithm development, the LDRD team developed a generalizable and interpretable ML method to accurately predict individual differences in cognition. The output of the ML revealed surprising features of the EEG data that, when interpreted by the cognitive science experts, provided novel insights to the underlying cognitive task.

Additionally, the outputs of the statistical methods show promise as a principled approach to quickly find regions within the EEG data where individual differences lie, thereby supporting cognitive science analysis and informing ML models. This work laid methodological groundwork for applying the large body of cognitive science literature on individual differences to high-consequence mission applications. An invited talk, "The Efficacy of Different Tasks for Modeling Individual Differences in Bilingual Language Proficiency," was given on the project at the 62^{nd} Annual Meeting of the Psychonomic Society. (PI: Kyra Wisniewski)

Sandia researchers wore caps like this one outfitted with EEG sensors while participating in an experiment that measures brain activity.

RECONFIGURING THE RESPIRATORY TRACT MICROBIOME TO PREVENT AND TREAT INFECTIOUS DISEASE.

Burkholderia pseudomallei, a bacterial respiratory pathogen that is intrinsically resistant to many antibiotics, is the causative agent of the infectious disease melioidosis, which has an estimated case fatality rate of approximately 35%. This LDRD sought to reconfigure the airway microbiome to enhance defense against respiratory pathogens like B. pseudomallei. Bacteria were recovered from the mouse airway, propagated in culture, and then re-introduced into the airway. Eight isolates, candidate probiotics (CP), consistently re-colonized the airway. Genome sequencing revealed that the six best colonizers are Bacillus strains. Both colonizing and non-colonizing Bacillus CPs were assessed for ability to mitigate respiratory infection caused by B. thailandensis, a surrogate for B. pseudomallei. The top-performing CP (a colonizer) robustly protected mice against otherwise lethal infection when administered as early as seven days prior to pathogen challenge. This successful proof of concept for airway probiotics uniquely positions Sandia and collaborators at Lawrence Livermore National Laboratory, and Alliance partners Georgia Tech and University of California Berkeley, to pursue translation to clinical and veterinary use, as well as development of engineered versions that produce therapeutic compounds or sensor molecules in situ. This three-year project has resulted in a Technical Advance on "Airway Probiotics to Counter Respiratory Infection" and a publication in *ACS Infectious Diseases*. (PI: Steve Branda)



CPs (10^6 CFU) were administered to the mouse airway via oropharyngeal aspiration (OPA). 3-7 days later, B. thailandensis ($5x10^5$ CFU) was administered via OPA. Mice were monitored for 10 days post-challenge. Results from 5-25 mice (1-5 studies x 5 mice/cohort) are shown. Green font: Colonizing CP. Red font: Non-colonizing CP. Blue asterisk: CP survival curve significantly differs from no-CP survival curve (pval < 0.001 in Cox-Mantel log-rank test with Bonferroni correction for multiple comparisons).

Treatment with candidate probiotics significantly increases the survival rate for mice challenged with an otherwise lethal dose of respiratory pathogen Burkholderia thailandensis.

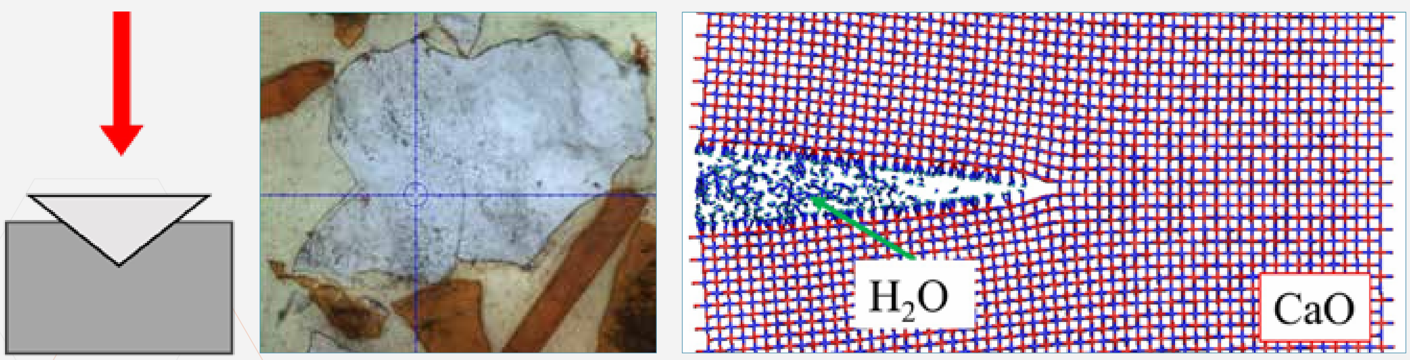
RELEASING, DETECTING, AND MODELING TRACE AEROSOLS AND GASES IN EARTH'S STRATOSPHERE.

Motivated by climate change and the growing international urge to implement or ban solar climate intervention through the release of aerosols, this project focused on the need to develop an accessible, transparent platform to make in-situ measurements in the lower stratosphere with respect to aerosols, gases, and temperature. Data was acquired from solar heliotrope balloons capable of flying payloads less than 6 lbs. and up to 17-23 km above Earth's surface for 4-12 hours in daytime free float. The temperature sensors were positively biased compared to global reanalysis data sets, and the gas sampler collected gases from the stratosphere, but had risks of contamination from the solder valve. The Optical Particle Counters reliably measured aerosols in the lower stratosphere with comparable results. This project, in collaboration with Sandia Alliance partners at the University of New Mexico and Texas A&M, Sandia National/Regional partners at the University of Washington, and also at Oklahoma State University, standardized stratospheric atmospheric sampling for the lower stratosphere or analyzation of targeted aerosol-emitting events. It also resulted in two journal publications, two Technical Advances filings, several conference presentations, and positive interactions with government and industry partners at the Federal Aviation Administration, and National Oceanic and Atmospheric Administration. (PI: Lauren Wheeler and Erika Roesler)

A gray plastic balloon just before launch into the lower stratosphere.

UNDERSTANDING MOLECULAR-SCALE EFFECTS ON FRACTURE CAN INFORM RESOURCE EXTRACTION AND HELP MAINTAIN THE NATION'S INFRASTRUCTURE.

Subcritical fracture controls deformation and permeability of rocks and degradation of manmade materials. To further understand the chemical mechanisms controlling subcritical fracture, this three-year project created nanomechanical and continuum-scale mechanics experiments to assess elastic, plastic, and brittle deformation of single crystals and multi-component rocks in reactive chemical environments. Additionally, Sandia researchers developed atomistic and continuum-scale modeling approaches to predict fracturing in silicate, carbonate, and oxide solids, mimicking those reactive environments. The team, in conjunction with Sandia Alliance partner University of Illinois at Urbana-Champaign is developing a new data analysis tool to assess scale-dependency during nanoindentation of laminated crystals. The experiments and models indicated that while calcium oxide phases are extremely sensitive to the presence of water, calcium carbonate undergoes only mild water-weakening and ion-specific interactions that can significantly decrease fracturing. Understanding molecular-scale effects on fracture could revolutionize the nation's use of subsurface systems for resource extraction, storage of CO_2 and nuclear waste, and help maintain essential infrastructure relevant to national security. The project's findings to date are reported in *Journal of Materials Science*, *The Journal of Physical Chemistry C*, and *Physical Review E*. (PI: Anastasia G. Ilgen)



(a) (b) (c)

(a) Liquid nanoindentation setup, (b) indentation site for individual grain, and (c) water inside crack tip in molecular dynamics simulations.

ACOUSTIC SENSING ON ARCTIC SEAFLOOR USING REPURPOSED TELECOMMUNICATIONS OPTICAL FIBER.

The Cryosphere/Ocean-Distributed Acoustic Sensing (CODAS) project completed eight ground-breaking data acquisition campaigns over a two-year period on Alaska's North Slope using Distributed Acoustic Sensing (DAS), an emerging technology that repurposes a standard telecommunications optical fiber into a kilometers-long seismic array. In this case, the seafloor fiber extends 37 km off Oliktok Point into the Beaufort Sea. The CODAS project was the first use of the DAS method in a polar coastal environment and in an area of transient sea ice. The collected data is a record of the sounds of the natural environment (ocean waves, sea ice vibration, icequakes, earthquakes) and anthropogenic sources (ships, trucks, hovercrafts). In collaboration with Sandia Alliance partner University of New Mexico, the team was able to determine both sea ice thickness and extent with unprecedented spatial and temporal resolution. Another unique accomplishment in collaboration with Sandia National/Regional partner University of Washington showed that DAS can reproduce buoy data by recording ocean wave parameters. Impacts to date include partnerships with industry including the Woods Hole Oceanographic Institute, invited and contributed talks sponsored by International Circumpolar Remote Sensing Society, National Science Foundation, Seismological Society of America, and the American Geophysical Union, plus an interview on the *Physics World Weekly* podcast. (PI: Robert Abbott)

Sandia researchers begin collecting the first-ever dataset from the Arctic seafloor using distributed acoustic sensing and a fiber optic cable. (Photo by Kyle Jones)

EXTRACTION AND SEPARATION OF RARE-EARTH ELEMENTS FROM DOMESTIC WASTE USING CITRIC ACID.

A secure, reliable, and sustainable domestic supply of rare-earth elements (REE) is essential to national security. The goal of this LDRD project was to develop an environmentally benign method to extract and separate REEs from coal and coal byproducts, the materials known to be enriched in REE contents. The work features a method that uses environmentally harmless citric acid in tandem with carbon dioxide to detoxify coal tailings by extracting critically needed rare elements and more harmful components at the same time. Further, the extraction improves the environment instead of destroying it as conventional mining may. Research was performed at various stages with Sandia National/Regional partner New Mexico State University and Alliance partner University of New Mexico, as well as National Energy Technology Laboratory and the University of Tennessee. This work, awarded a 2021 R&D 100 GOLD Special Recognition in Green Technology award, will also help ensure supply chain security and improve economic competitiveness for the nation. Credited to this LDRD work, two additional projects, \$187K and \$1.2M, respectively, were funded by DOE Office of Fossil Energy and Carbon Management to evaluate critical mineral resources in San Juan-Raton Basin, and in unconventional shale resources, respectively. (PI: Guangping Xu)

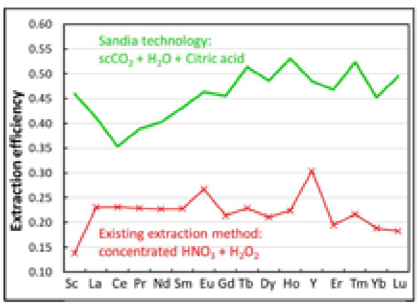


Fig. 1. Comparison of extraction efficiency between Sandia's environmentally benign technology and existing method using strong acids – concentrated nitric acid and hydrogen peroxide.

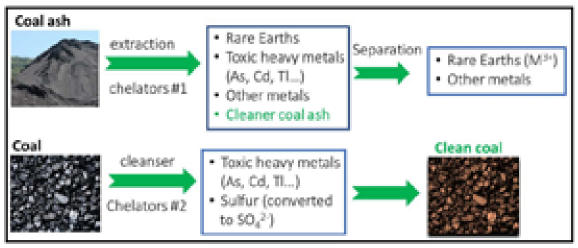


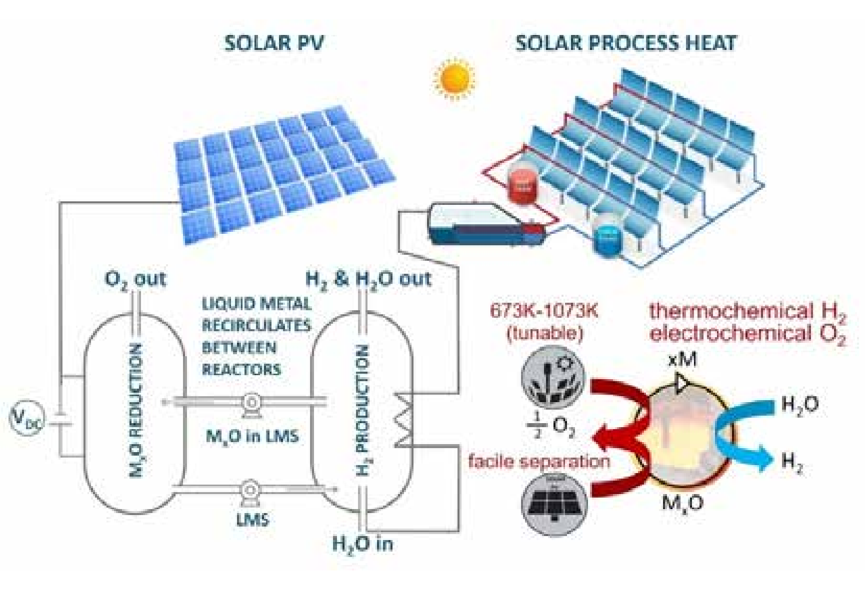
Fig. 2. Sandia technology can be used in extracting REE and other critical metals from coal ash, and also be used as coal cleanser to remove the toxic metals and sulfur.

A comparison of Sandia's method for extracting rare-earth metals to existing methods shows how using citric acid is more efficient.

Sandia researcher Guangping Xu adds coal ash into a citric acid mixture. This solution will be fed into a reactor—operating at about 70 times atmospheric pressure—where supercritical carbon dioxide aids citric acid in extracting rare-earth metals. (Photo by Rebecca Gustaf)

DEVELOPMENT OF NOVEL LIQUID METAL SOLUTION CHEMISTRY PRODUCES RENEWABLE HYDROGEN BY WATER SPLITTING.

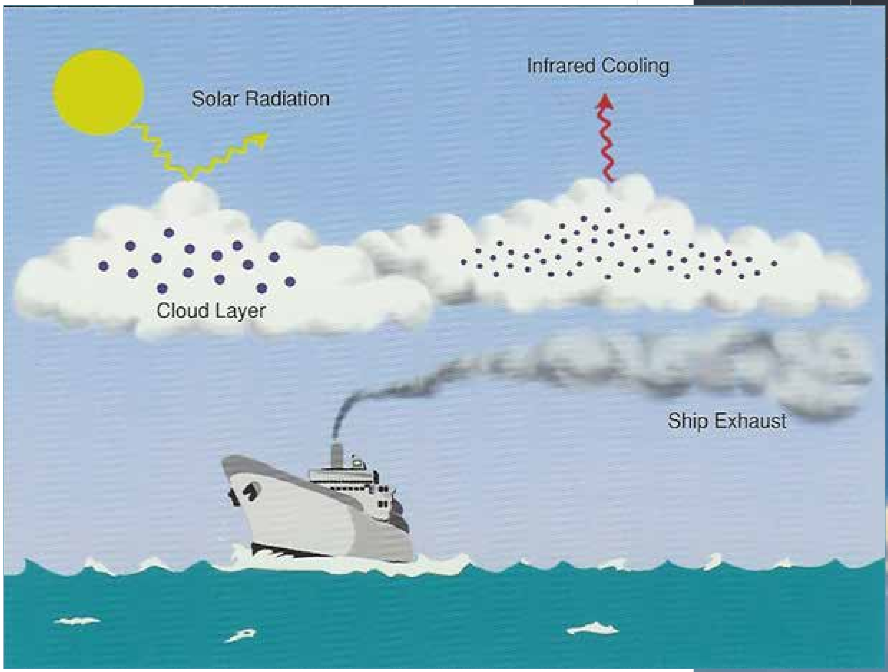
As an energy carrier, hydrogen (H_2) can be utilized as a domestic source of fuel, energy storage, and process heat. H_2 is sourced mainly by reforming hydrocarbons, which emits CO_2. Renewable pathways to H_2 are expensive and/or inefficient, so the goal of this LDRD project was to formulate a liquid metal solution (LMS) that could be integrated into a hybrid thermochemical-electrochemical process that utilizes heat and electricity from solar or nuclear power to renewably produce H_2 via water-splitting (WS). The Sandia team developed an ML algorithm to predict candidate LMSs, fabricated a novel flow reactor to characterize the LMS reaction, and demonstrated H_2 production via WS in a molten Sn-Zn alloy at temperatures below 500°C. This process demonstrates novel, carbon-free H_2 production adoptable by the nuclear and solar industries and will advance the nation toward DOE Earth shot Hydrogen 1-1-1 goal ($1/1 kg/1 decade). To date, two Technical Advances were generated, a non-provisional patent application is in prosecution, and follow-on funding was received through the DOE Solar Energies Technologies Office. Matthew Witman, a postdoc who contributed to the project and was later promoted to Sandia staff, was the co-winner of a 2021 Hydrogen Fuel Cell Technologies Office Postdoctoral Recognition Award.
(PI: Andrea Ambrosini)



Schematic of the liquid metal solutions approach for the combined thermochemical and electrochemical water splitting.

QUANTIFYING AEROSOL INJECTION BEHAVIOR FROM LARGE-SCALE SATELLITE IMAGERY USING STATISTICAL MODELING AND MACHINE LEARNING.

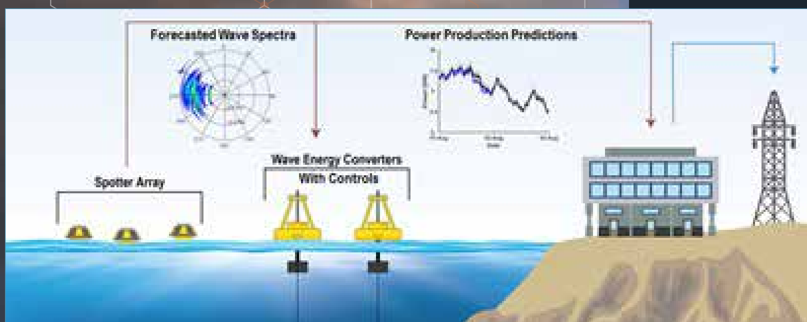
Solar climate intervention (SCI) strategies using aerosol injections exploit absorption and scattering properties to calibrate temperatures. However, true trajectorial dispersion of aerosols remains the largest source of uncertainty in climate models. To improve modeling accuracy, the Sandia LDRD team, in collaboration with Sandia National/Regional partner University of Washington, developed novel aerosol dispersion parametrizations at different spatio-temporal scales, one of which was highlighted in the cross-disciplinary journal *Environmental Data Science*. Machine and statistical learning algorithms created by the team have allowed for more understanding of dispersion fields from imagery and are to be exploited with complex climate models, leading to opportunities to improve aerosol SCI strategies for Sandia's climate intervention roadmap. In the project's second year, Sandia's large fog chamber will extend the experiments and analysis done using the table-top mini chamber built by the team by upscaling the domain of consideration from a single point to a 3D chamber on the order of tens of meters. The chambers will show the impact of scale on different parametrizations and what can be learned about atmospheric aerosols. (PI: Lekha Patel)



Satellite imagery can detect ship tracks, temporary cloud trails created via cloud seeding by the emitted aerosols of large ships traversing the world's oceans.

OVERCOMING WAVE ENERGY CONVERTER GRID INTEGRATION CHALLENGES BY PROVIDING A COMPLETE POWER FORECAST AT ELECTRICAL GRID CONNECTIONS.

Integration of renewable power sources into electrical grids remains an active R&D area, particularly for less developed renewable energy technologies, such as wave energy converters (WEC). High spatio-temporal resolution and accurate wave forecasts at a potential WEC (or WEC array) lease area are necessary to improve WEC power prediction and facilitate grid integration, particularly for microgrid locations. This project leveraged the availability of high-quality measurement data from recently developed low-cost measurement buoys to allow for operational assimilation of wave data into forecast models at remote locations where real-time data have previously been unavailable. In partnership with the University of Alaska Fairbanks, buoys were deployed offshore of the remote and 100% diesel-reliant community of Yakutat, AK (a potential wave energy deployment site). The buoy data was utilized for improved wave forecasting through data assimilation. This was integrated with WEC farm operational controls and energy storage systems to significantly increase accuracy and certainty of wave power forecasts into the grid, balance the energy variability, and obtain resiliency and security. Results from this project include nine publications, including "Extending Complex Conjugate Control to Nonlinear Wave Energy Converters" in the *Journal of Marine Science and Engineering*, and "Wave Sequential Data Assimilation in Support of Wave Energy Converter Power Prediction" in *arXiv* (preprint), one Technical Advance, and a patent application. (PI: Ann Dallman)



'Complete' wave power forecast: Incoming wave spectra forecast feeds into array and energy storage control, providing power forecast at grid connection.

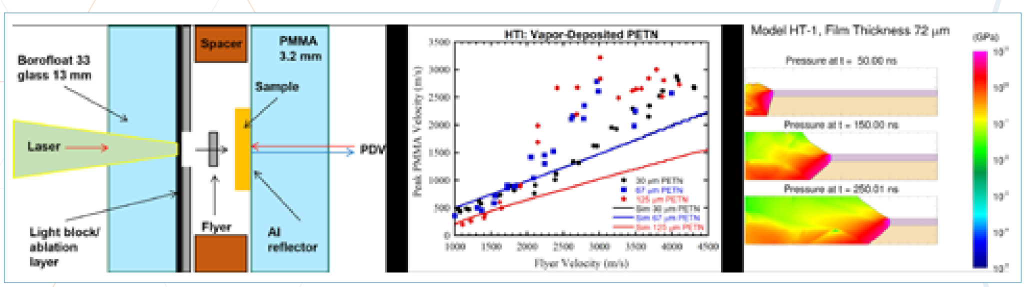
PI Ann Dallman received a Society of Women Engineers Distinguished New Engineer 2021 award for technical accomplishments and leadership in her first 10 years, which included leadership of this LDRD.

DESIGNING COMPOSITIONALLY COMPLEX OXIDE CATALYSTS TO CONVERT GREENHOUSE GASES INTO VALUABLE CHEMICALS.

Exploring a decentralized process for upgrading methane and carbon dioxide into valuable chemicals as a step toward displacement of flaring operations was the focus of this two-year LDRD project. The team's involved process converts methane and carbon dioxide into synthesis gas (an industrially valuable mixture of hydrogen and carbon monoxide) via the dry reforming of methane reaction. They successfully designed novel high- entropy oxide catalysts having aluminate spinel crystal structure, that are uniquely capable of structural regeneration. This characteristic overcomes issues with active particle sintering and excessive coke formation that plague conventional catalysts. Concentrated solar energy was integrated as process heat in the longest heated experiment conducted with the solar furnace at Sandia's National Solar Thermal Test Facility. The project, enabled in part through collaboration with Sandia Alliance partner University of New Mexico, resulted in one publication, three Technical Advances, and two provisional patents. (PI: Christopher Ryan Riley)

DETONATION IN MULTILAYER EXPLOSIVES: EFFECTS OF THE CHARACTERISTIC LENGTH SCALE OF MIXING.

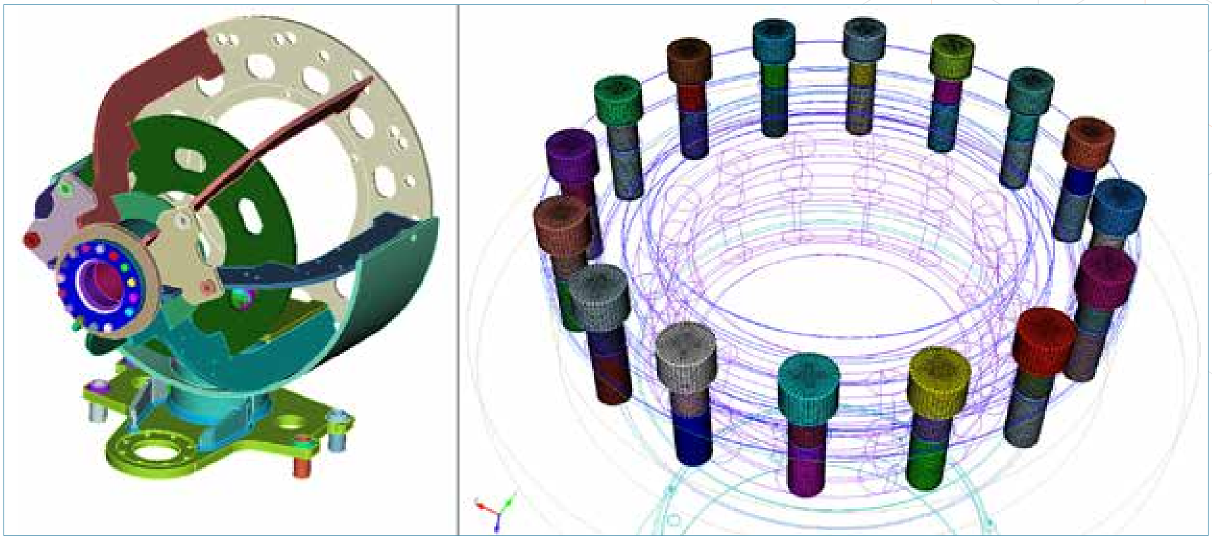
Predicting explosive performance at length scales near the minimum needed for a detonation to propagate is often a challenge—surrounding materials, non-ideal interfaces, sample geometry, and local microstructure variations can all significantly impact explosive output. For accurate predictions of performance, reactive burn models are needed that can capture the details around the growth or failure of reactions leading to detonation, which requires detailed experimental information for model parameterization. Researchers on this LDRD team developed a high-throughput experimental setup utilizing laser-driven flyers with photon Doppler velocimetry diagnostics and an array of vapor-deposited explosive films to characterize both initiation thresholds and the growth of reactions leading to detonation. This data was used to parameterize new burn models, which are enabling predictions of explosive performance at small scales, including the effects of non-ideal interfaces. This work led to two publications in the *Journal of Applied Physics* in 2022 using high-throughput initiation experiments to calibrate predictive simulations.
(PI: Robert Knepper)



Sandia's high-throughput initiation experiment uses an array of laser-driven flyers to impact small explosive samples (left), providing data on the growth of reactions leading to detonation (middle), which can be used to parameterize predictive simulations (right).

USING MACHINE LEARNING TO CREATE RAPID STRONGLINK MECHANISMS CAD-TO-SIMULATION-READY MODELS.

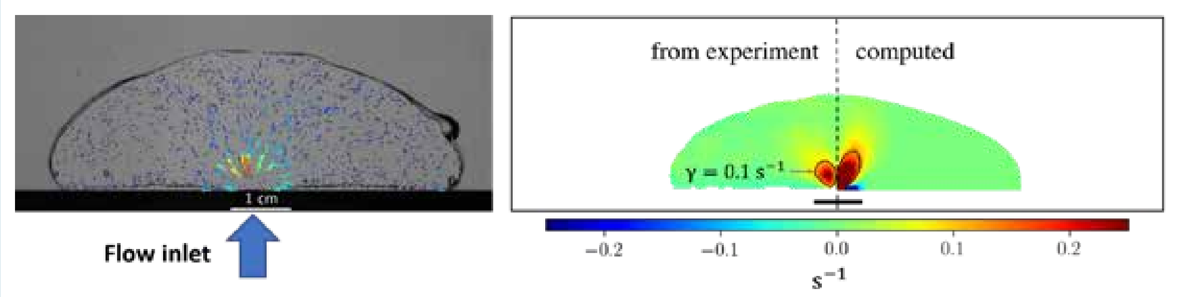
Computer aided design (CAD) to simulation workflows for nuclear deterrence (ND) have shown dramatic performance improvements with ML. This work targets some of the most inefficient, tedious, and error-prone bottlenecks using new ML-based methods. Common mechanisms such as fasteners and springs can now be quickly identified and reduced to simulation-ready proxies, significantly reducing the need for most human interactive geometry and meshing operations. Also developed is a new dynamic, in-situ classification tool that can be used as the basis for a common sharable knowledge base, capitalizing on the expertise of experienced engineers within a community of analysts. The time analysts need to prepare shell-based Finite Element Analysis models to simulate critical ND transportation systems was also dramatically impacted using a new multi-agent reinforcement learning algorithm that learns a complex procedure for dimensionally reducing a 3D CAD assembly to a simulation-ready set of interconnected sheet bodies. This project has led to two Technical Advances and a patent submission. Presentations were made at various conferences and symposia, including the Siemens Geometry and Meshing Lecture Series and the 16th and 17th U.S. Congress on Computational Mechanics. Additionally, it won the Best Technical Presentation award at the 2022 Society for Industrial and Applied Mathematics International Meshing Roundtable (IMR), and a published, peer-reviewed paper will be presented at the 2023 IMR in Amsterdam, Netherlands. (PI: Steven James Owen)



CAD model (left) with multiple fasteners (right), rapidly reduced to simulation-ready state using new ML methods.

ENABLING FULLY PREDICTIVE SIMULATIONS USING DISRUPTIVE COMPUTATIONAL MECHANICS AND NOVEL DIAGNOSTICS FOR FLUID-TO-SOLID TRANSITIONS.

Accurately capturing solidification of fluids and the development of residual stress is critical for fully predictive simulations for numerous applications in geoscience, nuclear safety, manufacturing, energy production, and bioscience. Researchers on this LDRD project developed, implemented, and demonstrated advanced constitutive models with yield stress to represent both fluid and solid behavior simultaneously. They also presented results from literature models and demonstrated the first finite element results for the Kamani-Donley-Rogers model that was developed by Sandia Alliance partners at the University of Illinois at Urbana-Champaign (Illinois). Predictions were compared to novel experimental results of gravitational settling of yield stress fluids in a Hele-Shaw cell. Both experiments and simulations showed solidification in regions of low applied stress near free surfaces and far from the inlet. These improved models for the birthing of residual stress will substantially improve predictions of Sandia's encapsulation processes. This project resulted in five publications consisting of one in *Physical Review Letters* in 2021, two in the *Journal of Non-Newtonian Fluid Mechanics* (1) (2), and the *Physics of Fluids* in 2022, and one in the *Journal of Rheology* in 2023. Additionally, this Sandia team had numerous collaborators from industry (3M, Proctor and Gamble), the government (U.S. Army Engineering R&D Center), and Sandia Alliance partners from Illinois, University of New Mexico, Georgia Tech, and the University of Utah. (PI: Rekha Rao)

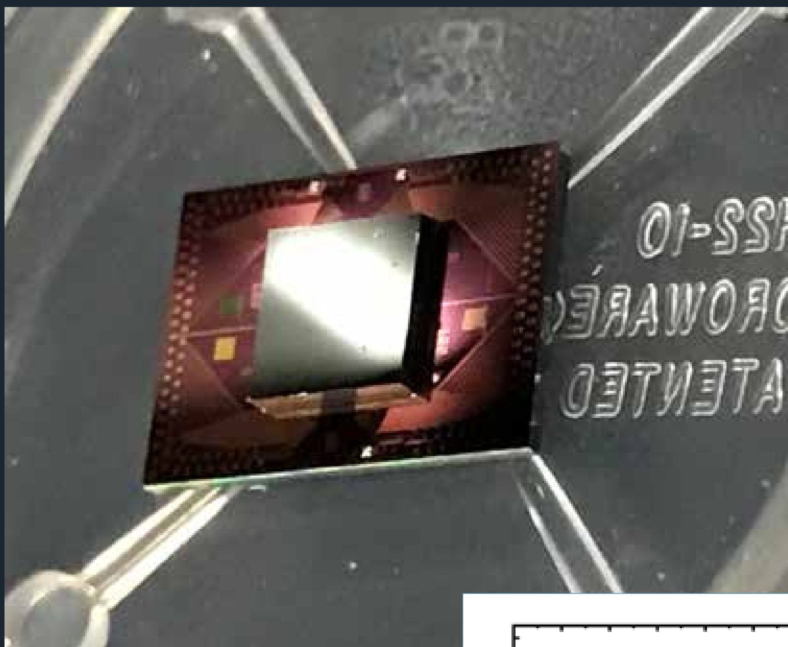


Stress birth and death of a fluid-to-solid transaction: (left) fluid birth, and (right) the solid transaction.

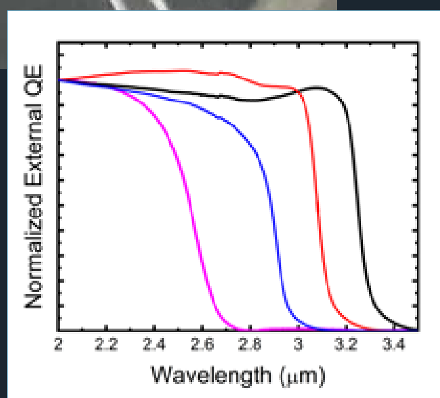
HIGH-SPEED DIAGNOSTIC AND SIMULATION CAPABILITIES FOR REACTING HYPERSONIC REENTRY FLOWS.

Hypersonic flight environments are often approximated in impulsively operated ground-test facilities, with test times of a few milliseconds at best, placing high-acquisition-rate measurements at a premium. Wavelength-tunable burst-mode laser capabilities for temperature and chemical species detection at 100-kHz rates were developed, improving on existing measurement speeds by 2-4 orders of magnitude and increasing data yield from a single laser shot to over 100 measurements during a single test. The team characterized nonequilibrium thermal environments and velocities in the shock-tunnel flow, capturing transient temperature changes in excess of 4000 K, and imaging hypersonic wake transients. These new capabilities are being applied for unique hypersonics data sets and informing new modeling and design tools at Sandia. The work was conducted in collaboration with Alliance partner Purdue University, who transferred expertise on tunable high-repetition-rate laser sources to Sandia. (PI: Sean Kearney)

DEVELOPING LARGE, HIGH-UNIFORMITY FOCAL PLANE ARRAYS FOR REMOTE SENSING THROUGH LOW-DARK-CURRENT EXTENDED-SHORT-WAVE DETECTORS.



Relative external spectral quantum efficiency for devices.

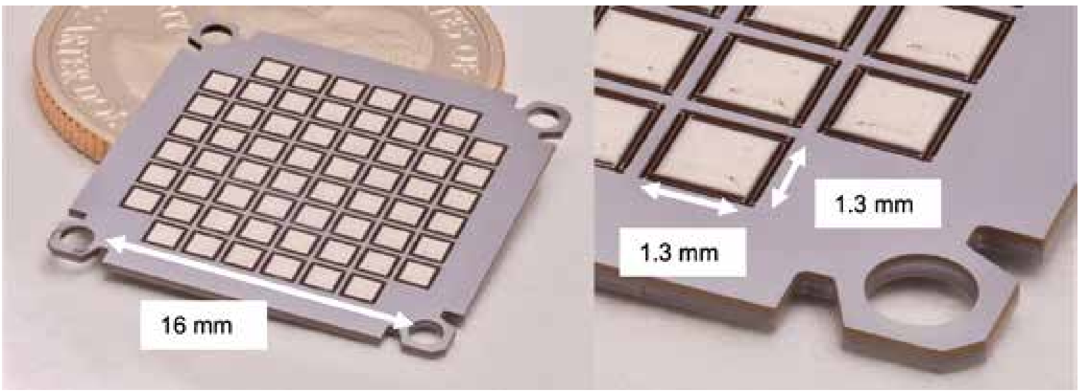


The team designed a focal plane array detector with cutoff wavelengths from 2.55 to 3.2 µm.

High-performance focal plane array detectors with long-wavelength cutoffs in the spectral range from 1.7 to 3.0 µm traditionally use mercury cadmium telluride (HgCdTe) as the photon-absorbing material. Detectors made from group-III and group-V elements offer potentially similar performance with reduced cost, improved manufacturability, and superior scaling to large arrays, but development of the required materials has lagged that of III-V detectors in the mid- and long-wavelength infrared. This Sandia LDRD team examined relatively unexplored III-V alloys for this application and obtained high-quality, single-phase quaternary materials, yielding detectors with cutoff wavelengths from 2.55 to 3.2 µm. Large-area detectors had high quantum efficiencies with dark currents like state-of-the art HgCdTe detectors for cutoff wavelengths longer than 2.9 µm. A new set of materials was identified through this effort that may be exploited to produce large, high-uniformity focal plane arrays for remote sensing. One publication resulted to date from this project, and two presentations were provided at events focused on military sensing technologies.
(PI: John Klem)

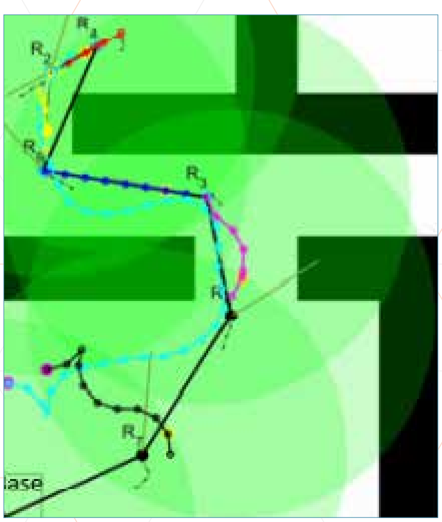
INVESTIGATION OF MICROCALORIMETER PHOTON DETECTOR PERFORMANCE TO ENABLE NONPROLIFERATION APPLICATION USE.

A fieldable microcalorimeter has the potential to provide energy resolution an order of magnitude better than the current high-purity germanium standard. This team sought to address current design limitations, such as detector deadtime and inconsistent performance between pixels caused by glue used to attach absorbers by hand. Ultimately, it was determined that electroplated gamma-ray absorbers could produce the same energy resolution as absorbers created from bulk tin material. Using this finding, the team designed and fabricated a 60-pixel integrated detector structure with tin electroplated into silicon cavities on one side of a wafer and thermal isolation trenches etched around each pixel. (The design calls for transition-edge sensors to be patterned on the opposite side.) The findings from this project, worked in collaboration with Sandia Alliance partner Texas A&M, the National Institute of Standards and Technology, and Los Alamos National Laboratory, forged a path toward the creation of an integrated microcalorimeter detector. The work resulted in one publication, three Technical Advances, and two patents that are currently in prosecution. (PI: Michael Hamel)



A 60-pixel integrated detector structure is shown with tin electroplated into silicon cavities on one side of a wafer and thermal isolation trenches etched around each pixel.

MOBILE JAM-PROOF WIRELESS TECHNOLOGY ALLOWS FOR MAINTENANCE OF LINE-OF-SIGHT NETWORK.



Simulations using line-of-sight maintenance allowed agents to navigate to user- or autonomously generated points of interest.

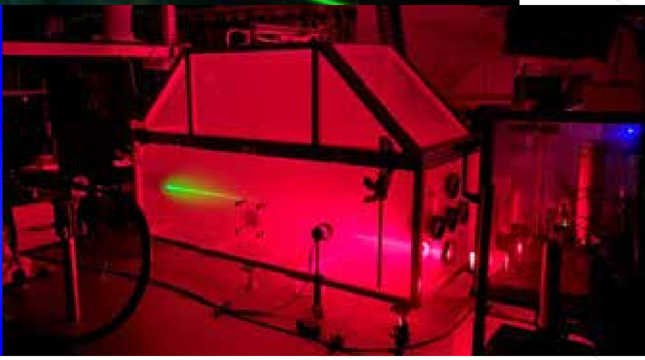
Bridging the technology gap required to bring highly reliable communication systems to autonomous mobile agents was the focus of this LDRD project.

After early exploration of technologies, it was determined that research in line-of-sight (LOS) maintenance for mobile agents could have the broadest impact beyond the initial project scope. Simulations allowed the team to examine various control strategies for maintaining a LOS network between agents while also navigating to user- or autonomously generated points of interest. The team presented findings for how the controllers, control parameters, and numbers of agents in the network influence the ability to achieve mission goals. (PI: Steven Spencer)

COMPUTATIONAL IMAGING FOR INTELLIGENCE IN HIGHLY SCATTERING AEROSOLS.

Aerosols like fog scatter and absorb light, creating degraded visual environments that cause unacceptable downtime for critical systems and operations. Rather than rejecting information in scattered light, this Sandia team sought improved solutions that can interpret the information. A computationally efficient light transport model was developed to achieve computational detection, localization, and imaging in fog at the Sandia Fog Chamber Facility. Through an academic collaboration with three graduate students and one faculty member at Sandia Alliance partner Purdue University, new sensing methods were developed using speckle intensity correlations that allowed characterization of fog, imaging of hidden objects, and an ability to distinguish objects on a far-subwavelength scale. This LDRD project represents significant developments that challenge the limits of imaging through dynamic scattering media and open important application spaces. This project resulted in nine journal articles, three invited and seven contributed talks at high-profile conferences such as those sponsored by the Society of Photographic Instrumentation Engineers, Optical Sensors and Sensing Congress, American Physical Society and the Optical Society of America, and the American Association for Aerosol Research. It also allowed for strong collaborations with industry and government partners, including NASA and Teledyne FLIR. (PI: Brian Bentz)

Members of Sandia National Laboratories' fog chamber research team inside the facility after setting up for an experiment. (Photo by Randy Montoya)



Left: Sandia's fog facility creates repeatable and well-characterized fog that is helping Sandia researchers and partners from NASA's Revolutionary Aviation Mobility group and Teledyne FLIR test sensing capabilities.

Right: The Sandia team created two bench-top fog chambers to support collaboration with Alliance partner Purdue University. Sandia is studying and characterizing the fog generated by its new bench-top fog chamber, while Purdue is using its twin system to perform experiments. (Photo by Randy Montoya)

CUSTOMIZED LITHIUM BATTERIES FOR MISSION APPLICATIONS.

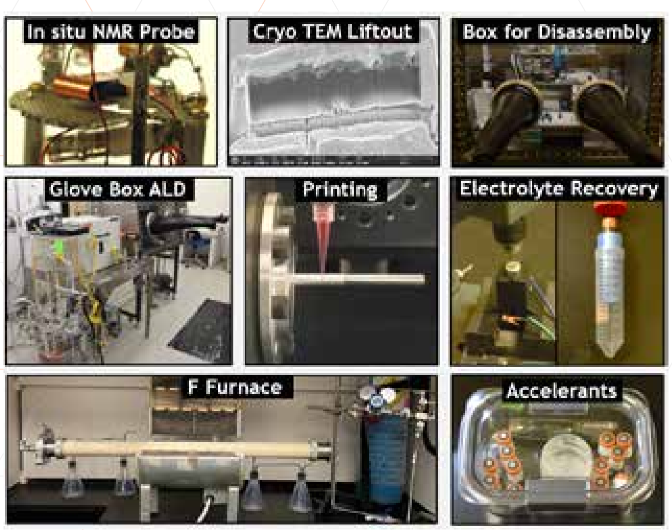
Development of complex-shaped batteries will have value for national security missions and other applications where higher power and custom form could be maximized by capitalizing on the available battery space. By employing new nuclear magnetic resonance experimental designs and diagnostic tools (a cutting-edge capability for Sandia), this LDRD Grand Challenge team was able to observe processes in situ, rather than having to employ destructive testing. They also identified aging mechanisms through multi-year accelerated aging studies, addressed major national security mission and industry issues, and ultimately advanced fundamental understanding of the relationships between rechargeability, aging, and electrode architectures in model lithium anode and conversion cathode batteries.

One aspect of the lithium battery project involved investigating the rechargeability behavior of carbon monofluoride (CFx). This research resulted in the team authoring one of the most comprehensive studies on CFx currently available. They also experienced early wins by serving as a consultant on battery failure and applying project-derived techniques for battery aging characterization. This understanding will enable batteries that cycle reliably for 2-10 cycles, can maintain long shelf life, and be customized for high power and custom form.

The key understanding of rechargeability, aging, electrode architectures, battery designs, and diagnostic tools has potential for meeting broad industry demand for custom-shaped batteries including commercial and military drone systems that have limited recharge capability but need high energy and power density, and space applications such as launch vehicles that require short-term and high-power battery capabilities.

PI Katie Harrison, left, and Katie Jungjohann are part of the Lithium Ion Battery LDRD Grand Challenge team. (Photo by Bret Latter)

The team collaborated with faculty at Sandia Alliance partner Purdue, University of Maryland, Sandia National/Regional partner University of California Los Angeles, and University of California San Diego. In addition, they partnered with ThermoFisher Scientific, ABQMR, and Lawrence Berkeley National Laboratory. To date, this project has resulted in 37 publications, 12 invited talks, and presentations at several society meetings including Materials Research Society, Microscopy and Microanalysis, Electrochemical Society, and Reactive Metal Processing, and high-profile conferences including the 2020 Battery Gordon Conference and the Chemical, Bioengineering, Environmental and Transport Systems 2020 virtual conference. The PI also served as a guest editor for the journal *Nanotechnology* for a special issue: "*Focus on Nanophase Materials for Next-generation Lithium-ion Batteries and Beyond*."
(PI: Katie Harrison)

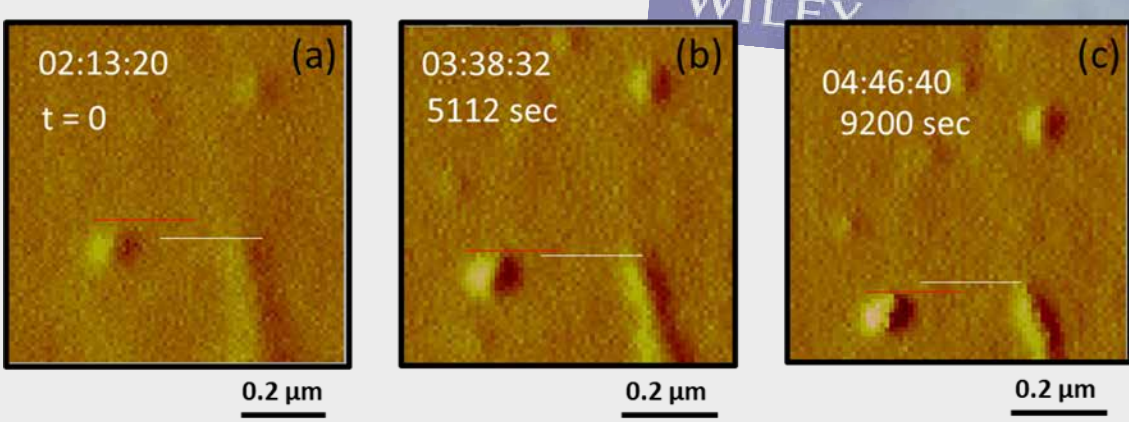


Shown are some of the tools and capabilities developed during the Lithium Ion Battery LDRD Grand Challenge.

STRESS INTENSITY THRESHOLDS FOR DEVELOPMENT OF RELIABLE BRITTLE MATERIALS.

Brittle material failure can appear random and unpredictable at subcritical stresses. A fundamental understanding of how structural and environmental factors impact fracture propagation is necessary to predict fracture in these systems. Through this project, a physics-based model of glass fracture was developed to limit uncertainties in predicting crack growth. An experimental and computational approach composed of molecular dynamic (MD) simulations, numerical modeling, and atomic force microscopy (AFM) was used. AFM characterization identified crack growth rates as slow as 10-13 m/s. MD simulations identified the role of inelastic relaxation in crack propagation including evolution of the local atomic structure during relaxation. A numerical model for the existence of a stress intensity threshold was developed and is being incorporated into mission programs. The project included collaboration with faculty and students from Sandia Alliance partner Purdue University and with the Missouri University of Science and Technology. This work has resulted in five publications, with one, "Inelastic relaxation in silica via reactive molecular dynamics," selected for the cover of the *Journal of the American Ceramic Society*. PI Jessica Rimsza was also selected to participate in the 7th World Materials Research Institutes Forum Workshop for Early Career Scientists for her work on fracture in nuclear waste forms. (PI: Jessica Rimsza)

Cover of the Journal of the American Ceramic Society.



Three examples of inelastic relaxation in cracks propagation.

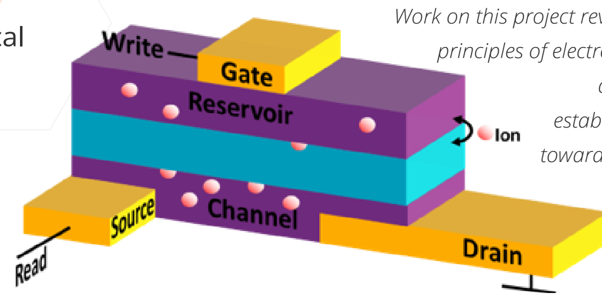
SMART MATERIALS FOR HIGHLY COMPLEX OPTICAL TAGS WITH ENVIRONMENTAL RESPONSE.

As counterfeiting methods become more sophisticated, countermeasures must be developed at the same pace. In this Sandia LDRD project, unique exemplars of next-generation anticounterfeiting optical tags were developed that leverage the luminescent properties of materials for encoding. The research team also gained a fundamental understanding of how both structure and composition affect the energy transfer pathways that govern photoluminescent properties in these materials, and they enabled the precise manipulation of the resulting photophysical properties. They collaborated with Sandia Alliance partners from Georgia Tech and the University of Illinois Urbana-Champaign who provided complementary modeling and organic synthesis expertise, respectively. Collectively, this project produced new and differentiating technologies enabling Sandia to develop advanced concept solutions for materials assurance. This work generated two patent applications, seven journal publications with one making the cover of *Angewandte Chemie*, and a recently published article in *Nature Communications*. (PI: Dorina Sava Gallis)

Cover of the Journal of the German Chemical Society Angewandte Chemie International Edition

FIN-ION TUNABLE TRANSISTOR FOR ULTRA-LOW POWER COMPUTING.

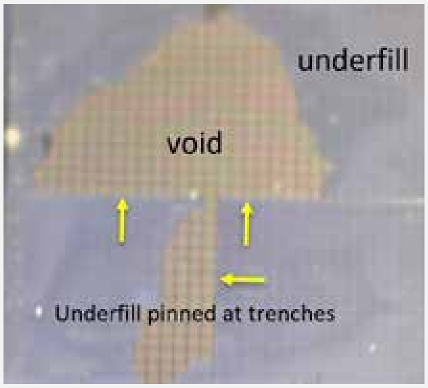
Data-heavy workflows such as AI require in-memory computing, so this LDRD team focused on creating analog resistive nonvolatile memory to increase system efficiency. Work on this project revealed fundamental principles of an electrochemical random-access memory, established a viable path toward its integration, and leveraged correlated phenomena to enable on-demand architectural reconfigurability of computing fabrics. Anticipated impacts include computing systems with orders of magnitude improved energy efficiency and radiation hardness. This project resulted in three Technical Advances and six publications, including "Nonvolatile Electrochemical Random-Access Memory under Short Circuit" published in *Advanced Electronic Materials* and Filament-Free Bulk Resistive Memory Enables Deterministic Analogue Switching published in *Advanced Materials*. The project benefited from collaborations with faculty and students at Sandia Alliance partner UT Austin, Sandia National/Regional partner University of Michigan, and faculty at Sandia Alliance partner Texas A&M University, and Sandia National/Regional partners Stanford and Arizona State University. The Science Magazine Board of Reviewing Editors appointed PI Alec Talin to the board for his demonstrated expertise. (PI: A. Alec Talin)

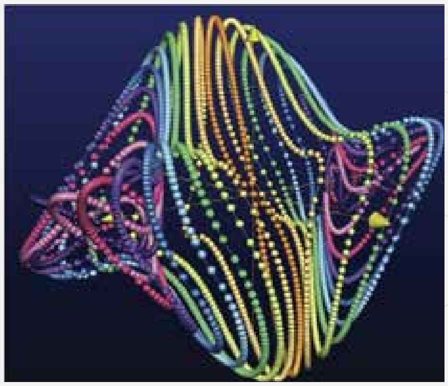


Work on this project revealed fundamental principles of electrochemical random-access memory and established a viable path toward its integration with complementary metal-oxide-semiconductor.

NEW TECHNOLOGY FOR HETEROGENEOUSLY INTEGRATED DEVICES ALLOWS FOR UNDERFILLING OF COMPLEX GEOMETRIES USING DRIVEN FLUIDS.

Underfilling is a widely used manufacturing process that helps stabilize and reinforce solder joints in electronic parts. However, heterogeneously integrated (HI) devices are challenging to underfill using standard capillary flow methods, due to large areas with narrow gaps—trenches that act as strong flow barriers, and high bump density that cause filler particle segregation. Through this LDRD project, the team developed a magnetic underfill that can be driven with multiaxial magnetic fields having key symmetries to create vorticity in the fluid, enabling it to fill narrow gaps, cross barriers in any orientation, and uniformly disperse the filler particles. This approach was demonstrated using driven fluids consisting of epoxy and magnetic nanoparticles. A new Sandia capability was developed to create vorticity vector orbits with low frequency triaxial magnetic fields. It was discovered that significant torque density can be generated in viscous particle suspensions, enabling driven underfilling of complex geometries—a viable new technology for HI devices. Discoveries during this two-year project led to new concepts for low moisture permeation coatings now under study and generated one Technical Advance. (PI: Lauren Shea Rohwer)

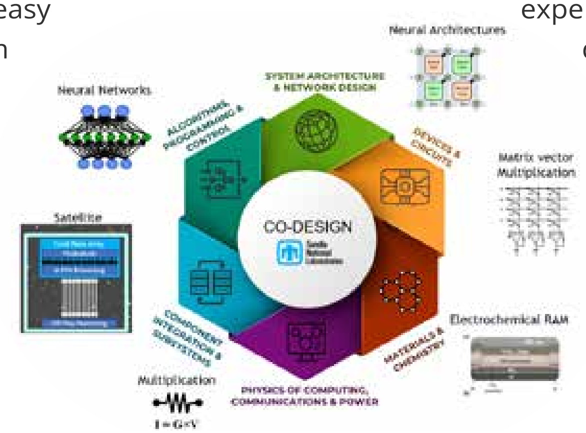




(Left) Without a magnetic field, there are voids in the HI devices. (Middle) Using the phase-modulated 1+dc:2:3 magnetic field, the HI device is void-free, completely gap filled, with no filler particle segregation. (Right) A set of vorticity vector orbits computed for a phase-modulated 1+dc:2:3 field.

NEW 2.5D NEUROMORPHIC DISCOVERY PLATFORM WILL ENABLE AI-ENHANCED CO-DESIGN.

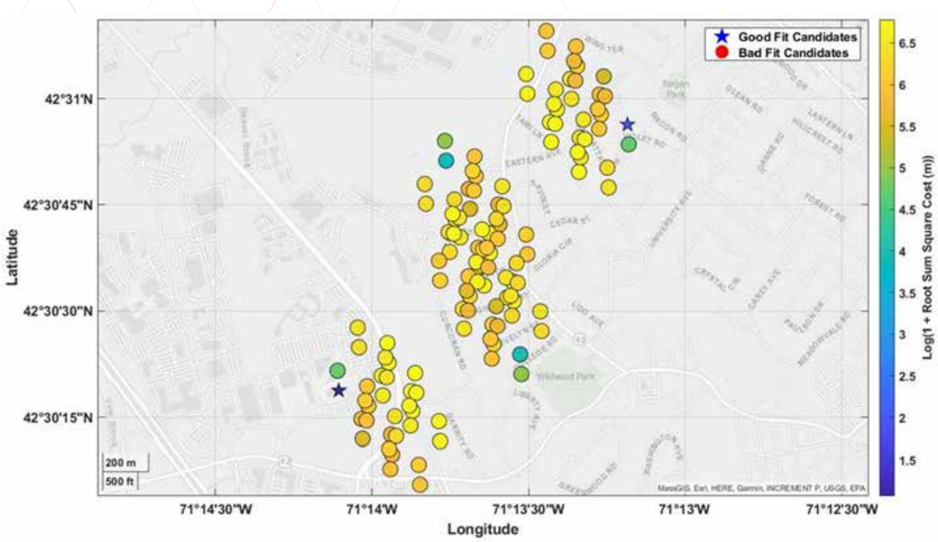
Novel material and device concepts previously took years for iteration. Discoveries in this LDRD project will now allow them to be iterated on in weeks thanks to a new easy fabrication substrate platform for novel devices. The team designed and taped out a microelectronics discovery platform or a "lab-on-a-chip" that has high-speed pulsing and high-resolution sensing that permits researchers to gauge fundamental limits of atomic switching in novel microelectronic devices including ECRAM and ReRAM. Additionally, the team released an updated microelectronics co-design software, CrossSim 2.0, a GPU-accelerated, Python-based crossbar simulator that allows researchers to take experimental data from the discovery platform and immediately model system-level performance for sensor processing mission applications. A strong relationship with Arizona State University and a partnership with former Sandian, Matt Marinella, is providing a talent pipeline to multiple U.S. citizen students working on microelectronics co-design. (PI: Sapan Agarwal)



AI-enhanced co-design will be enabled through Sandia's 2.5D neuromorphic discovery platform.

TWITCHER: MOTOR DITHER CORRELATION FOR THE SURVIVAL OF GLOBAL NAVIGATION SATELLITE SYSTEM SPOOFING ATTACKS.

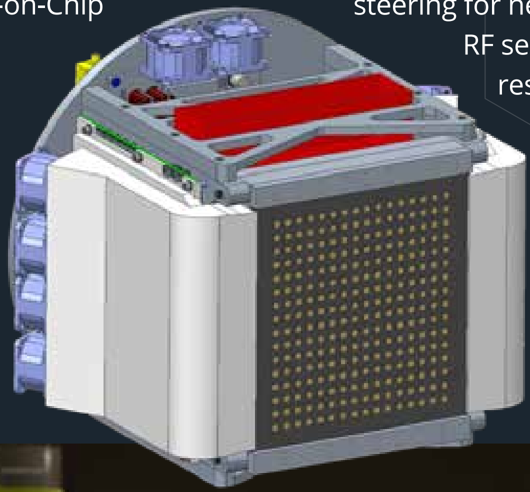
Global navigation satellite system (GNSS) receivers are vulnerable to deception jamming attacks (e.g., spoofers, repeaters), that inject false signals into receivers to change perceived position and time. In this LDRD, Sandia researchers developed a methodology of defending GNSS receivers from complex deception jamming attacks through modification to GNSS receivers: (1) a Constellation Binner tracks duplicate peaks that purport themselves to be the same signal, and then organizes those signals into unique position solutions, and (2) a Jitter detector identifies which signal is true and which is false. The Constellation Binner has been validated in anechoic chamber tests on a hardware platform to produce two position solutions from a GPS receiver in the event of spoofer attacks, and both solutions can be parsed through various spoofer detection algorithms to identify true and spoofed solutions. (PI: Connor Brashar)



Geometric mapping of candidate scores

ADMMA PROJECT ENABLES BEAM-AGILE RF SENSING AND PROMISES UNPRECEDENTED FLEXIBILITY AND PERFORMANCE.

The Advanced Digital Multi-Mission Aperture (ADMMA) project tackled the technical challenge of radio frequency (RF) device physics limiting ultra-wide-band (UWB) antenna electronic beam steering performance. It does this by implementing real-time UWB digital-signal-processing algorithms using state-of-the-art RF System-on-Chip devices to achieve unparalleled beam, frequency, and signal agilities. Such an approach not only increases system resistance to electronic jamming but also reduces probability of interception for radar and high-bandwidth data/communication links. This project created a high-power antenna aperture prototype utilizing emergent high-efficiency gallium nitride devices and developed novel digital beam formation/processing/calibration techniques that enabled UWB electronic beam steering for next-generation multi-mission RF sensing. ADMMA's flexibility and resiliency improves our nation's ability to achieve RF superiority/ dominance in complex electromagnetic contested environments. (PI: Jacques Loui)

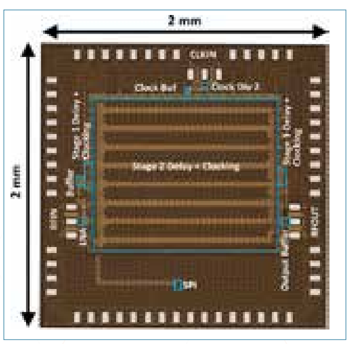


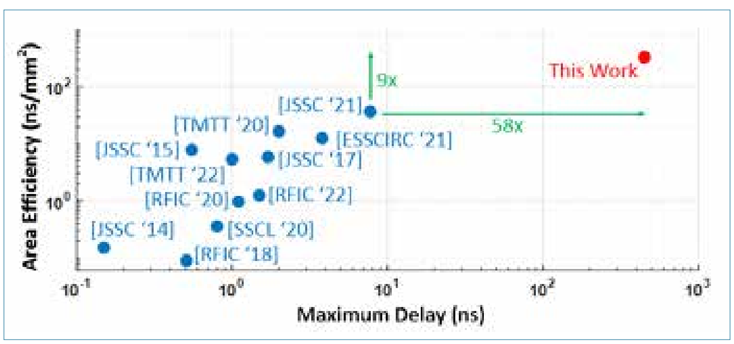
A computer-aided design rendering of the ADMMA prototype.

PI Jacques Loui, left, and a firmware developer are part of a team redesigning high-performance radar as a flexible, multipurpose sensor. (Photo by Craig Fritz)

ENABLING NEW MISSION SPACE WITH MINIATURE PROGRAMMABLE DELAY ELEMENT FOR ELECTRONIC WARFARE APPLICATIONS.

Achieving large delays at GHz frequencies with significant bandwidth and programmability is key for applications including radar testers, digital RF memory, and emerging full-duplex communications. While many mission applications desire hundreds of nanoseconds of programmable delay in the signal path, only a maximum of 2 ns of programmable delay had been achieved prior to this project. As a result, these systems relied on either Surface Acoustic Wave devices (lossy and have no programmability) or digital systems (consume watts of power and have limited minimum delay taps). In this project, the team developed a 2.55-448.6 ns programmable delay element using a time-interleaved, multi-stage, switched-capacitor approach on a CMOS integrated circuit covering a span of 0.2-2 GHz with 4 mm^2 area, consuming < 100 milliwatt and operating over a full temperature range. The approach departed prior delay line approaches and exceeded state of the art by project end by 58x in maximum programmable delay, 9x in area efficiency, and 2x in bandwidth. The device is enabling new mission space in tagging, tracking, and locating and electronic warfare applications and has seen interest in consumer cellular applications. This project was done in collaboration with Sandia Alliance partner University of Texas at Austin and supported by a graduate student. One publication on the project was an Industry Best Paper Award Finalist at the 2022 IEEE Radio Frequency Integrated Circuits (RFIC) Symposium. This represented Sandia's first-ever accepted paper at IEEE RFIC. (PI: Travis Forbes)



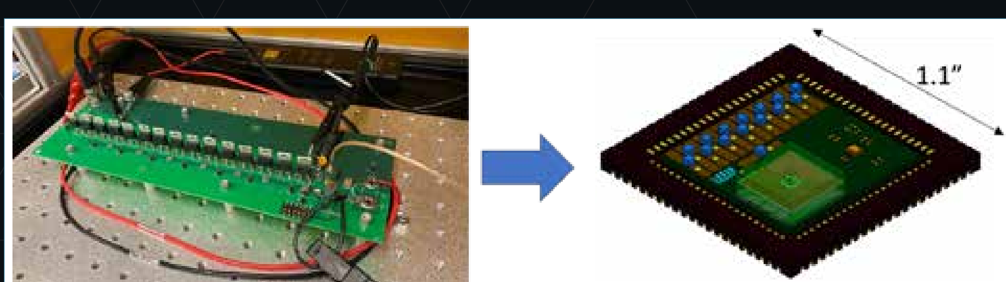


Left: Programmable delay element device.

Right: Maximum delay achieved vs. area efficiency scatter plot of prior art

RADIATION-HARD, HIGH-VOLTAGE, CHIP-SCALE POWER CONVERTER DELIVERS LARGE

Heterogeneous integration refers to the integration of separately manufactured components into a higher-level assembly package that, in the aggregate, provides improved operating characteristics. Numerous high-consequence systems and national security applications have advanced high-voltage components that rely on bulky and heavy power converters. This project uses advancements



Model of original high-voltage power converter (left) compared to chip-scale power converter (right) shows reduction in scale for similar capabilities.

ENVIRONMENTAL LEARNING METHODOLOGIES FOR REMOTE SENSING POWER OPTIMIZATION.

Understanding the environment that an unattended sensor is being placed in is critical to developing accurate models that drive design, especially when the sensor's power use is directly coupled with the environment's stimuli. Knowledge of the deployment environment is used to design and configure a sensor to meet a specific service life requirement. Sensors deployed in environments that are understudied or dynamic pose a problem to the design process of guaranteeing that a sensor will remain functional throughout its required service duration. This research developed a fusion of unsupervised learning, parametric optimization, and anomaly detection algorithms to design a robust, adaptable framework for in-situ power optimization to preserve and extend service life of remote sensor systems in the field. This technology affords a reduction in deployment planning time and deployment risk, affording quicker response to opportunities. (PI: Aaron Hill)

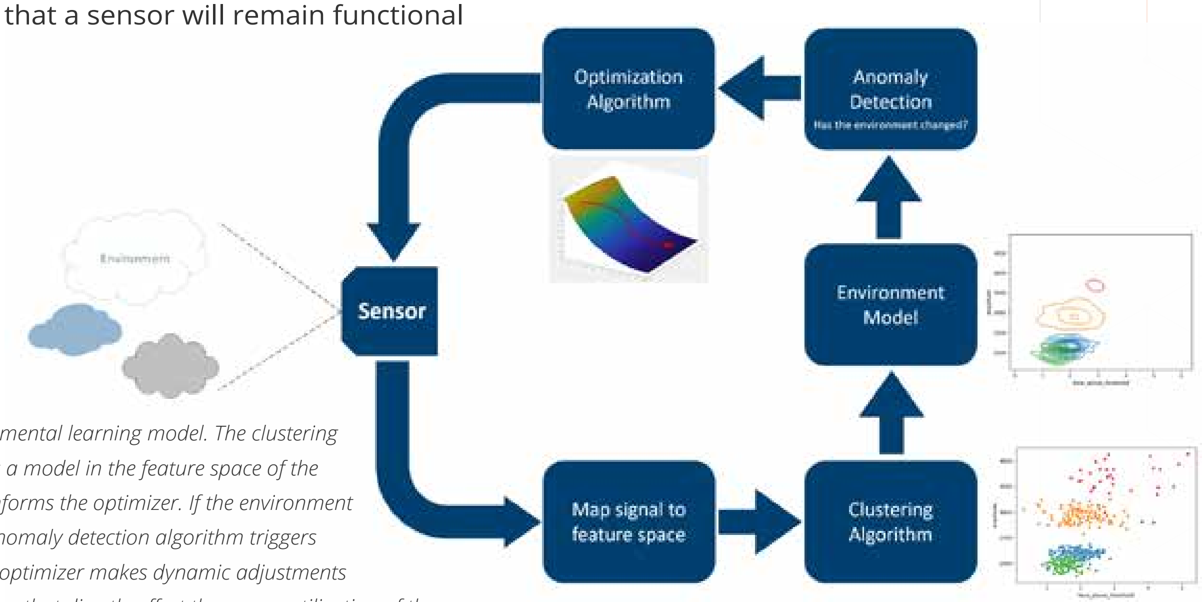


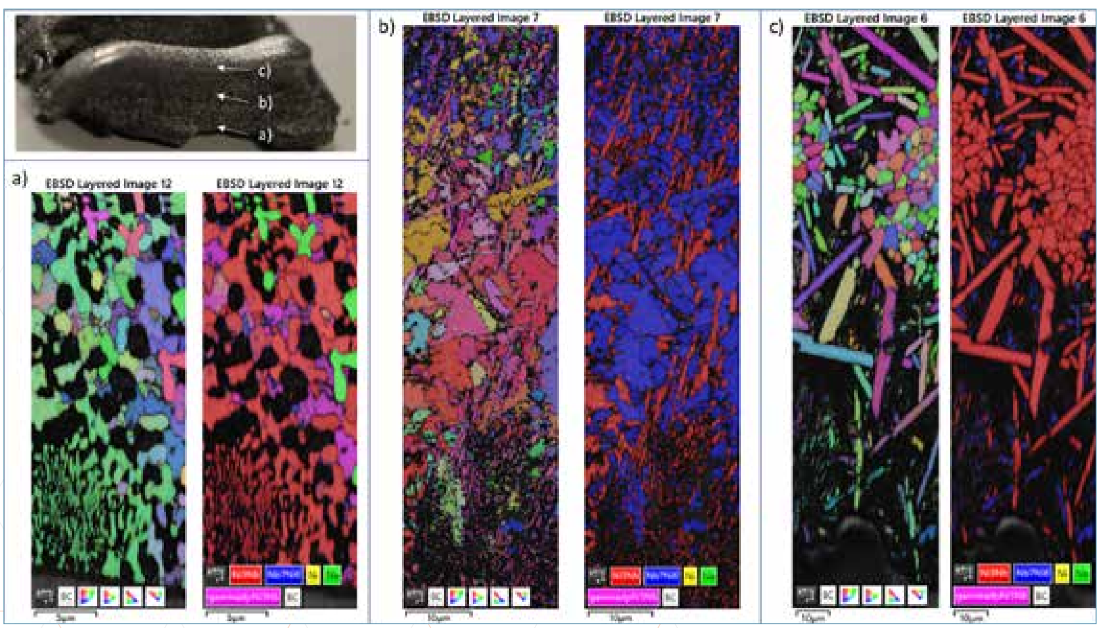
Diagram of environmental learning model. The clustering algorithm produces a model in the feature space of the environment that informs the optimizer. If the environment has changed, the anomaly detection algorithm triggers the optimizers. The optimizer makes dynamic adjustments to system parameters that directly affect the energy utilization of the system to better match the present environment.

BENEFITS IN A COMPACT PACKAGE.

in heterogeneous integration to reduce high-voltage power conversion to a single packaged component: a radiation-hard, high-voltage, chip-scale power converter. This effort exploits Sandia's microelectronics development capabilities to realize a compact converter with high-boost gain, reasonable conversion efficiency, good voltage stability, and resilience in extreme environments. To date, the team has demonstrated a feasible conversion circuit at the printed circuit board level; designed, fabricated, and demonstrated a custom integrated circuit (IC) to control switching using one of Sandia's resilient IC platforms; built and begun testing a chip-scale power inductor; and fabricated an interposer with novel embedded high-voltage components. Demonstration of the chip-scale power converter is expected in FY23.
(PI: Jason Neely)

DESIGNING FUNCTIONALLY GRADED METALLIC COMPOSITES TO ENABLE INTERFACIAL PROPERTIES TAILORED TO MISSION-SPECIFIC NEEDS.

Functionally graded materials have properties that gradually change throughout the material body to enable tailorable responses to external stimuli. The goal of this project was to design tailored, multifunctional, metallic composites with materials properties far surpassing conventional technologies. Enabled by additive manufacturing, this work focused on maturation of near-net shape-processing capabilities targeting a multifunctional materials framework with highly tunable properties to establish a trajectory toward agile, materials-by-design solutions for a wide-range of Sandia and DOE mission-relevant applications. The team used laser-engineered net shaping with multiple powder hoppers to print functionally graded material with extraordinarily high hardness (~15 GPa) and fracture toughness (~70-90 MPa-m1/2) in the transition region. These results were verified on single composition prints with multiple techniques, including nanoindentation and scratch testing. High-resolution microscopy and simulations revealed that plasticity is controlled through the creation of slip planes that are unable to cross phase boundaries. This three-year project has nine published journal articles including ones at *Physical Review Letters*, *Journal of Materials Research*, and *Acta Materialia*, with two others currently in preparation. The team collaborated with faculty at Johns Hopkins University, and Sandia Alliance partners University of Illinois at Urbana-Champaign and University of Texas at Austin. (PI: Michael Chandross)

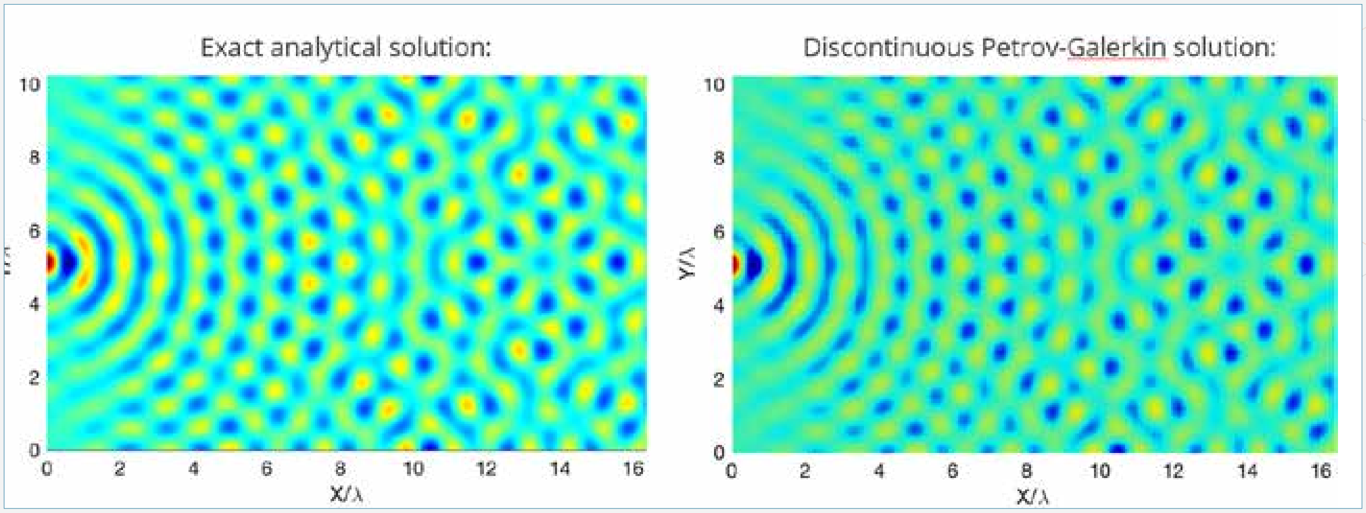


The structural and compositional analysis of an undeformed Ni59.5Nb40.5 alloy built on a Vitreloy 105 substrate using electron backscatter diffraction. Inverse pole figures and phase maps are shown for (A) the region near the substrate, (B) the middle region, and (C) the top region.

Sandia has spent decades developing new additive manufacturing tools and processes to fulfill its unique national security mission. Preview the latest advancements in multi-material AM available for licensing and partnerships. Visit ip.sandia.gov to learn more.

CUTTING-EDGE METHODS AND TECHNIQUES ALLOW ACCURATE PREDICTION OF UHF WAVE PROPAGATION IN MISSION APPLICATIONS.

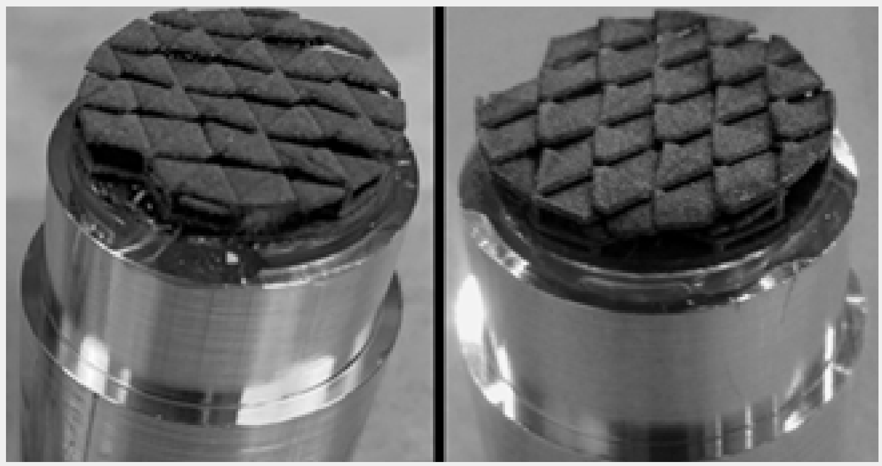
Predicting ultra-high frequency (UHF) wave propagation is important to many civilian and defense applications. Traditional finite element (FE) methods in the Sierra Mechanics code suite provide accurate prediction of structural response up to mid-frequencies. As frequency increases, pollution error limits prediction accuracy. This project developed and implemented cutting-edge numerical methods and techniques allowing accurate prediction at ultra-high frequencies. Pollution-mitigating higher-order elements were extended to elastodynamics in Sierra/Structural Dynamics. The pollution-limiting Discontinuous Petrov-Galerkin (DPG) method, developed by Professor Leszek Demkowicz at Sandia Alliance partner University of Texas at Austin, was implemented as a stand-alone application within the Sierra framework. The Trilinos Project was leveraged for faster implementation, code portability, and graphics processing unit capability. A novel preconditioner was developed in conjunction with matrix-free methods to reduce computational cost. Some achievements, crucial to the success of the current Resilient & Agile Deterrence Mission Campaign projects were applied and will extend to Sierra Mechanics. Recent publications include an article in the *SIAM Journal on Scientific Computing*. (PI: Jerry Rouse)



A two-dimensional time-harmonic acoustics problem was used to verify the DPG implementation. The problem is shown on the right (forcing at midspan on left side, absorbing boundary on the right). Below, the exact solution (derived analytically) is shown on the left, and the DPG prediction is on the right. The length and width are normalized by the wavelength (X/lambda, Y/lambda). There is good agreement with the exact solution for the high-frequency acoustic waves in this problem, which confirms the implementation is working properly.

SANDIA'S MULTIPHYSICS METAMATERIAL LATTICES REDUCE STRESS IN HARSH SHOCK AND VIBRATION ENVIRONMENTS BY 100X.

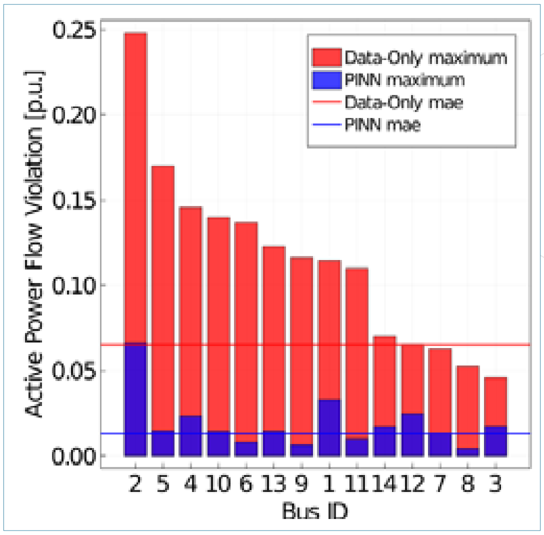
Mechanical metamaterials are an emerging class of materials for mitigating harsh shock and vibration environments. Mechanical metamaterials, here in the form of structural lattices, can be designed to exhibit desirable stiffnesses, vibrational responses, and compressibility to filter, direct, or absorb mechanical energy. The Sandia metamaterial design captures energy in lattices containing triangular-shaped petals. This lattice reduces peak stresses transmitted to the underlying structure. Lattices were additively manufactured at Sandia in 316L steel and tested using lab-scale nanosecond laser impulses and Sandia's larger SPHINX and Z machine facilities. The lattices reduced transmitted stresses by 100x—in some cases to below the measurement noise floor. Sandia Alliance partners at Georgia Tech designed, fabricated, and tested a one-dimensional nonlinear metamaterial for passive, amplitude-dependent energy transmission filtering, demonstrating a complementary approach. (PI: Laura Biedermann)



A steel lattice with triangular-shaped petals mitigated an incident shock with no identifiable damage. (Left and right images show the lattice before and after the incident shock.)

REDLY: RESILIENCE ENHANCEMENTS THROUGH DEEP LEARNING YIELDS OFFER BENEFITS FOR POWER SYSTEMS.

The planning, operation, and real-time security assessment of power systems require the solution of complex optimal power flow problems that are computationally intractable. Contemporary approaches leverage sub-optimal approximations of the power flow physics that limits the ability of operators to protect the grid against threats leading to interrupted service or physical damage. This LDRD addressed these challenges by developing a complete framework for the design, validation, and deployment of physics-informed neural network (PINN) surrogates for power systems. The LDRD team applied Lagrangian-based regularizations of power flow physics to design surrogates with up to 3x improvement in prediction accuracy and 10x improvement in worst-case errors over baseline approaches. The project resulted in the design of the Optimization and Machine Learning Toolkit that demonstrated improved verification of PINNs across multiple applications. It also provided an opportunity to collaborate with Imperial College and Carnegie Melon and facilitate growth opportunities for a PhD intern from Alliance partner Georgia Tech and an undergraduate from National/Regional partner University of Florida. Journal publications from 2022 include *Computer Aided Chemical Engineering* and *Computers & Chemical Engineering*. (PI: Michael Shannon Eydenberg)



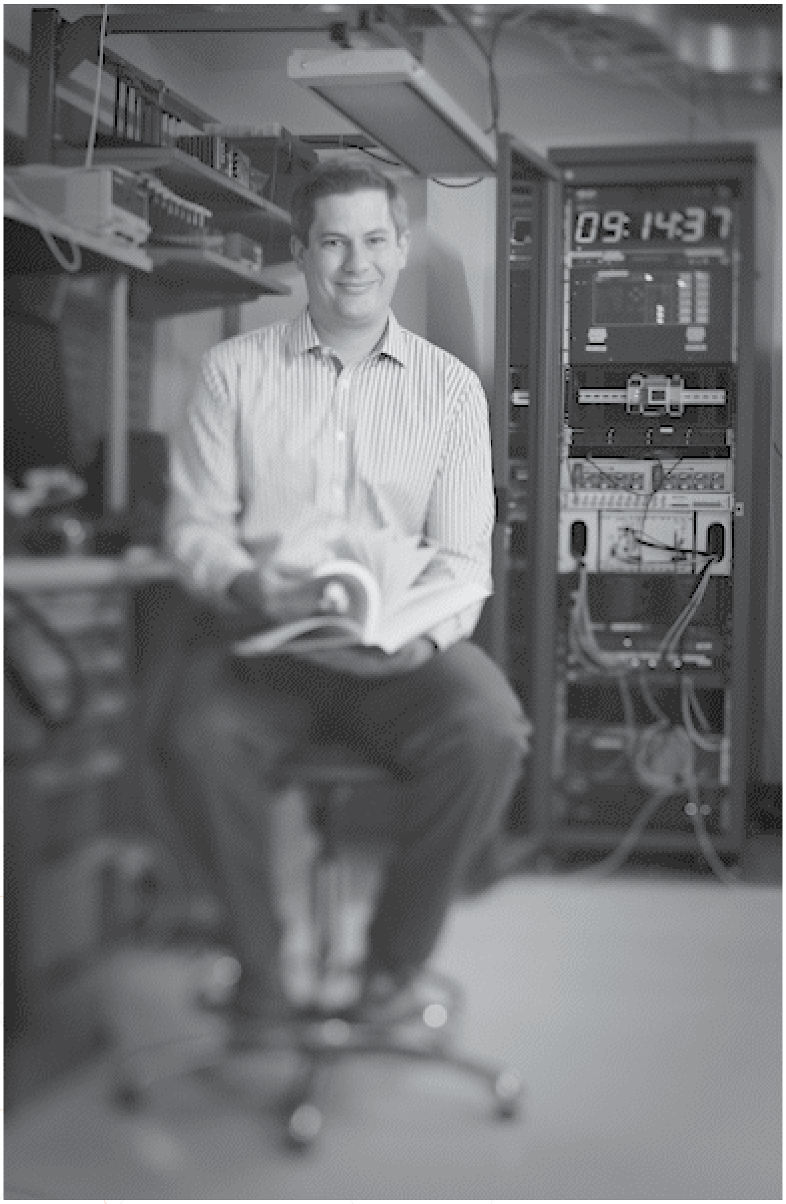
REDLY PINNS (blue) demonstrate significantly improved worst-case violation error over non-PINN baselines (red).

MITIGATING POWER ATTENUATION AND ENABLING MEGASONIC COMMUNICATION IN DEFENSE APPLICATIONS THAT RELY ON HERMETICALLY SEALED FARADAY CAGES.

The electronic shielding necessitated by different mission applications requires new approaches to power transmission and mechanical communication (transduction). This project, which leveraged Sandia's high performance computing and Sierra's massively parallel implementation of the adjoint method for partial differential equation-constrained optimization, enabled a new set of tools for the design and optimization of piezoelectric-based ultrasonic mechanical transduction channels. The risk-averse optimization methods developed in the project enable wide bandwidth data rate communication while mitigating power attenuation. This was accomplished by developing electrical-mechanical-coupled physics modeling, simulation and optimization capabilities that optimized electrical circuit parameters, including thermal preloads, material properties, geometries, and signal optimization. In addition, a posteriori error-based reduced order modeling techniques were combined with optimization under uncertainty in order to minimize computational expense while achieving optimal designs that are robust to model uncertainties. Several follow-on projects are currently leveraging the new modeling and optimization capabilities for early design studies. (PI: Timothy Walsh)

SIGNAL-BASED FAST-TRIPPING PROTECTION SCHEMES FOR ELECTRIC POWER DISTRIBUTION SYSTEM RESILIENCE.

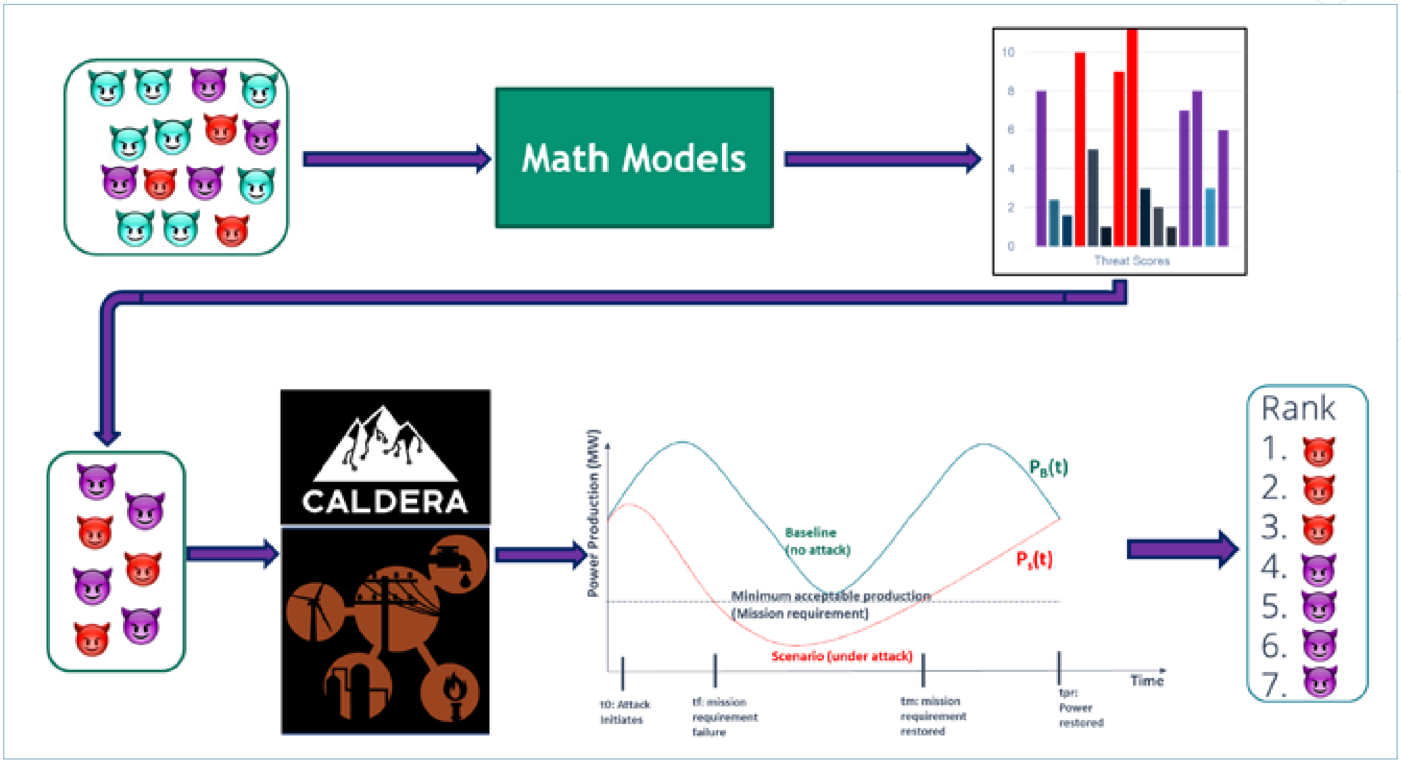
When it comes to national security, it is imperative to accurately detect and quickly remove electrical faults for power system resilience and minimize impacts to defense critical infrastructure. This LDRD team developed novel methods to detect faults in the electric power grid, which are dramatically faster than today's protection systems. Their new signal-based fast-tripping schemes will improve grid stability during disturbances and allow additional integration of renewable energy technologies with low inertia and low fault currents, as they use the physics of the grid and don't rely on communication to reduce cyber risks for safely removing faults. Highly accurate fault location methods were developed for distribution systems, AC and DC microgrids, using high-frequency sensors and signal processing techniques. The algorithms will use less than 0.5 ms of data and compute the fault location within 2 ms for fast tripping protection schemes. This project generated 20 publications, received the best paper award at the 2020 IEEE Kansas Power and Energy Conference, and resulted in several Technical Advances and patents being filed. Faculty, postdoc, and graduate students from Sandia Alliance partner University of New Mexico, Sandia National/Regional partner New Mexico State University, Alliance partner Georgia Tech, and Clemson University collaborated on the project, as did industry partners Siemens, Emera Technology, and Quanta Technology. (PI: Matthew Reno)



PI Matthew Reno worked with IEEE to develop the first standards for microgrid protection.

ADROC: AN EMULATION EXPERIMENTATION PLATFORM FOR ADVANCING RESILIENCE OF CONTROL SYSTEMS.

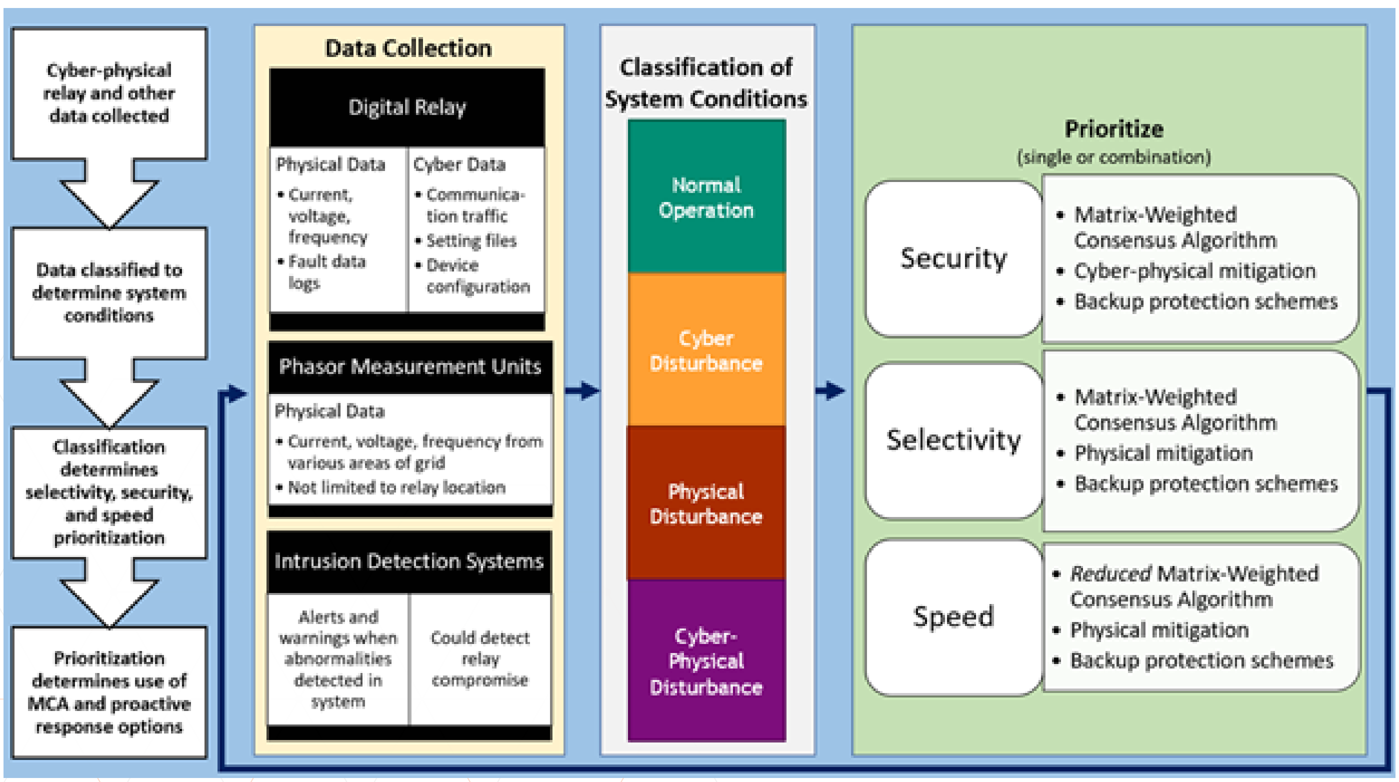
Industrial control systems have increasingly been targeted by cyberattacks, so it is crucial that system owners have tools to understand their systems' resilience to them. Many existing tools, however, are qualitative, generic, or driven by subject matter expertise, making thorough cyber resilience analysis a challenge. The ADROC project, under the Resilient Energy Systems Mission Campaign, developed a two-phase system modeling platform for data-driven resilience analysis and threat prioritization in collaboration with Sandia Alliance partner University of Illinois at Urbana-Champaign. Math models efficiently filter out threat scenarios of low concern, and emulation models enable more detailed analysis for threats of high concern. Data extracted from the experiments are used to calculate cyber resilience metrics and prioritize threats. ADROC can be used to analyze proposed system designs, cyber threats, and more. The work of ADROC, published at the Sat-CPS '22: Proceedings of the 2022 ACM Workshop on Secure and Trustworthy Cyber-Physical Systems, will be extended through future efforts to develop capabilities so critical system owners can understand and improve the cyber resilience of their systems. (PI: Jamie Thorpe)



Overview of the workflow of the ADROC platform.

DEFENSIVE, WIDE-AREA SPECIAL PROTECTION SCHEME PRESERVES ELECTRIC GRID OPERATION BY PROCESSING CYBER-PHYSICAL DATA.

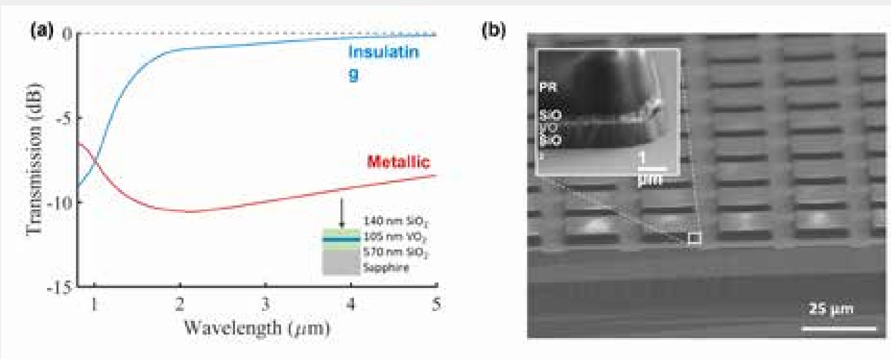
To meet the needs of future special protection schemes (SPS), Sandia and a research team at Sandia's Alliance partner Texas A&M University, proposed a defensive, wide-area SPS that learns system conditions, mitigates cyber-physical consequences, and preserves electric grid operation under diverse disturbances. The Harmonized Automatic Relay Mitigation of Nefarious Intentional Events (HARMONIE) SPS processes cyber and physical data from relay and out-of-band measurements and learns actual system conditions using transformer-based and graph convolution neural networks to adapt to both predictable and unpredictable disturbances. Additionally, it deploys proactive response actions to prevent cascading impact. Through several real-time, cyber-physical emulation disturbance experiments, HARMONIE-SPS demonstrated how processing cyber-physical data for assessing system conditions and informing response provides more comprehensive, effective protection of the electric grid. Six publications on the impacts of this research, achieved in part through collaboration with the Public Service Company of New Mexico, include one presented at the 2021 Resilience Week Conference.
(PI: Shamina Hossain-McKenzie)



HARMONIE-SPS defends the electric grid by processing cyber-physical data, classifying system conditions, and informing response.

PROTECTING SENSORS USING PIXELATED OPTICAL SHUTTERS.

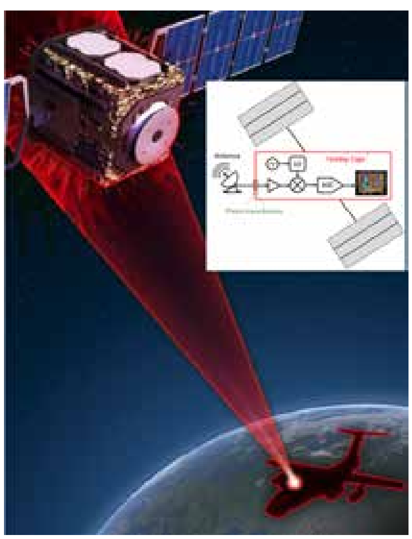
Sensitive optical detectors are subject to permanent damage when exposed to high-intensity laser light, but this can be mitigated using optical limiters or shutters. With the goal of protecting sensors, this LDRD team designed, fabricated, and developed high fill-factor, optically triggered optical limiter arrays based on the phase transition in vanadium dioxide (VO_2). Techniques for depositing and patterning VO_2 thin films were matured, as well as two different computation approaches for designing limiter arrays in this platform. Development of one of these computational techniques was led by Sandia Alliance partner University of Illinois at Urbana-Champaign, who used a two-stage neural network to model and optimize sub-wavelength structures capable of thermally efficient optically limiting. (PI: Michael Wood)



(a) Simulated transmission spectrum of the stacked optical shutter element.
(b) Angled-view scanning electron micrograph of an etched pixel array. Photoresist (PR) is still intact in the image but was removed before optical testing.

ELECTROMAGNETIC THREAT RESILIENCE VIA A PROTECTIVE FARADAY CAGE.

Several key mechanical transduction advancements were made for electromagnetic (EM) resilience in space systems during this LDRD project, including modeling tools to accurately predict performance of prospective Faraday cages and an optimized design that provided measured shielding effectiveness exceeding 80 dB for frequencies up to 20 GHz. The most compelling accomplishment was demonstration of the threat-hardened autonomous watchdog (THAW) concept, where a protected subsystem was operated through a simulated EM attack strong enough to destroy an exposed antenna and overwhelm unprotected electronics. At various stages of this project, Sandia partnered with National/Regional partners University of Colorado Boulder and New Mexico Institute of Mining & Technology, and also leveraged the expertise of a graduate student at Sandia Alliance partner Georgia Tech. Key impacts, which were reported in one publication and six presentations, include providing Sandia space missions with novel architectures for protecting critical assets, enabling capabilities not previously possible for other governmental agencies, and improving robustness for commercial space operations. This project advanced the tools and knowledge base that will empower space system designers to integrate barrier transduction solutions into satellites for increased EM resilience. (PI: Charles Reinke)



The use of a Faraday cage provides shielding effectiveness to space systems such as satellites when subjected to an EM attack.

SPACEWEASEL: A LOW SWAP, CYBER-ANOMALY DETECTION CAPABILITY FOR SATELLITES.

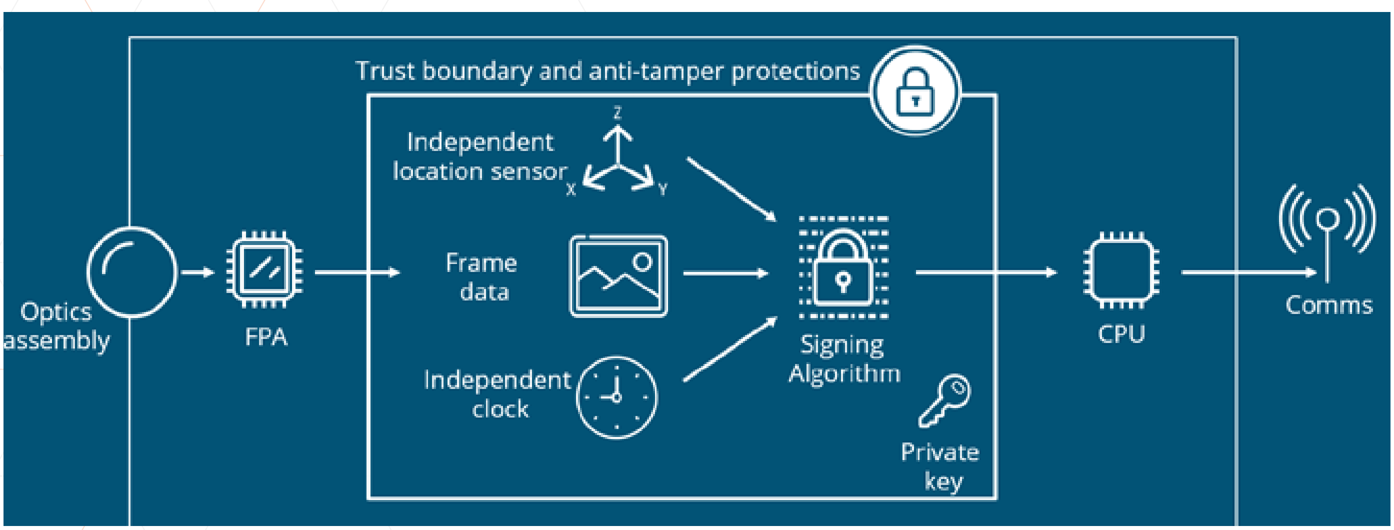
With increasing concerns about cyberattacks on satellites, demand for cyber-resilient systems is rising. Anomaly and threat detection, the first design principles of cyber-resilience, remain in a nascent state for satellites. Current sensor and detection schemes cannot differentiate between normal failures (hardware, environmental, etc.) and a cyber-attack. To address these challenges, this project developed a distributed sensor in software. The team implemented the software capability, one that can detect cyber anomalies in real-time while meeting space, weight, and power constraints with no negative impacts on the primary mission, and tested it in a Sandia satellite-cluster operating system. The solution is novel as it does not require extra hardware to qualify for the space mission and can also be extended for implementation in existing satellite resources by using small portions of extra computing and memory without the need for radiation hardening or other hardware-related requirements. (PI: John Montoya)

INTEGRITY BOX ASSURES THE AUTHENTICITY OF DATA PRODUCED BY THIRD-PARTY SATELLITE VENDORS.

Increased access to space has opened the door to many satellite vendors. The project team identified certain requirements for trusting imagery from third-party vendors and then designed hardware, software, and systems of controls to meet those requirements for Earth-imaging satellites. The trusted hardware provides assurance of capture time, location, and preserves the content and origin by capturing and digitally signing the original data, enabling end users to make trust decisions about the data. The Sandia hardware functions as an independent witness that oversees and signs off on satellite collection activities.

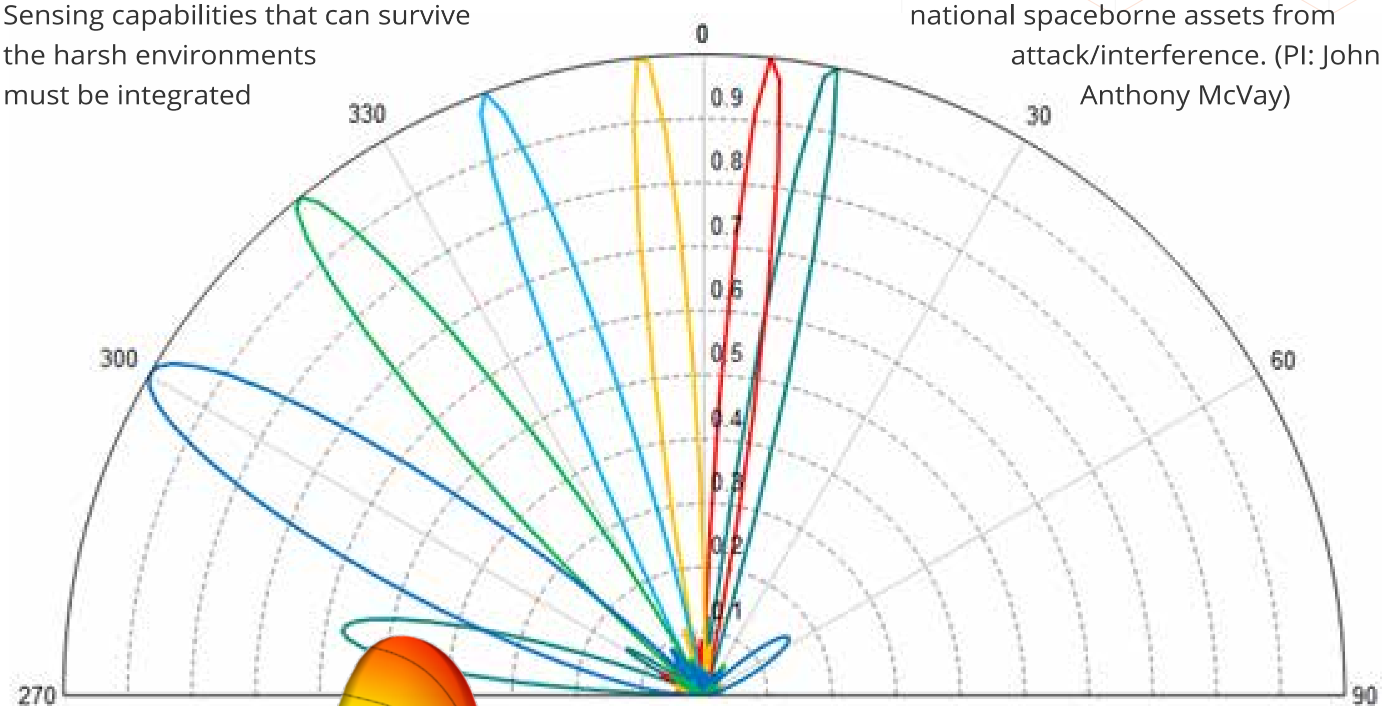
Anti-tamper, inspection, and verification measures are essential in protecting and verifying the secure operation of the team's hardware. Satellite operators using this approach in their satellites and operations will offer their end users greater assurance in the authenticity of the produced satellite imagery products. The project PI spoke about the work, "On Trusting Third-party Satellite Data," at the 36th Annual Small Satellite Conference in 2022. (PI: Sean Michael Crosby)

Sandia's Integrity Box architecture provides independent assurance of a satellite collection by signing the data which includes collection time and location information.

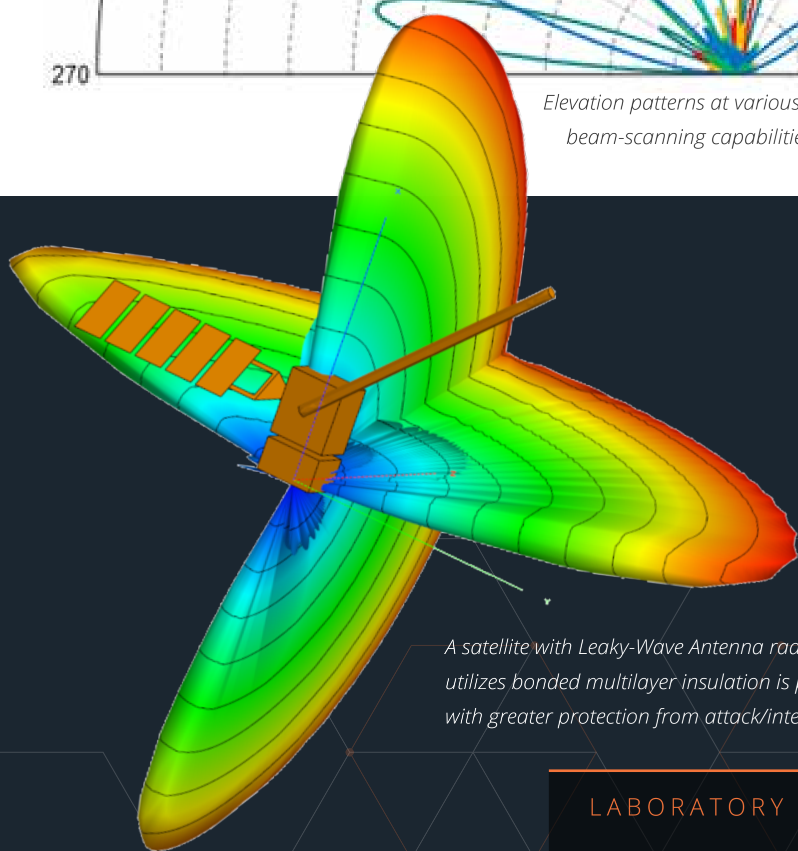


SATELLITES ENVELOPED WITH STITCHED ENGINEERING SENSORS FOR DETECTION OF APPROACHING OBJECTS.

In contested space, spaceborne assets are vulnerable and must be able to monitor their surroundings. To protect sensitive electronics, the assets utilize multilayer insulation (MLI) to provide a stable operating environment. The environmental stability underneath the MLI is exploited for those components not able to survive outside in the extreme temperatures. Sensing capabilities that can survive the harsh environments must be integrated to the asset's exterior. In this project, a Leaky-Wave Antenna radar was designed and fabricated using bonded MLI materials, and the radar was integrated onto the MLI. Uncertain material parameters, including material electrical permittivity and loss tangent, were extracted and estimated for bonded spaceborne MLI. The capability provided by this design will help defend national spaceborne assets from attack/interference. (PI: John Anthony McVay)



Elevation patterns at various frequencies of operation within the 5-12 GHz band showing the beam-scanning capabilities of the Leaky-Wave-Antenna with bonded multilayer insulation.



A satellite with Leaky-Wave Antenna radar that utilizes bonded multilayer insulation is provided with greater protection from attack/interference.

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.

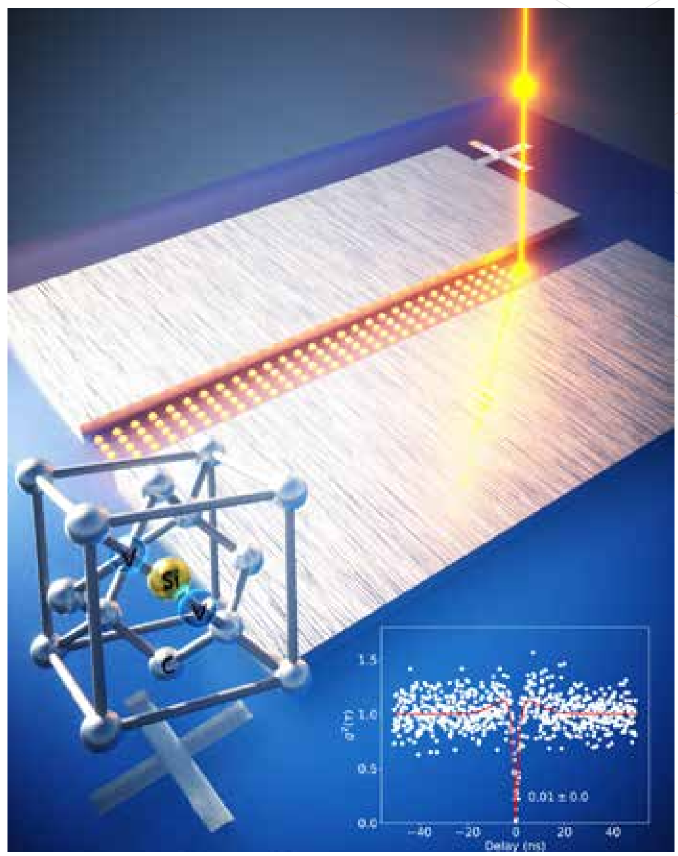
WIDE-BANDGAP SEMICONDUCTORS BENEFIT FROM DEVELOPMENT OF SINGLE-PHOTON SOURCES IN GALLIUM NITRIDE.

Gallium nitride (GaN) is a very hard, mechanically stable wide-bandgap (WBG) semiconductor that permits devices to operate at much higher voltages, frequencies, and temperatures, and is a key component in LEDs, lasers, and certain radio frequency applications. Single-photon emitting color centers (defects or substituted atoms with optical transitions within the host's bandgap) in WBG semiconductors are an important platform for quantum information sciences and can provide both on-demand single photons and long-lived quantum spin states.

Andy Mounce, Sandia researcher and PI of the "Development of Single Photon Sources in GaN" project, was one of four employees in the nation to earn DOE's Early Career Research Award in 2022.

Recent demonstration of single photon emission in GaN and the utility of GaN for LED lighting and high-power electronics led the LDRD team, which included faculty member Kevin Jones at Sandia National/Regional partner University of Florida and faculty member Victor Acosta at Sandia Alliance partner University of New Mexico, to investigate the creation and understanding of single photon emitters in GaN. The energy levels of color centers from defects and transition metal substitutions in GaN were calculated using Sandia-created SeqQuest density functional theory (DFT) code, which avoids typical inaccuracies of DFT for wide-bandgap semiconductors, to better understand the origin of recently observed (and to be created) single photon emission in GaN.

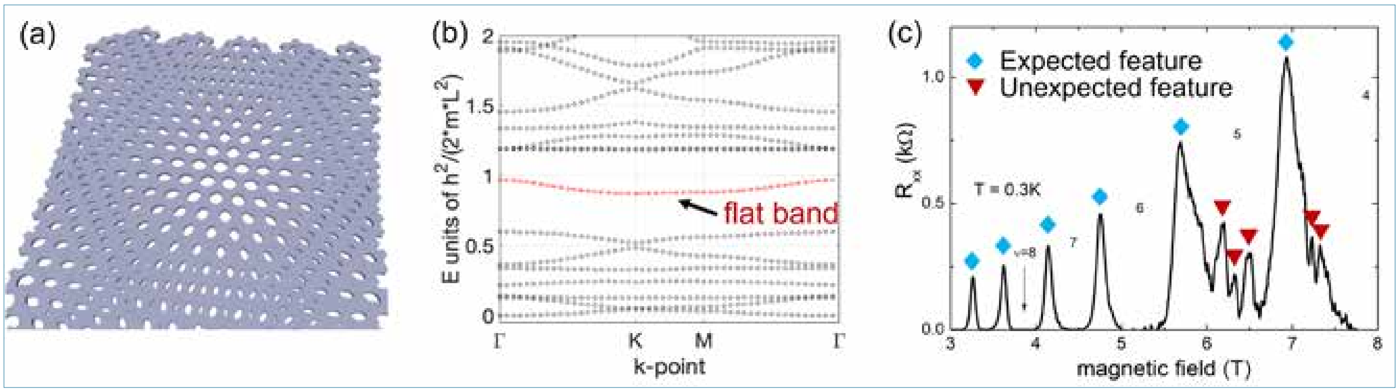
Through this project, the team developed new techniques for improving the accuracy of Sandia's unique nano-focused ion beam implantation capabilities and created new capabilities for characterizing color centers through focused ion beam implantation. These techniques and capabilities benefit WBG semiconductors used in military, radio and power conversion applications, and act as a foundational technology for new electrical grid and alternative energy devices and vehicles. (PI: Andrew Mounce)



Single-photon sources based on atom-like features in solid-state materials offer the prospect for integrated, on-demand solid-state platforms and are being intensively explored for numerous mission-related quantum information technologies. New techniques for improving the accuracy of Sandia's unique nano-focused ion beam implantation capabilities were developed through this LDRD project.

SEMICONDUCTOR TWISTRONICS WILL ENABLE FUTURE QUANTUM INFORMATION SCIENCE APPLICATIONS.

The three-year semiconductor twistronics project aims to advance the field of moiré quantum materials (MQM) for quantum information science (QIS) applications by exploring MQMs composed entirely of compound semiconductors. Four years after the exciting discoveries in magic-angle twisted bilayer graphene, traditional MQMs face daunting issues. These challenges are inevitable in new quantum states and correlated phases. By making semiconductor MQMs a new QIS materials platform, future QIS applications can build on, and be compatible with, the sophistication and maturity of the state-of-the-art semiconductor industry. This project, conducted in collaboration with Sandia Securing Top Academic Research Talent at Historically Black Colleges and University

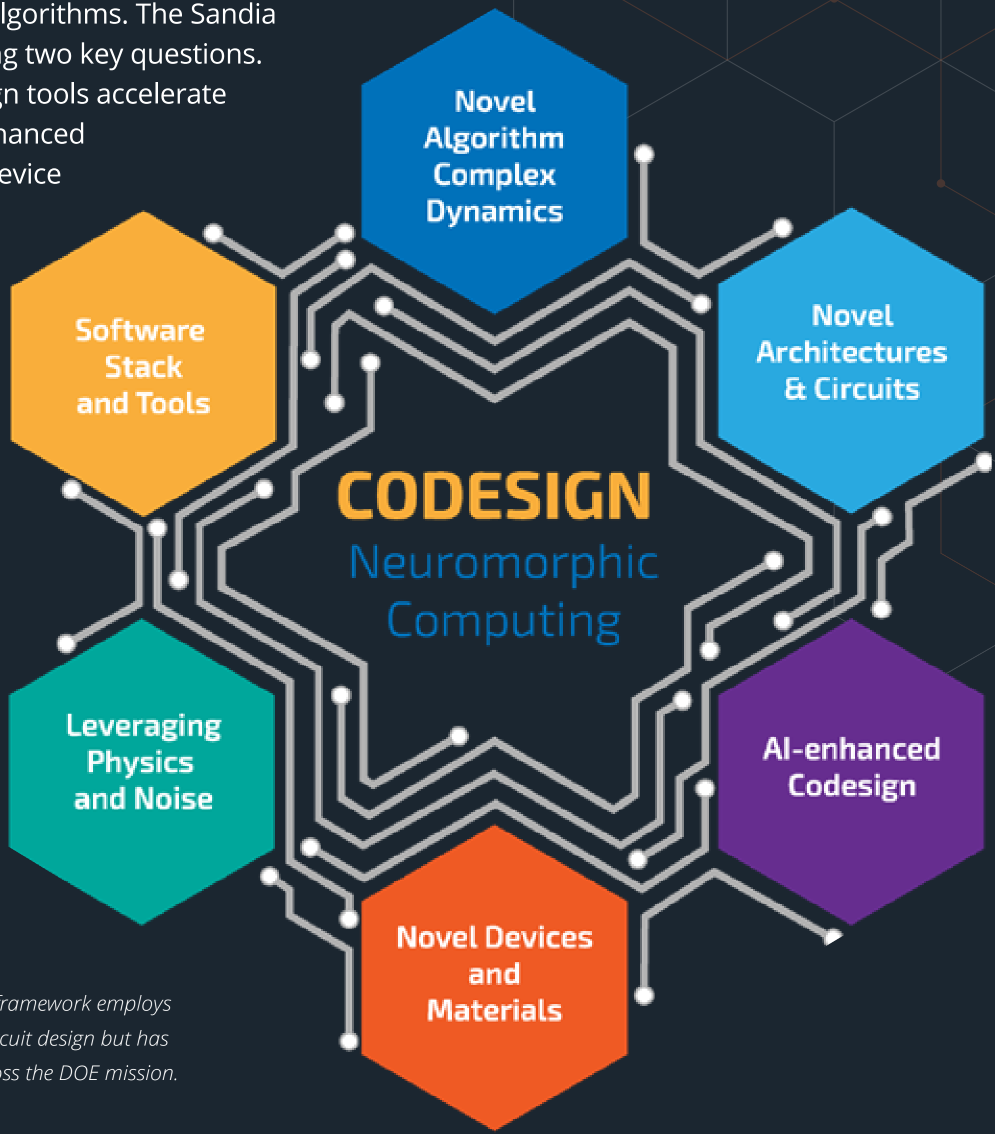


(a) A schematic showing two hexagonal patterns etched into the 2D electron gas of an Indium Arsenide (InAs) quantum well, twisted to form a moiré pattern. (b) Theoretical modeling showing the presence of a flat band separated from other continuous bands. (c) Preliminary observations, in a prototype semiconductor moiré structure, of unexpected quantum transport features (triangles). These features are in addition to the usual peaks (diamonds) and are reminiscent of exotic quantum states observed in twisted bilayer graphene. They are absent in InAs structures without moiré patterning.

traditional MQMs due to reliance on mechanical exfoliation of flakes to create one-off devices. The Sandia research eliminates major device-to-device variations by using lithographically defined semiconductor MQMs. This further enables controlled parameter tuning over wide ranges. Such tunability is essential to unravel mysterious quantum materials phenomena that is already observed but poorly understood, and to discover (START HBCU) partners Norfolk State University and Prairie View A&M University, Sandia Alliance partner University of Illinois at Urbana-Champaign, and the University of Southern California and University of Texas at Dallas, has resulted in a publication in *Nanotechnology*, three Technical Advances, and two patent applications that are in prosecution. (PI: Wei Pan)

AI-ENHANCED CODESIGN FOR NEXT-GENERATION NEUROMORPHIC CIRCUITS AND SYSTEMS.

Circuit design involves an assembly of interconnected circuit elements that perform a specific objective function. Neuromorphic computing is a prime candidate to employ AI-enhanced methods in developing circuits, systems, and architectures due to plethora of novel devices, diverse methods of encoding/decoding of inputs/outputs, and neuro-inspired algorithms. The Sandia research focused on answering two key questions. One, can AI-enhanced codesign tools accelerate circuit design? Two, can AI-enhanced tools be leveraged for novel device discovery? The team, in collaboration with Sandia Alliance partner Georgia Tech, focused on design rather than just circuit optimization solutions and leveraged reinforcement learning and evolutionary algorithms. The result was a new AI-enhanced framework for automated circuit design and approaches for novel device discovery. The complete framework can be extended beyond circuit design and will be useful for mission-relevant applications in nuclear deterrence, code generation, and supply chain management. The PI from this one-year project was invited to give two presentations, and the team filed a Technical Advance, with plans for a patent application. (PI: Suma George Cardwell)



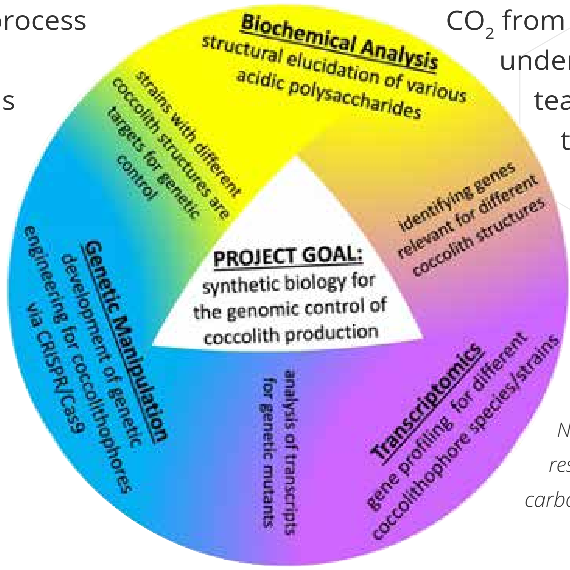
New neuromorphic computing framework employs AI-enhancements to facilitate circuit design but has many opportunities for use across the DOE mission.

USING PHAGE-BASED, SPECIES-SPECIFIC EDITING OF THE ALGAE MICROBIOME TO IMPROVE ECONOMIC VIABILITY OF ALGAE GROWTH AS FEEDSTOCK.

The major challenge with using algae as a feedstock is growing it economically, which hinges strongly on the ability to prevent pond crashes due to biotic factors, like bacteria. Phages, the viruses of bacteria, offer an unexplored solution to this problem. In contrast to antibiotics, phages are typically species-specific and might be used to rescue pathogen-infected cultivations without affecting the native microbiome. To test this idea, Sandia identified a highly virulent pathogen of an elite algae strain and showed that phages rescue the algae culture from the pathogen. The next step showed that algae lacking a microbiome are more susceptible to the pathogen. Finally, the microbiome was moved from the control algae to the culture lacking a microbiome, showing that the transplanted microbiome restores the protective effects against the pathogen. In summary, there were two countermeasures identified that can be used to improve resilience and increase productivity of algal biomanufacturing systems. (PI: Jesse Cahill)

BIOMIMETIC CALCIFICATION FOR CARBON SEQUESTRATION FROM SEAWATER.

An integrated data science and experimental approach is being taken to the challenges of direct capture of CO_2 from the ocean. A large group of marine microalgae, coccolithophores, produce calcium carbonate (calcite) plates referred to coccoliths. This calcification process is linked to inorganic carbon acquisition for photosynthesis and plays an important role in the global carbon cycle. Researchers on this project discovered the genetic controls of the biological calcification processes, characterized the chemical mechanisms that drive calcite formation, and, ultimately, decoupled the calcification process from photosynthetic carbon fixation. This will allow achievement of the project goal of increasing the per cell rate of calcification, thus removing more CO_2 from seawater. In the long term, by understanding the in vivo process, the team will be able to reconstitute the process in a hybrid bio/inorganic system able to carry out calcification without the biological limitations thus enhancing CO_2 capture. (PI: Todd Lane)



Numerous objectives are involved in helping researchers work on biomimetic calcification for carbon sequestration from seawater.

IMPROVING/TESTING ML METHODS FOR BENCHMARKING SOIL CARBON DYNAMICS REPRESENTATION OF LAND SURFACE MODELS.

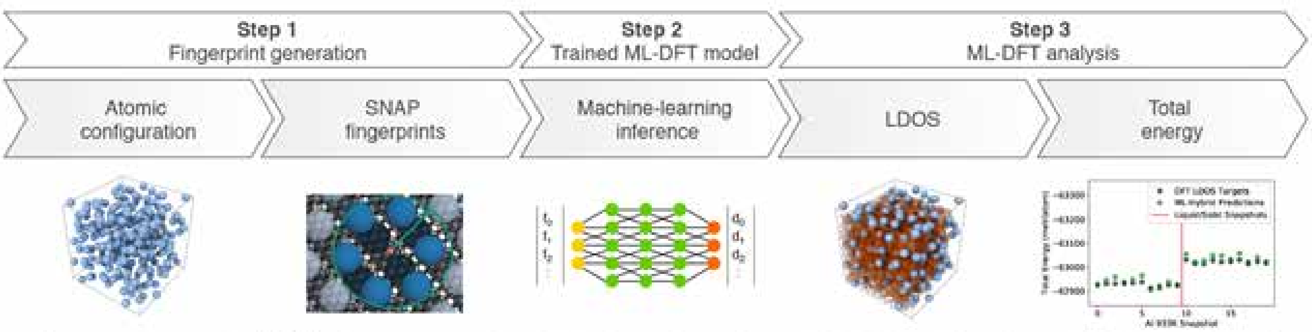
Representation of soil organic carbon (SOC) dynamics in Earth system models (ESM) is a key source of uncertainty in predicting carbon climate feedbacks. The magnitude of this uncertainty can be reduced by accurate representation of environmental controllers of SOC stocks in ESMs. In this study, researchers used data of environmental factors, field SOC observations, ESM projections and ML approaches to identify dominant environmental controllers of SOC stocks and derive functional relationships between environmental factors and SOC stocks. Derived mathematical relationships were derived to benchmark the coupled model intercomparison project phase six ESM representation of SOC stocks, and divergent environmental control representation in ESMs were found in comparison to field observations. Representation of SOC in ESMs can be improved by including additional environmental factors and representing their functional relationships with SOC consistent with observations. This project was highlighted in the *Soil Science Society of America*.
(PI: Umakant Mishra)

UTILIZING NONLOCAL INTERFACE PROBLEM ALLOWS FOR 7X SPEEDUP IN LARGE SCALE SIMULATIONS.

Multimaterial problems exist in mission applications such as mechanics and subsurface transport. To capture effects arising from long-range forces at the microscale and mesoscale that aren't accounted for by classical partial differential equations, the MAThematical foundations for Nonlocal Interface Problems (MATNIP) project team developed a mathematically rigorous interface theory employing nonlocal models that use integral as opposed to differential operators. By applying their theory to domain decomposition methods, the team was able to achieve speedups of up to 7x in solve in solve time in large-scale simulations. The issue of parameter selection for nonlocal models from experimental data was successfully tackled using both adjoint optimization and ML approaches. The Sandia team collaborated with Los Alamos and Oak Ridge National Laboratories, as well as Florida State University, Sandia Alliance partner UT Austin, and Lehigh University. The project team had fifteen publications, presented talks, and a former team member, Marta D'Elia, was nominated for the SIAM Wilkinson Price in Scientific Computing and Numerical Analysis for contributions to nonlocal modeling. (PI: Christian Glusa)

ACCELERATING MULTISCALE MATERIALS MODELING WITH MACHINE LEARNING.

Multiscale materials modeling provides fundamental insight into microscopic mechanisms that determine materials properties in nuclear stockpile applications that leverage radiation-harden semiconductors, advanced manufacturing, shock compression, and energetic materials. This LDRD team including three postdoctoral researchers developed a new ML surrogate model for density functional theory using deep neural networks to accurately predict total energies of 100,000 atom systems when trained on only 256 atoms. When compared with direct numerical simulation of 2048 aluminum atoms, the error in electron density of the new surrogate model is under 1%, but computation is three orders of magnitude faster. Promising methodologies such as optimal experimental design techniques and novel Graph Neural Networks were explored in training smaller data sets and will be researched further in the future to continue accelerating first-principle data generation and increase the fidelity and robustness of predictive atomistic materials simulations. An ML model designed for aluminum has already been successfully leveraged in Sandia's Electronics Parts Program milestone. (PI: Sivasankaran Rajamanickam)



(a) Snapshot of an atomic configuration.

(b) Bispectrum components at each point on a Cartesian grid

(c) Feed-forward neural network.

(d) ML-DFT prediction of the local density of states (LDOS) on Cartesian grid.

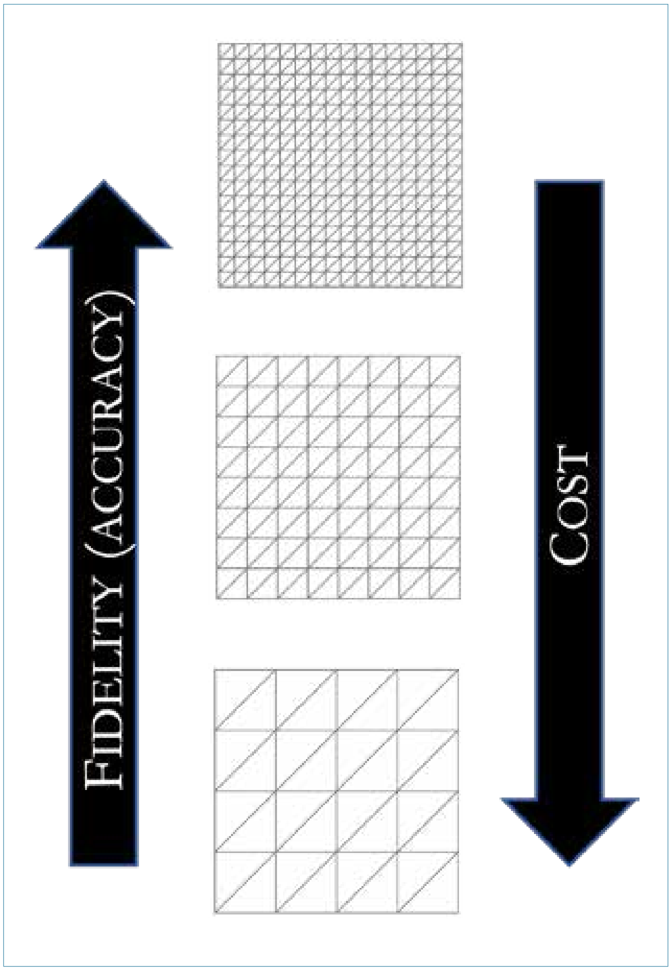
(e) ML-DFT prediction of the total energy for both solid and liquid phases.

OPTIMIZING MACHINE LEARNING DECISIONS WITH PREDICTION UNCERTAINTY.

While ML classifiers are widespread, their output is often not part of a follow-on decision-making process because of lack of uncertainty quantification. Through this LDRD, the team developed decision analysis methods that combined uncertainty estimates for ML predictions with a domain-specific model of error costs. In the project, they explicitly weighed whether ML models under evaluation were qualified to make any prediction by producing general algorithms that minimized prediction error costs by validating these algorithms through demonstrations on cyber security and image analysis cases. The developed and trained ML classifier ultimately provided a framework for: (1) quantifying and propagating uncertainty in ML classifiers; (2) formally linking ML outputs with the decision-making process; and (3) making optimal decisions for classification under uncertainty with single or multiple objectives. Methods developed through this project are currently being incorporated into applications that impact national security domains by directly addressing questions of automated decision. (PI: Michael Darling)

REDUCING THE COST OF QUANTIFYING UNCERTAINTY USING MULTI-FIDELITY FUSION AND RESOURCE ALLOCATION.

Quantifying uncertainty in computationally expensive numerical simulations via repeated evaluation of the highest-fidelity model is often intractable. Approximations of the highest fidelity model (e.g., simplified physics, reduced order, or ML models) can be used to reduce the computational cost of quantifying uncertainty but can introduce significant error. This two-year project developed novel multi-fidelity methods that judiciously integrate limited high-fidelity data alongside data from multiple cheaper models to both: (1) construct accurate ML models; and (2) produce unbiased estimates of uncertainty. The team's methods have repeatedly reduced the cost of quantifying uncertainty by 1-3 orders of magnitude when applied to applications spanning plasma physics to ice-sheet models and can increase the utility of ML models, by leveraging them alongside high-fidelity simulation to make validated predictions with quantified uncertainty. This project resulted in five publications and numerous invited and contributed talks to several high-profile societies. The team partnered with students, postdocs, and faculty at various universities, including Sandia National/Regional partner University of Michigan, Sandia Alliance partner Texas A&M University, Notre Dame, University of Southern California, University of Utah, and Michigan State University. (PI: John Davis Jakeman)



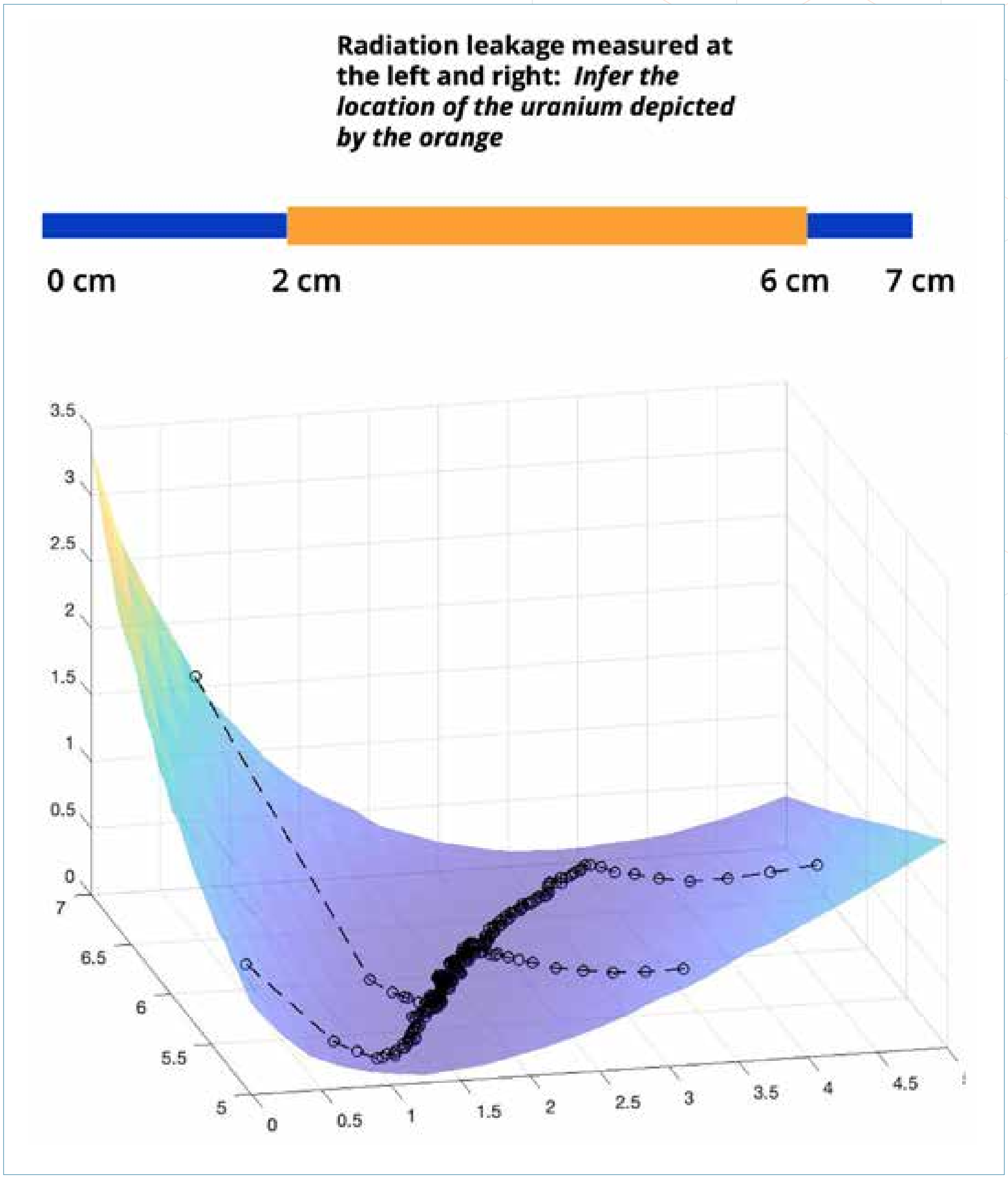
By using novel multi-fidelity methods that integrate limited high-fidelity data alongside data from multiple cheaper models, the team repeatedly reduced the cost of quantifying uncertainty by 1-3 orders of magnitude in various applications from plasma physics to ice-sheet models.

IDENTIFYING AND CHARACTERIZING DISINFORMATION RISKS IN NATIONAL SECURITY MISSIONS.

Cyber-influencing via foreign disinformation campaigns is a fundamental challenge that poses a serious threat to national security missions, especially since the rise of social media platforms has lowered the adversary's cost of operations. This work expanded the quantitative analytic methods available to the national security community by producing software based on a mathematical formalism called the non-abelian Fourier transform. The software, which combines the accurate identification of adversarial tactics with digital media context, determines likely indicators of a foreign disinformation campaign, and is already impacting Sandia missions in emerging spaces. It will also support future early-warning systems. (PI: Michael Brzustowicz)

ACCOMPLISHING MORE WITH LESS COMPUTATION USING MONTE CARLO SAMPLING-BASED PARTICLE SIMULATIONS.

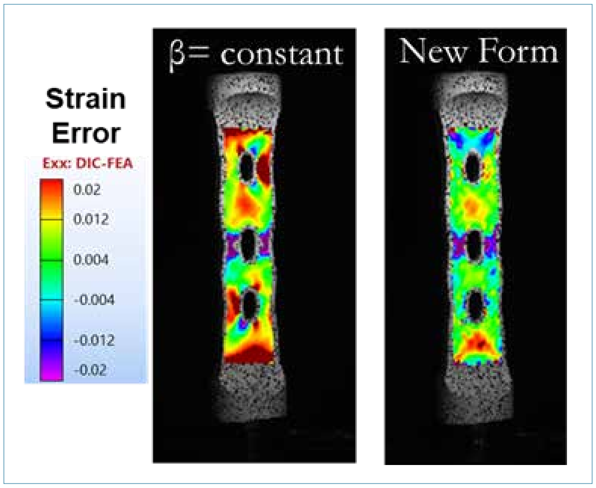
Particle models for Brownian dynamics, radiation transport, low-density fluids, and plasmas lack a gradient-based optimization capability for various problems of interest, e.g., inverse problems. Such a capability enables the particle simulation communities to go beyond forward simulation by accomplishing more with less computation. Gradient-based methods crucially depend upon sensitivities, which are synonymous with the calculation of a derivative that measures the change in a quantity with respect to a change in another quantity. The team, who partnered with faculty at Tulane University, University of Delaware, and Sandia National/Regional partner North Carolina State University, provided a proof-of-concept demonstrating a gradient-based optimization capability for Monte Carlo sampling-based particle simulations is possible. The PI for this two-year project gave two invited talks and two contributed talks on the research. (PI: Richard Lehoucq)



An example problem involves inferring the location of the orange material along the horizontal axis given radiation leakage measurements at the left and right. The example, showing four different gradient descent iterations computed via reuse of Monte Carlo samples for the desired values of 2 cm and 6 cm overlaying the surface, is proof-of-concept that a gradient-based optimization capability for Monte Carlo sampling-based particle simulations is possible.

UNDERSTANDING THE COUPLING BETWEEN HEAT GENERATION AND MECHANICAL WORK IN LARGE DEFORMATION PLASTICITY.

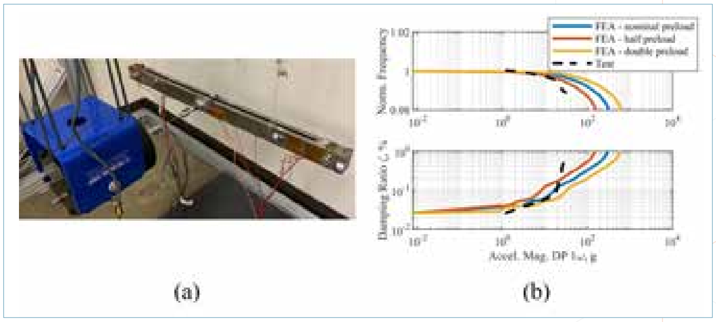
Accurately predicting material failure is of high value to any number of applications including accident/ crash scenarios. When metals deform plastically, a large amount of energy is generated, which is classically understood to be either stored in the metal or dissipated, usually as heat (described by a single, constant parameter β). The dissipation as heat leads to a temperature rise, increasing the local strain rate in a feedback loop, until ductile failure. The key impacts from this LDRD project include a comprehensive thermomechanical dataset, simulation development (including a functional form for β), and a mechanism to quantitatively compare coupled mechanical behavior to simulation. The dataset includes use of emerging microstructural analysis tools to quantify energy stored in the microstructure and full-field diagnostics. The wide range of states interrogated allows careful evaluation of model form error, which will lead to predictive thermomechanical models. This project resulted in one patent, numerous conference presentations (including the 16th International Conference on Advances in Experimental Mechanics [the British Society for Strain Measurement] where it won a Best Paper Award, a proceedings paper at the ASME Conference in 2021, and two journal publications (*Measurement Science and Technology*, *Strain, An International Journal for Experimental Mechanics*). (PI: Amanda Jones)



Coupling between heat generation and mechanical work with high amounts of generated energy shows plastically deformed metals.

ADVANCING STRUCTURAL DYNAMICS CAPABILITIES WITH NONLINEAR MODAL ANALYSIS.

Linear modal analysis has served as the cornerstone of computational and experimental structural dynamics for many years. Nonlinearity, such as frictional contact or nonlinear materials, may invalidate the assumptions necessary to model the dynamics with linear system theory. The Sandia LDRD team set out to extend the computational and experimental modal analysis framework to characterize, identify, and predict vibration response of nonlinear mechanical systems. The novel "nonlinear phase resonant mode" theory provides a consistent mathematical definition for both simulation and test methods. The nonlinear modes are identified experimentally using active controllers to maintain a phase quadrature condition. The simulation counterpart uses the multi-harmonic balance method with continuation to efficiently compute the periodic orbits from nonlinear models. The generalized, nonlinear modal analysis framework is applicable to arbitrary conservative and non-conservative nonlinearity. This project resulted in ten publications including recent articles in *Mechanical Systems and Signal Processing* and *IOPScience*, and numerous conferences and society meeting presentations. The LDRD team collaborated with Sandia Alliance partners from the University of New Mexico, Georgia Tech, and Texas A&M University. They also collaborated with the Sandia National/Regional partners from New Mexico State University, ETH Zurich, Los Alamos National Laboratory, and ATA Engineering. (PI: Robert Kuether)



Nonlinear phase resonant mode testing shows: (a) a Phase resonance test of a nonlinear beam assembly, and (b) a correlation of measured and predicted amplitude dependent natural frequency and damping ratio.

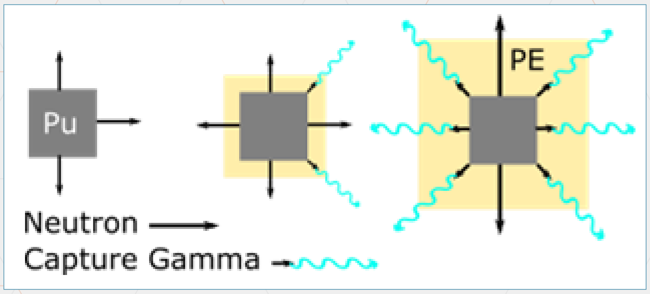
MALGEN: MALWARE GENERATION WITH SPECIFIC BEHAVIORS TO IMPROVE MACHINE LEARNING-BASED DETECTORS.

Damage caused by malware to applications in the national security sector is increasing at exponential rates. Leveraging ML techniques for its detection can achieve greater than 99% classification accuracy on benchmark datasets, but performance drops significantly in deployed settings The Sandia MALGEN LDRD team, in collaboration with Sandia National/Regional partner New Mexico Tech, explored and addressed this gap by proposing a novel evaluation method that held out a malware family from training and determined this type of evaluation provided more realistic results. Malware was detected by discerning commonly exhibited behaviors such as Dynamic Link Library injection and process hollowing, which goes beyond signature-based methods by (1) assuming a set of behaviors common to most malware samples exist, and (2) the detection of behaviors will generalize to novel malware. Performance was further improved by generating additional synthetic malware with specific behaviors. The methods determined through this three-year project lay a foundation for improved integration of ML that have been highlighted in two journals and four conferences/workshops. (PI: Michael Reed Smith)

NUMEROUS MISSION APPLICATIONS MAY BENEFIT FROM NEUTRON-CAPTURE GAMMA MULTIPLICITY COUNTING MEASUREMENTS.

Neutron multiplicity analysis is a technique used for estimating the mass and multiplication of special nuclear material configurations. However, in heavily moderated configurations, neutron leakage is reduced due to thermalization and subsequent capture of neutrons. As neutron leakage is reduced, measurement efficiency decreases, resulting in increased measurement times and larger uncertainty in mass and multiplication estimates based on standard neutron multiplicity analysis. In this collaborative project, which included researchers at Oak Ridge and Los Alamos National Laboratories, the team experimentally validated the viability of the neutron-capture gamma multiplicity signature through a series of experiments in which they measured a 4.5 kg mass of weapons-grade plutonium in various moderator configurations and accurately estimated assembly multiplication. These results, which demonstrate significant promise for potential application to the emergency response, warhead verification, and nuclear safeguards communities, were presented at the Institute of Nuclear Materials Management Annual Meeting. (PI: Kyle Polack)

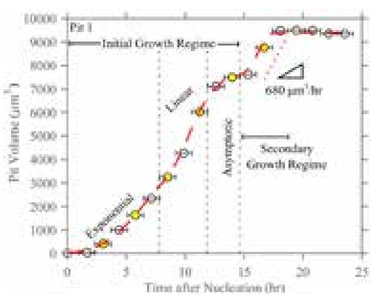
Measurement of a 4.5 kg sphere of weapons grade plutonium moderated by 6" of high-density polyethylene (HDPE) using an array of sodium iodide detectors (rear). In this photo, the moderating sphere is half assembled, which allows the plutonium and the nested HDPE shells to be seen. The measurements were performed using a fully assembled moderating sphere. The nested shells made it possible to assess the performance of the technique using a parametric study over a range of HDPE thicknesses.

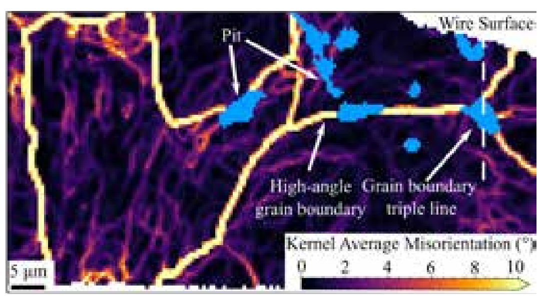


A cartoon depicting a plutonium source surrounded by an increasing amount of moderator. As the polyethylene (PE) surrounding the plutonium (Pu) grows, the neutron leakage increases due to rising neutron multiplication but eventually diminishes as neutrons are absorbed to emit characteristic gammas. These capture gamma rays can act as surrogates for captured neutrons.

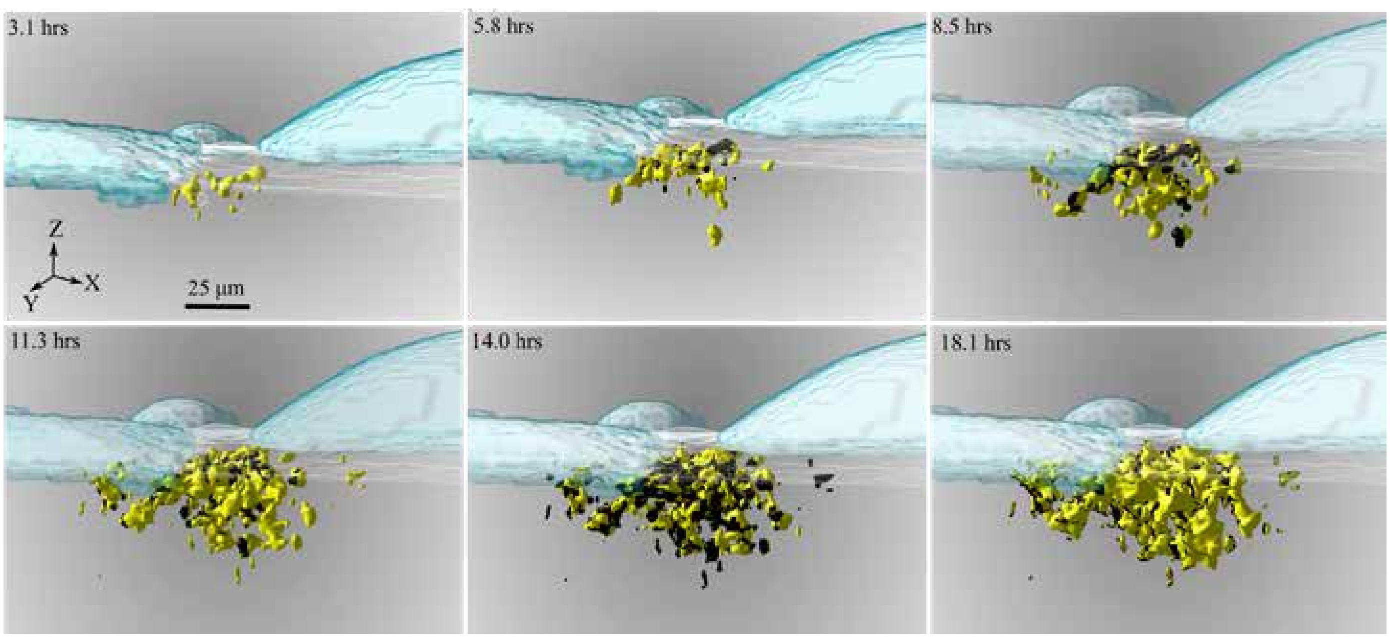
REVEALING THE KINETICS OF ATMOSPHERIC CORROSION DAMAGE THROUGH IN-SITU X-RAY COMPUTED TOMOGRAPHY AND MACHINE VISION.

Atmospheric corrosion is a critical materials degradation problem, yet the ability to predict its kinetics remains elusive. Conventional approaches provide no information about how localized damage evolves, giving limited predictive capabilities in common scenarios. The goal of this Sandia LDRD team was to employ in-situ X-ray computed tomography to directly observe how corrosion damage evolves, enabling the mechanistic relationships between environmental drivers, microstructural triggers, and the kinetics of atmospheric corrosion to be uncovered. To exploit the insights held within hundreds of 3D datasets, custom machine-vision algorithms were developed to automatically identify critical features. Ohio State University conducted electrochemical experiments to unravel these relationships and revealed that corrosion rates are closely tied to the evolution of the electrolyte and the local microstructure, enabling the development of predictive tools for Sandia missions. Other academic collaborators who contributed to this work were Sandia Alliance partners Georgia Tech and the University of Texas at Austin. This work has resulted in five journal publications including one in *npj Materials Degradation*, one in *Corrosion – The Journal of Science & Engineering*, and two in *Journal of The Electrochemical Society*, and four presentations. (PI: Philip Noell)



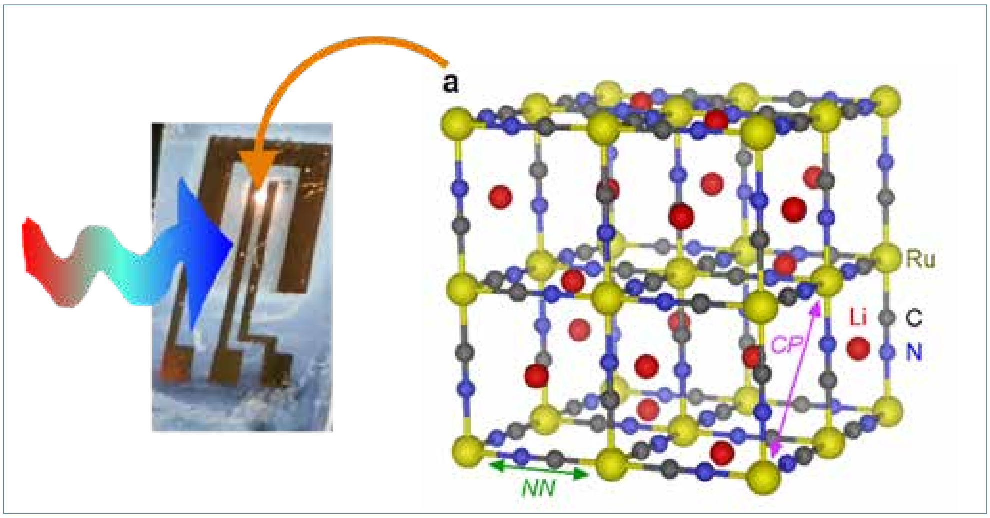


In-situ XCT enables both the growth rate and morphology (yellow) of pits to be directly characterized in relationship to the evolving electrolyte (blue) and prior stages of pit morphology (black).



PROTON-TUNABLE ANALOG TRANSISTOR FOR LOW-POWER COMPUTING.

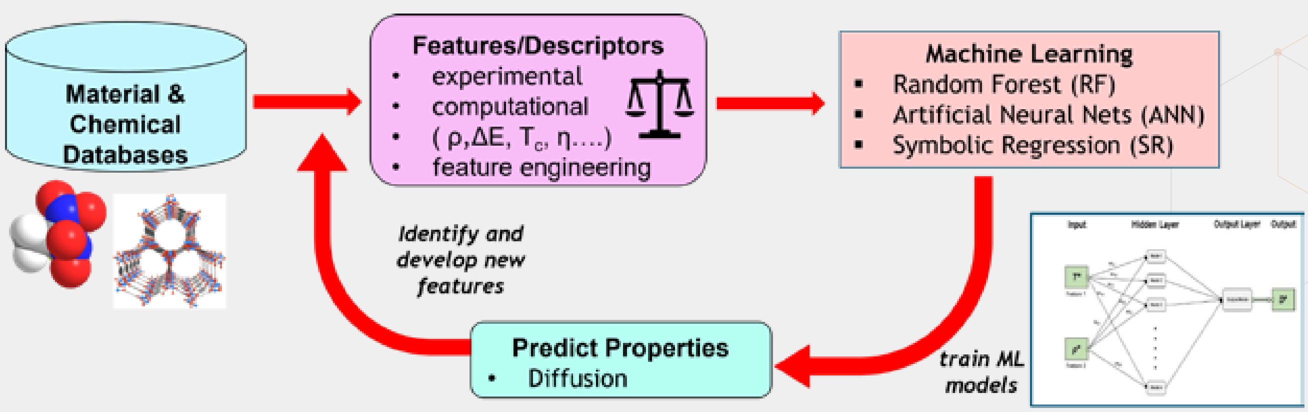
Motivated by the need for efficient analog signal processing, this Sandia LDRD team discovered that mixed valence coordination compounds called Prussian Blue Analogue (PBA) can be used for inkjet-printed flexible artificial synapses that reversibly switch conductance by more than four orders of magnitude based on electrochemically tunable oxidation state. Retention of programmed states is improved by nearly two orders of magnitude compared to the extensively studied organic polymers, which enable in-memory compute and avoid energy costly off-chip access during training. They demonstrated dopamine detection using PBA synapses and biocompatibility with living neurons, evoking prospective application for brain-computer interfacing. Application of electron transfer theory to in-situ spectroscopic probing of intervalence charge transfer elucidates a switching mechanism. When this occurs, the degree of mixed valency between N-coordinated Ru sites controls the carrier concentration and mobility. This work was published in a recent article "Tunable Intervalence Charge Transfer in Ruthenium Prussian Blue Analog Enables Stable and Efficient Biocompatible Artificial Synapses" in the *Journal of Advanced Materials*, as well as five other articles. The Sandia team worked with the Arizona State University and the Sandia National/Regional partner Stanford University. PI A. Alec Talin was recently invited to join the Science Magazine Board of Reviewing Editors. (PI: A. Alec Talin)



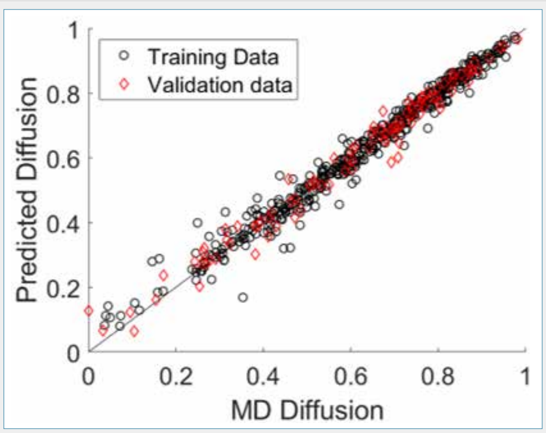
In-situ spectroscopy reveals a new charge transport mechanism and how to control it.

MACHINE LEARNING TO GO BEYOND THE DARKEN EQUATIONS IN MULTICOMPONENT MIXTURES.

Prediction of fluid transport properties—particularly in confined environments—can accelerate the materials discovery process for applications including energy storage, separations, catalysis, and drug delivery. Transport properties of fluid mixtures in porous environments are extremely difficult to obtain experimentally, and extensive modeling efforts are required to thoroughly sample the composition space needed for material prediction. To overcome these challenges, the Sandia LDRD team used ML to predict individual diffusion rates quickly and accurately for single and multi-component fluids in bulk and porous environments. By integrating different response functions directly in the model development process, the underlying relationships describing the physics and chemistry controlling diffusion were identified. The resulting ML-derived models provide extremely fast diffusion prediction for a wide range of fluid systems and pore architectures. This work has resulted in nine publications with numerous invited and contributed conference talks. One publication was highlighted on the Kudos Research Showcase website (click the Read Article section to view this article). Another publication was an Editor's Pick for inclusion in a collection of hottest articles of 2021 in the journal *Physical Chemistry Chemical Physics*. (PI: Jeffery Greathouse)



The workflow for the development of ML-derived models for diffusion prediction involves iterative refinement of the features and algorithm.

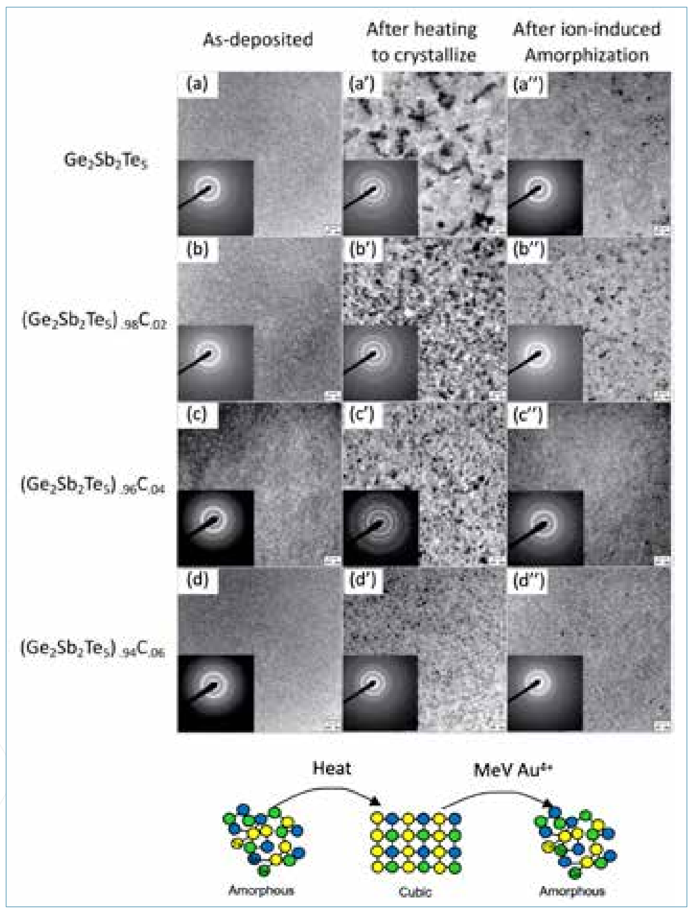


ML model development enables quick and accurate prediction of individual diffusion rates for single and multi-component fluids.

UNDERSTANDING THE EFFECTS OF RADIATION ON RECONFIGURABLE PHASE CHANGE MATERIALS.

Chalcogenide thin films that undergo reversible phase changes show promise for next-generation nanophotonics, metasurfaces, and other emerging technologies. This general class of thin films can be switched rapidly between amorphous and crystalline phases which exhibit contrasted optical and electronic states. Despite the successful development of benchmark $Ge_2Sb_2Te_5$ for some applications, there is a desire to identify new materials with improved performance. The Sandia LDRD team focused on the behavior of sputter-deposited $(Ge_2Sb_2Te_5)xC1-x$ [0 < 1-x < 0.12] films and investigated the phase stability and key unknowns of several promising quaternary compositions. This study confirmed increased crystallization temperatures of C-doped $Ge_2Sb_2Te_5$ consistent with enhanced amorphous phase stability. Additional experiments involving high energy, and heavy ion irradiation explored the stability of films subjected to collision-induced disordering. Detailed characterization showed that crystalline films can be amorphized by ion irradiation (metamictization) and quaternary addition affects radiation tolerance. This study provides new insight into chalcogenide phase stability offering design pathways for future applications. The project involved collaborations with students and faculty from Sandia Alliance partner Purdue University and National/Regional partner University of Florida. This work generated multiple publications including one extensive article in the *Journal of Physics*. PI David Adams was also recently elected Fellow and President of American Vacuum Society: Science and Technology of Materials, Interfaces and Processing.
(PI: David Adams)

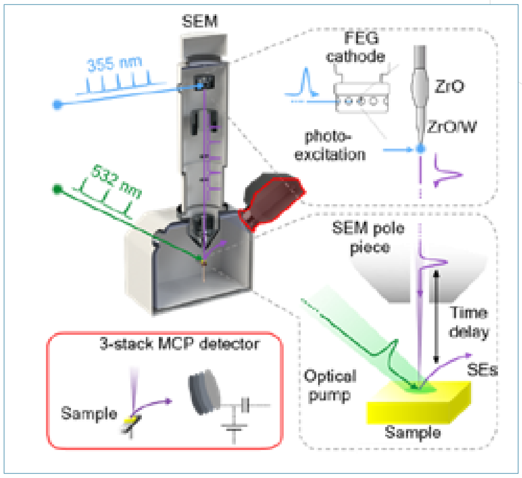
David Adams was elected Fellow and President of American Vacuum Society: Science and Technology of Materials, Interfaces and Processing in 2023.



Plan view transmission electron micrographs and electron diffraction patterns comparing a non-doped film with three films of varied, doped composition. Films are shown after deposition, heating to crystallize, and MeV Au ion irradiation to high dose. Lack of distinct spots in the diffraction patterns post-irradiation is evidence of amorphization.

DEVELOPMENT AND UTILIZATION OF QUANTITATIVE SECONDARY ELECTRON IMAGING FOR THE STUDY OF QUANTUM COMPUTING MATERIALS.

Electronic components are approaching their fundamental limits in terms of energy, speed and size. To be able to predictively design sub-10 nm components, accurate measurements of the thermodynamics of the underlying materials (their terminal states) are needed, and also of the kinetics of the energy carriers that dictate speed and energy limits. The scanning ultrafast electron microscope (SUEM) successfully measured picosecond-resolved carrier kinetics with an unprecedented combination of spatial, temporal, depth and surface potential information. This Sandia LDRD team worked on optoelectronic materials gallium arsenide and indium arsenide (InA), and measured, for the first time, the carrier time constants in InAs. The SUEM tool revealed surprising negative-time kinetics influenced by a combination of surface and vacuum potentials. This cutting-edge technique will speed up manufacturing of electronics via predictively choosing and designing materials without having to manufacture and measure entire electronic devices. This work generated one paper under publication, and several conference talks sponsored by the Materials Research Society. Due to this work, Chris Perez, a Sandia a year-round intern, graduated with his PhD from Stanford University and was awarded a doctoral fellowship at the Advanced Light Source at Lawrence Berkely National Laboratory. (PI: Suhas Kumar)



The SUEM measuring a combination of electrical components showing spatial, temporal, depth, and surface potential information.

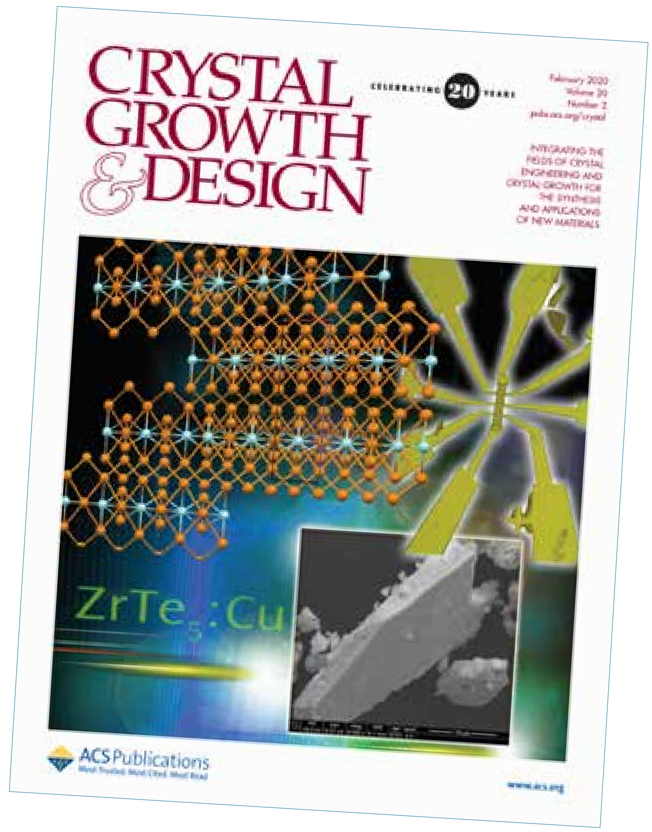
PHONONIC MEMORY AND OPTICAL TELEPORTATION USING OPTOMECHANICS: HARDWARE ACCELERATORS FOR QUANTUM COMPUTERS.

Linking quantum computers via transparent optical networks would enable significant progress in the development of quantum information systems. This LDRD project investigated transduction of a superconducting qubit microwave photon to a flying optical photon in fiber utilizing a piezoelectric transducer and optomechanical crystal. This approach takes advantage of the individual components; as superconducting qubits excel in computation, optical photons are efficient for long-distance communication, and long-decoherence-time phonons are suitable to serve as an intermediary.

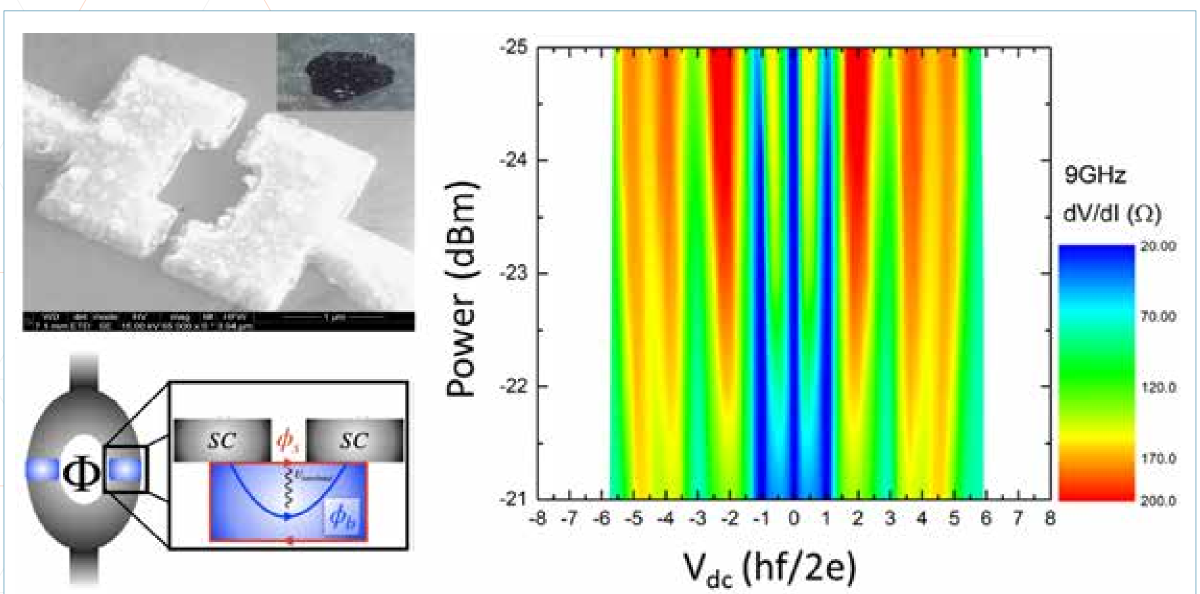
In this project, the superconducting qubit, piezoelectric transducer, and optomechanical crystal were developed on the same silicon membrane platform. Moreover, the team developed a theoretical framework to optimize the control and operation of these components to form quantum networks. The work from this LDRD project was published in *npj quantum information*, *Journal of Physics A,* and *Physical Review Research,* and was developed in collaboration with Sandia Alliance partner University of Texas at Austin. (PI: Matt Eichenfield)

SINGLE PHOTON DETECTION WITH ON-CHIP NUMBER-RESOLVING CAPABILITY.

The ability to detect single photon quanta plays a key role in fundamental science and advanced engineering applications. Rapid development of quantum information applications is now necessitating on-chip single photon detection (SPD) with deterministic number resolution in the microwave range of the EM spectrum. In this project, the Sandia team achieved high quality materials synthesis, and experimentally explored and theoretically simulated microwave response and SPD in superconducting quantum interference devices (SQUID) realized in topological Dirac semimetals (DSM). Importantly, these initial results reveal that DSMs are a promising material system for SPD at the needed microwave frequencies. The studies of the microwave response of DSMs, conducted in collaboration with the College of William & Mary and Sandia Alliance partner Georgia Tech, led to a high-impact discovery of the presence of the Leggett mode, a collective quantum phenomenon predicted more than 50 years ago. This project produced nine high impact journal publications, five Technical Advances, and one submitted U.S. patent application.
(PI: Wei Pan)



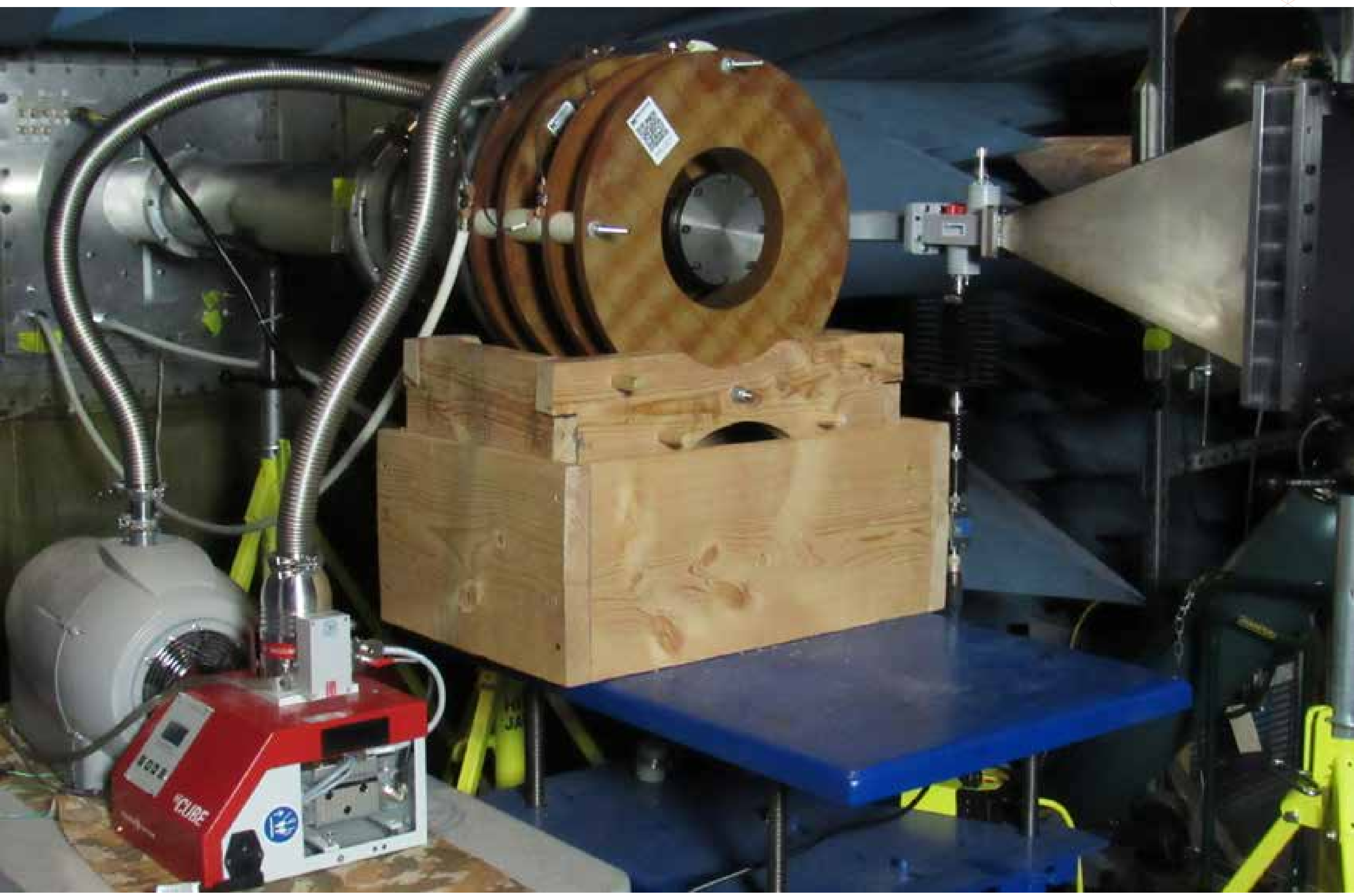
One publication, Single-Crystal Synthesis and Characterization of Copper-Intercalated $ZrTe_5$, was featured on the cover of Crystal Growth & Design.



The top left shows the as-grown single crystal and a SQUID. The superconducting (SC) proximitized surface (ϕ) and bulk (ϕ) channels are coupled via interband pairing ($U_{interband}$), giving rise to a Leggettt mode. The suppression of the even Shapiro steps (high dV/dI value) at 9 GHz is due to the Leggettt mode.

MULTIPLE HIGH-POWER PHASE-LOCKED HPM SYSTEMS HAVE THE ABILITY TO INCREASE DIRECTED ENERGY STRIKE EFFECTIVENESS.

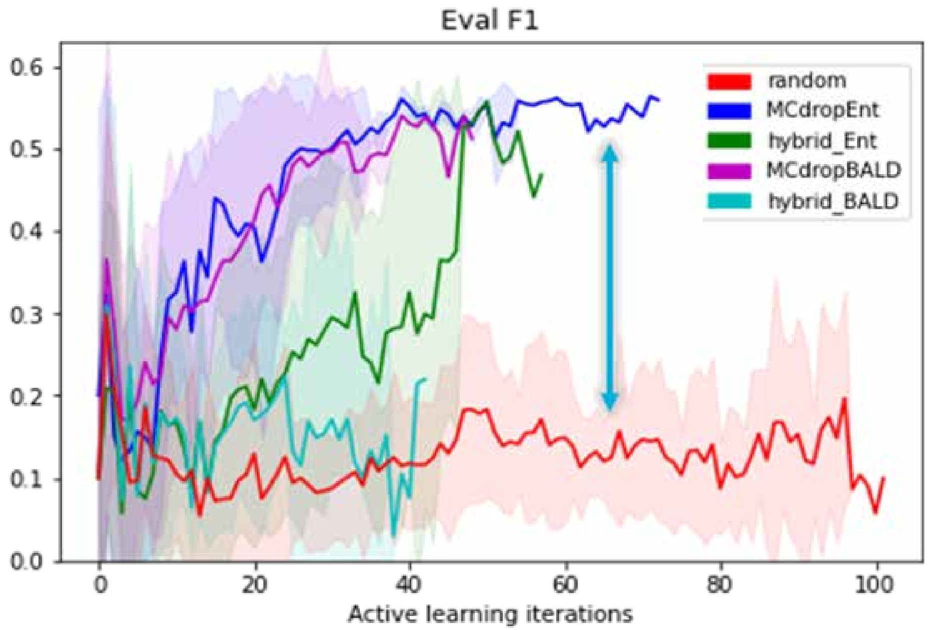
Advantages to a phased array of high-power microwave (HPM) systems include increased power and range of engagement in various defense applications. The pinnacle challenge to achieving such systems lies in controlling the initial random phase of the HPM. This LDRD explored seed-locking the gigawatt (GW)-class HPM source to an orders-of-magnitude lower seed signal. Seed-locking is achieved by creating the electromagnetic fields in the HPM tube prior to plasma oscillations to lock the plasma mode to these established fields. During this three-year LDRD, a GW-class, S-Band HPM system was constructed to oscillate at two narrowband frequencies. In collaboration with the Air Force Research Laboratory, a one-megawatt, commercial-off-the-shelf magnetron was integrated into the HPM system as the seed. Ultimately, evidence of phase-locking between the two sources was not concluded. Timing between the seed source and the HPM pulsed-power is critical, and the shot-to-shot jitter varied tremendously. This HPM system will serve as a testbed for new and ongoing research into distributed HPM systems. (PI: Andrew Sandoval)



GW Class S-Band high-power microwave system.

IMPROVING ACTIVE LEARNING FOR LANGUAGE MODEL TO COMBAT DISINFORMATION.

Various supervised language-modeling techniques can help decipher and dismantle disinformation campaigns, but they rely heavily on large, human-labeled training datasets. This LDRD addresses this problem by deploying active learning (AL) to generate labeled datasets and optimize human input. Task adaptive pretraining was used to leverage the unlabeled data and boost the performance of the classifier. A disinformation rhetoric metric was created to measure the presence of common disinformation rhetoric, for both the classifier and human to leverage. The DRM was combined with an uncertainty criterion to create a hybrid acquisition method. A sophisticated and robust stopping strategy was developed to save human time from being wasted on iterations that would not significantly benefit classifier performance. This work laid the foundation to continue using AL in the disinformation data annotation domain and to shift the AL paradigm to optimize human input. This project was sponsored by Sandia Fellow Bill Miller. (PI: Emily Kemp)



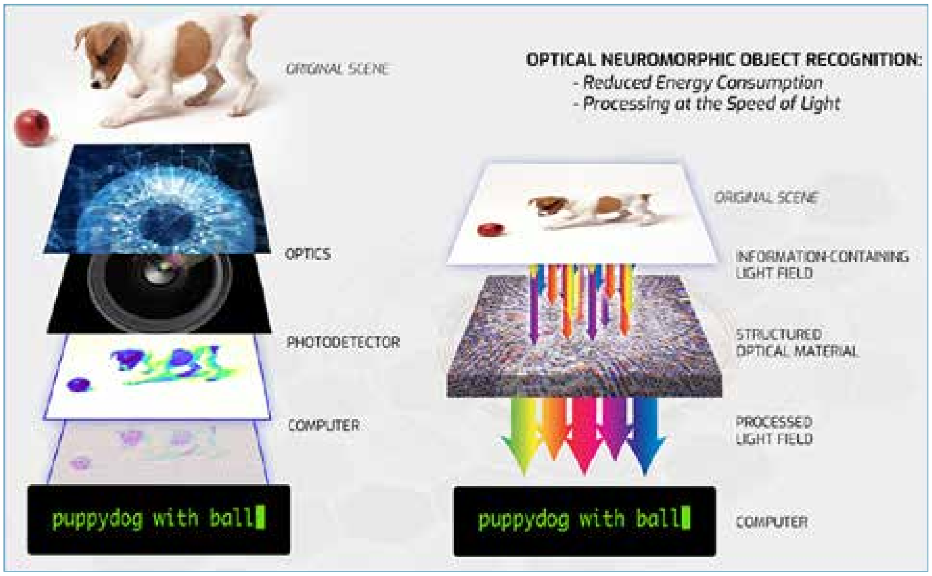
Averaged AL simulation results.

EXPERIMENTAL QUANTUM-ENABLED, SUPER-RESOLUTION IMAGING TECHNIQUE IS A '

Rayleigh diffraction limits the obtainable imaging resolution from conventional imaging techniques by making it hard to discriminate an object's geometrical features smaller than the wavelength of probe light. Rayleigh-diffraction-limited imaging resolution is explained in quantum mechanics as a consequence of light-noise fluctuation (i.e., shot noise). Sandia developed a super-resolution quantum imaging technique where a much smaller (enhanced) imaging resolution can be obtained by employing squeezed light, where light noise is significantly reduced below the shot noise. This LDRD team advanced the technology by delivering squeezed light with 10 dB less noise than the shot noise. Such a large noise reduction allows a significant advance in performance as compared to Rayleigh-diffraction-limited conventional imaging. This quantum imaging technique will be a game changer in biology and chemistry, where super-resolution optical diagnostics will elucidate the underlying physical processes. This project was co-sponsored by two Sandia Fellows – Ed Cole and Dave Chandler. (PI: Daniel Soh)

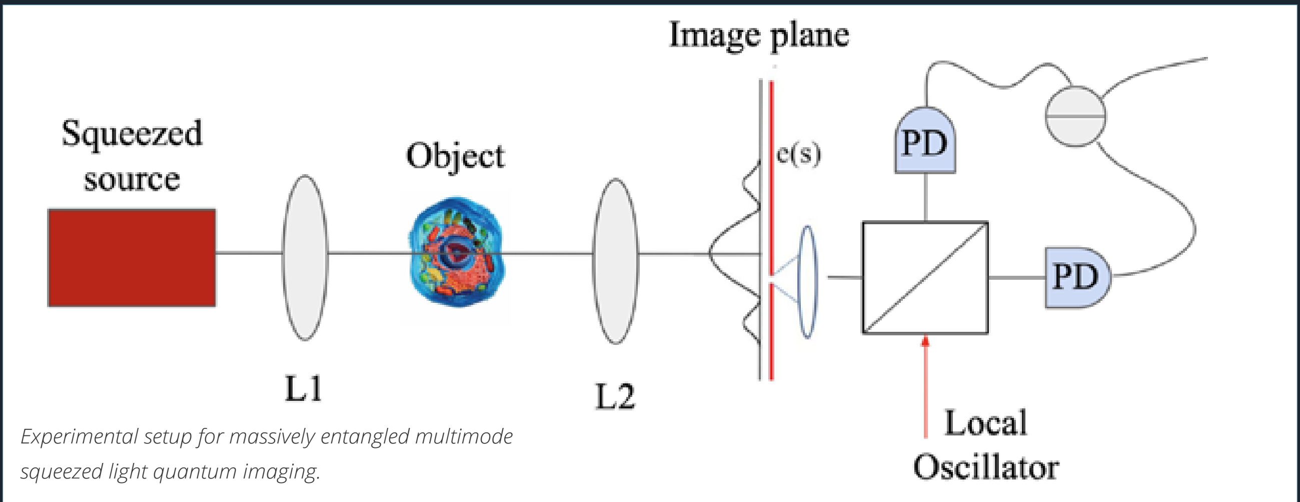
NEUROMORPHIC INFORMATION PROCESSING BY OPTICAL MEDIA OFFERS ENERGY EFFICIENCY AND INCREASED SPEED.

Identifying features in a scene from emitted or reflected light is at the core of many applications such as remote sensing, autonomous driving, and biological imaging. Usually, this is accomplished by converting the incoming photons to electrons using a camera, and then analyzing the digital images using algorithms running on computers. This approach requires significant energy and time. In this LDRD, Sandia explored a radically different approach where a passive material can directly process the incoming light and act as a neuromorphic classifier at the speed of light. This demonstrates that such systems can be as good as electronic neural networks, but with much lower energy consumption and faster speeds. While this work focused on optical fields, the approach can be generalized to other fields (e.g., temperature, strain), opening a rich area of research that requires contributions from many scientific disciplines. This work resulted in two key publications published in *Optics Express* and *ACS Photonics*. The PI facilitated collaborations with Sandia Securing Top Academic Research Talent at Historically Black Colleges and Universitites partner Norfolk State University, where five students supported work focused on optical learning. (PI: Francois Leonard)



Side by side comparison of electronic (left) and optical (right) neuromorphic recognition processes.

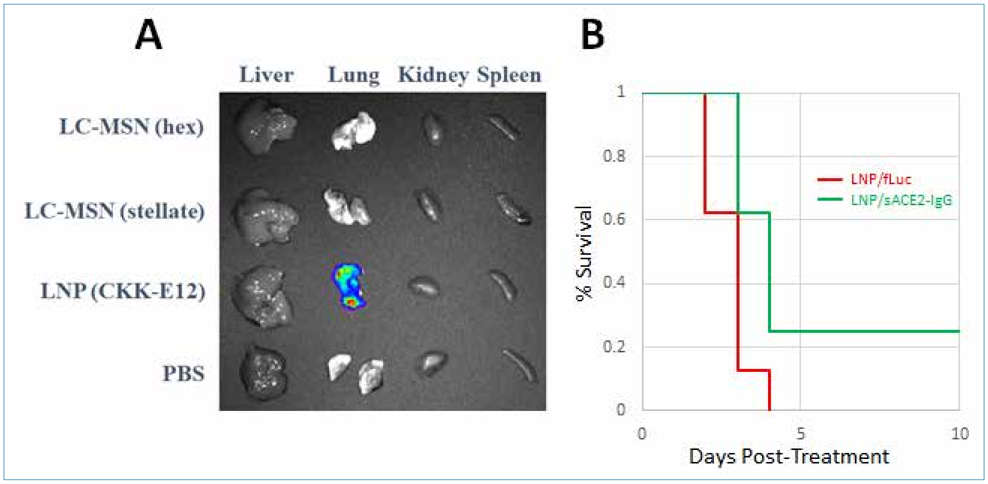
"GAME CHANGER" FOR OPTICAL DIAGNOSTICS USED IN BIOLOGY AND CHEMISTRY.



Experimental setup for massively entangled multimode squeezed light quantum imaging.

NANOPARTICLE-MEDIATED DELIVERY OF THERAPEUTIC mRNA FOR PROTECTION AGAINST LUNG DAMAGE.

Researchers developed a generalized approach to nanoparticle (NP) mediated delivery of messenger RNA (mRNA) to the lung, for use in transient programming of host cells to produce proteins that counter lung damage. In initial studies, reporter mRNA (fLuc, encoding luciferase) was delivered using lipid-coated mesoporous silica NPs (LC-MSN) and lipid NPs (LNP), the latter proving more reliable. Then, mRNA encoding known protein therapies were delivered using LNPs. The control formulation (LNP/fLuc) showed some toxicity in mice with lung damage. Despite this intrinsic toxicity, several test formulations were modestly therapeutic; these included mRNA encoding modified ACE2 (sACE2-Ig), a cytokine receptor antagonist (IL-1RA), and a glycoprotein that promotes vascular development (ANGPT1). This work advances the state of the art for mRNA delivery to the lung and provides a foundation for evaluating and characterizing mRNA-based lung therapies, including three that appear exceptionally promising. (PI: Steve Branda)



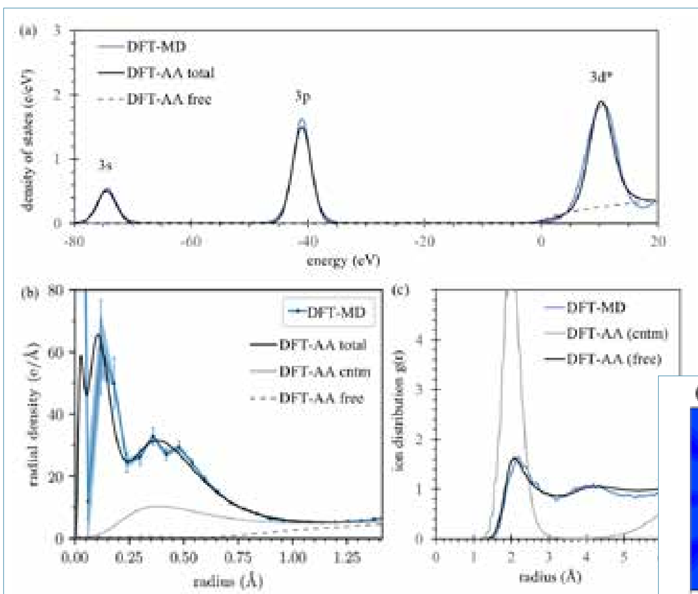
A. NPs (100 ug) loaded with fLuc MRNA (5 μg) were administered to C57Bl/6J mice via OPA (3 mice per treatment condition); PBS served as a negative control. At 6 h post-treatment, d-luciferin (3 mg) was administered via IP injection, and 5 min later tissues were collected for measurement of luminescence (indicative of luciferase expression) via IVIS analysis (565 nm emission). Representative ivis images (tissues from one mouse per treatment condition) are shown. B. aGalCer (5 μg) and LPS (150 μg) were sequentially (2 d interval) administered to C57Bl/6J mice via OPA to induce lung damage. At 1 d post-LPS administration, an LNP/mRNA formulation (2 μg mRNA) was administered via OPA (8 mice per treatment condition). Mortalilty was monitored for 10 d following treatment.

QUANTUM-ACCURATE MULTISCALE MODELING IN HIGHLY COMPRESSED METALS.

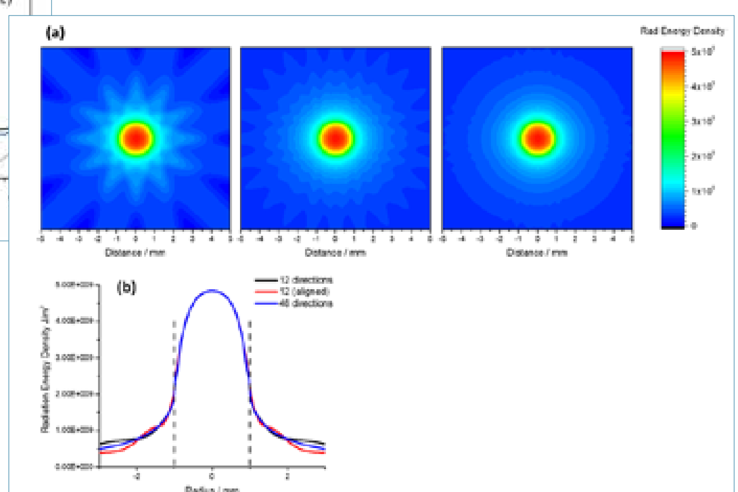
The development of equations-of-state and transport models in areas such as shock compression and fusion energy science is critical to DOE programs. Notable shortcomings in these activities are phase transitions in highly compressed metals. Fully characterizing high-energy density phenomena using pulsed power facilities is possible only with complementary numerical modeling for design, diagnostics, and data interpretation. This team constructed a multiscale simulation framework based on a combination of high-fidelity electronic structure data, ML, and molecular dynamics enabling quantum-accurate, computationally efficient predictions. This provides kinetics of magneto-structural phase transitions along shock Hugoniots and ramp compression paths in the equations of state, and transport properties such as viscosity, electrical and thermal conductivities. Findings from this project were published in the *Journal of Material Science* and *npj computational materials*. (PI: Mitchell Wood)

IMPROVING PREDICTIVE CAPABILITY IN REHEDS SIMULATIONS WITH FAST, ACCURATE, AND CONSISTENT NONEQUILIBRIUM MATERIAL PROPERTIES.

Predictive design of experiments in Radiation, Electrical, and High Energy Density Science (REHEDS) requires knowledge of material properties (e.g., equations of state (EOS), transport coefficients, and radiation physics). Interpreting experimental results also requires accurate models of diagnostic observables (e.g., detailed emission, absorption, and scattering spectra). These properties and observables are all typically tabulated with dedicated models that are not mutually consistent and are restricted to Local Thermodynamic Equilibrium (LTE). This project developed a relatively fast and accurate non-LTE average-atom model based on density functional theory that provides a complete set of EOS, transport, and radiative data. That model was tested against first-principles multi-atom models and extended to non-LTE; a tabular scheme was developed that compactly captures non-LTE effects, and the tables were implemented in both the GORGON simulation code and a new post-processor—significantly advancing REHEDS modeling capabilities. The research, done in collaboration with Sandia Alliance partner University of Illinois at Urbana-Champaign, Michigan State University, Cornell University, Princeton University, and Lawrence Livermore National Laboratory, and has resulted in nine publications including 2022 articles in *Scientific Reports*, *Journal of Physics B: Molecular and Optical Physics*, and *Physical Review Letters*. Postdoc Alina Kononov was selected for a 2022 APS Metropolis award "For trailblazing contributions to the computational modeling of materials physics, including large-scale simulations of irradiated materials and advances in time-dependent density functional theory." (PI: Stephanie Hansen)



A comparison of multi-center density functional theory (DFT) and DFT-molecular dynamics (DFT-MD) data and our DFT-average atom (DFT-AA) model for iron at ρ = 7.9 g/cc and T = 1 eV: (a) valence-shell electronic densities of state, (b) radial electron densities with error bars representing averages over ions for DFT-MD and two plausible definitions of ionized electrons in DFT-AA, and (c) radial ion distributions for the two definitions of ionization.



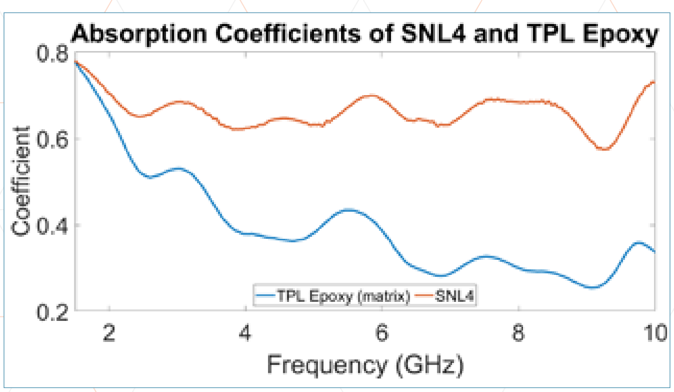
Steady-state K-shell group radiation energy density for a uniform plasma cylinder of aluminum with ni = 1020 ions/cc and Te = 500 eV [7] using 12, 24, and 48 rays for radiation transport, (b) lineouts of radiation energy density from the 12-angle case aligned (red) and between (black) rays, and from the 48-angle cases between rays (blue); black dashed lines denote the edges of the plasma cylinder.

PIRAMID: PHYSICS-INFORMED, RAPID AND AUTOMATED MACHINE-LEARNING FOR COMPACT MODEL DEVELOPMENT.

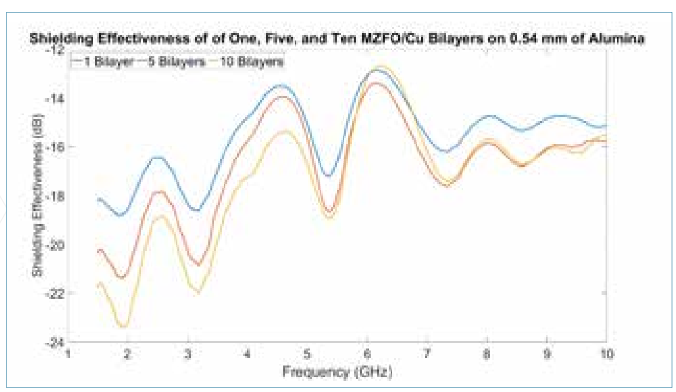
The PIRAMID LDRD project advanced the possible realization of multi-scale modeling between Radiation Analysis, Modeling and Simulation for Electrical Systems (RAMSES) simulation codes Charon and Xyce. The project team developed a workflow to train a novel ML architecture on continuum semiconductor physics simulation data from Charon for incorporation within a circuit simulation in Xyce. Compact models typically require manual calibration which might demand Charon analysis. The team workflow enables analysts to immediately leverage Charon data to produce models for use within circuit analyses. The enabling mechanism is incorporation of physics conservation laws in an ML architecture. The team's approach extends to other domains and will be explored through collaboration with Nathaniel Trask's DOE Early Career project. Treating other Radiation, Electrical, and High Energy Density Science models at Sandia similarly will allow for broader multi-scale modeling. The team collaborated with Xiaozhe Hu, James Adler, and Casey Cavanaugh at Tufts; George Slota and Chris Brissette at RPI; and Jack Garbus at Brandeis. An article on this project's research was published in the *Journal of Computational Physics*. (PI: Andy Huang)

HIGH FIELD AND FREQUENCY ELECTROMAGNETIC (HIFI-FREE) SHIELDING.

The goals of the HiFi-Free LDRD project were: (1) create a novel physics-based model of EM shielding for cylindrical symmetries, (2) develop hybrid absorbers with shielding effectiveness (SE) greater than mu-metal at reduced density/thickness from 100 MHz–10 GHz, and (3) investigate multilayer thin film shielding. The team, who collaborated with faculty at Penn State on some aspects of the project, characterized the absorption, reflection, shielding effectiveness and complex permittivity/permeability of 35 µm Mn1-xZnx ferrite, in steps of x=0.1, and discovered the x=0.4-0.7 stoichiometries to be the most absorptive from 1–10 GHz. Four hybrid absorbers were fabricated with one third the density of mu-metal and created a 0.34 mm shield that absorbed 60%–80% of incident power from 1.5–10 GHz. The team fabricated 100 nm thick Cu and $Mn_{0.5}Zn_{0.5}Fe_{2O4}$ multilayers and found one bilayer provided 14–18 dB of SE from 1.5–10 GHz, with negligible improvement from additional layers. A novel physics-based model of EM shielding was developed and tested that provides accurate results for dielectric and magnetic shielding from 100 MHz–1 GHz. (PI: Andrew Scott Padgett)



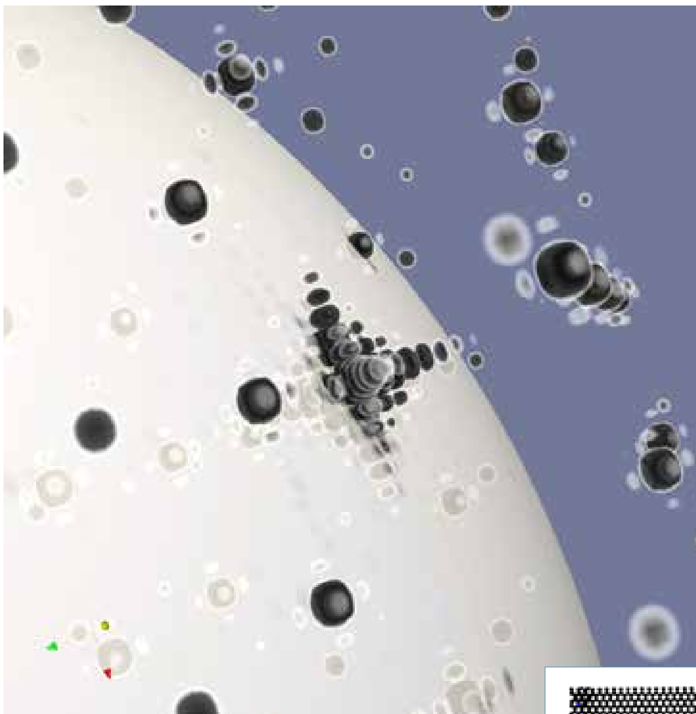
Absorption coefficients of SNL4 and TPL Epoxy.



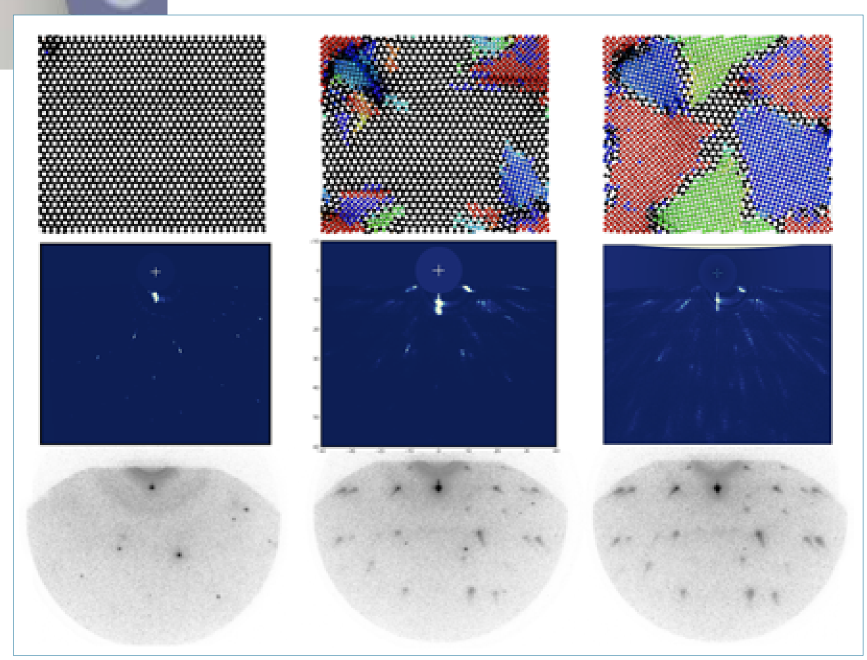
Shielding effectiveness of one, five, and ten MZFO/Cu bilayers on 0.54 mm of alumina.

SIMULATED X-RAY DIFFRACTION AND MACHINE LEARNING FOR OPTIMIZING DYNAMIC EXPERIMENT ANALYSIS.

In-situ X-ray diffraction (XRD) from ns dynamic compression experiments is shedding light on atomistic processes at extreme pressures. As experiments develop, new computational analysis tools are necessary to make sense of the data. This one-year LDRD project successfully established a simulated XRD capability and proved the concept of applying ML image analysis to interpret experimental data. The team developed code and validated new LAMMPS tools for 2D XRD pattern creation, produced cadmium sulfide (CdS) 2D XRD training data for two structures, incorporating broad X-ray spectrum. ML pattern recognition models (convolutional neural network-based) were trained from this dataset for orientation analysis and noise filtering. The ability to simulate and analyze X-ray diffraction data is crucial to interpreting a new class of dynamic high-pressure experiments. The success of this one-year project, presented at multiple American Physical Society conferences, advances predictive capability within weapons science. (PI: J. Matthew D. Lane)



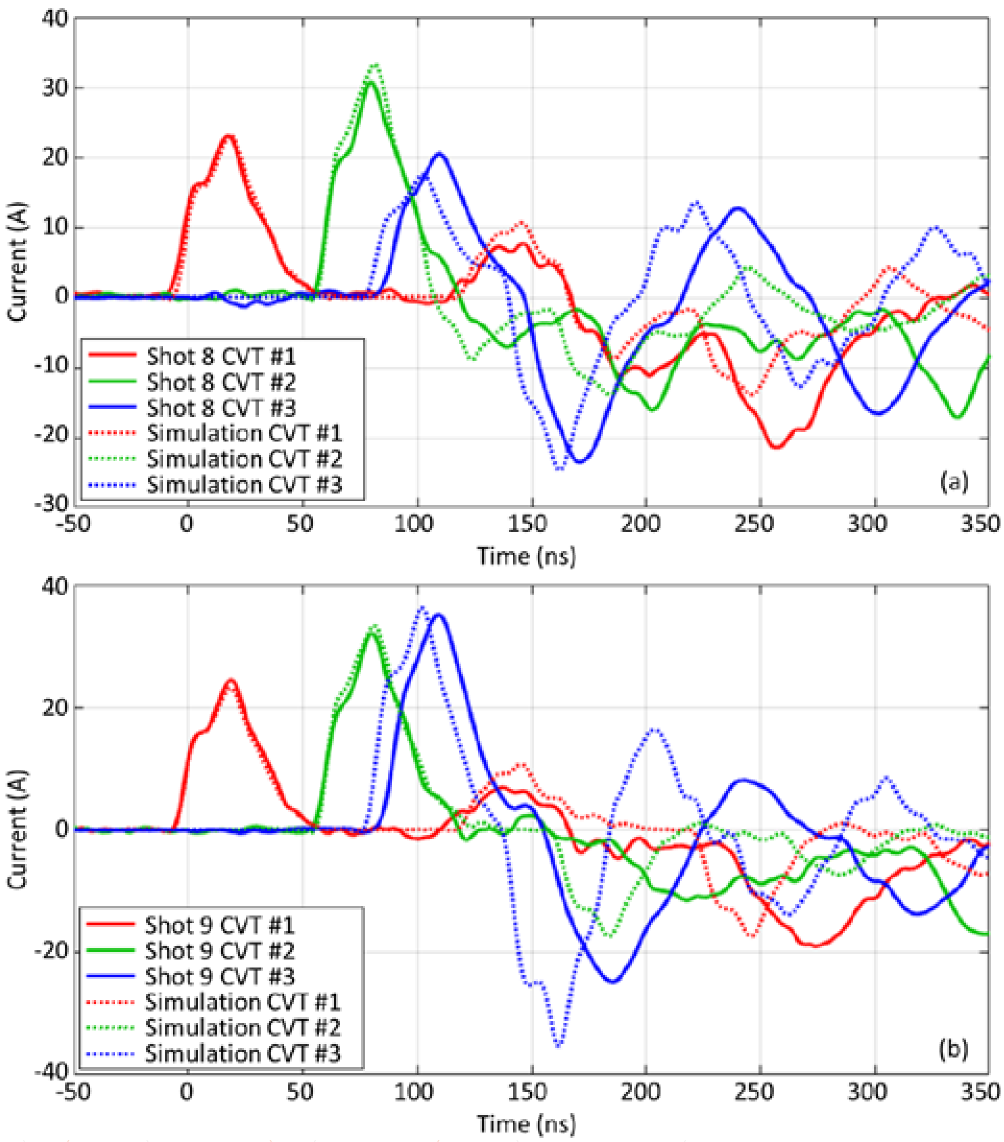
Representation of a reciprocal lattice density (black) and Ewald sphere construction (white) in k-space. The points intersecting the Ewald sphere of radius 1/λ represents the monochromatic diffraction pattern for that energy X-ray. The orientation of the sphere is determined by the incident k vector. The 2D diffraction pattern is mapped on the spherical surface with angular coordinates θ and φ.



Top: Real-space atomistic representations of CdS phase transition under high-pressure (> 5.5 GPa) shock compression colored by lattice type and orientation. Wurtzite is black. Rock salt is green, red or blue, based on orientation. Middle: Simulated diffraction patterns from the atomistic simulations, produced with energy spectrum and angular geometry corresponding to experiments. Because DCS X-rays are highly collimated, a single incident angle was used. Bottom: Experimental patterns showing evolution from wurtzite to rock salt structures. Time progresses from left to right. Experiments correspond with experimental times -43, 110, and 263 ns.

DEVELOPMENT OF HYBRID SYSTEM-COMPONENT MODEL DEVELOPMENT FOR LOW-COST HIGH-ALTITUDE EMP TESTING.

This LDRD project developed a methodology for modeling cable configurations in a substation or generation plant circuit to predict high-altitude electromagnetic pulse (HEMP) propagation through a system. This approach seeks to address gaps in how HEMP vulnerability assessments are performed by enabling better prediction of threat environments at critical equipment, which is vital for cost-effective mitigation planning. The one-year effort of this project focused on defining the methodology for a termination cabinet example case supported by experimental data and focused EM field modeling of cabinet features. It was discovered that transmission line models defining cables with respect to the nearest ground metal were well aligned to experimental data, and that many typical features of cabinet configurations were too small to significantly impact conducted HEMP propagation. The process used in this work can be applied to build model libraries in a future vulnerability assessment tool. (PI: Tyler Bowman)

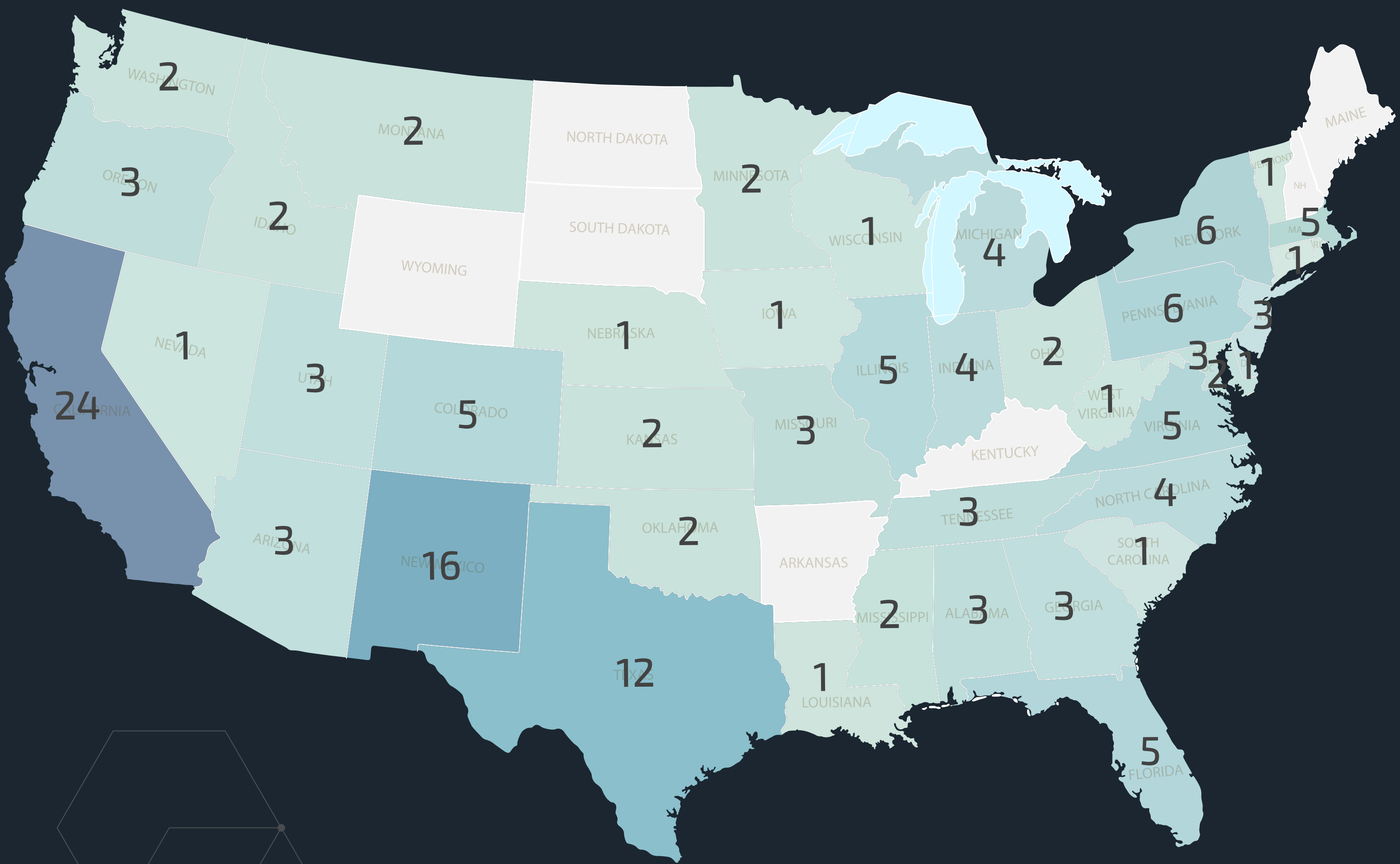


Comparison between experimental data from current viewing transformers (CVT) and circuit simulation of a termination cabinet with (top) a high output impedance or (bottom) a low output impedance.

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 2022 through LDRD, but they give a glimpse of how significant the program is to the country and to the world.

FY22 LDRD PROJECTS LEVERAGE A RICH NETWORK OF COLLABORATORS



This map highlights the distinct number of collaborating institutions during the 2022 fiscal year. There were 278 LDRD projects that worked with a total of 109 academic institutions, 25 government institutions, and 41 industry partners. Academic collaborations are important for nurturing the talent pipeline. In the 2022 fiscal year, 278 projects worked with a total of 580 university collaborators, including faculty (408), postdocs (14), graduate students (146), and undergraduates (12).

On February 16, 2022, Sandia hosted its first Distinguished Visitor virtual visit with Secretary of Energy Jennifer Granholm, with NNSA Administrator Jill Hruby also in attendance. Former LDRD PI and 2021 Ernest Orlando Lawrence Awardee Andrew Landahl, one of only six scientists selected to brief Sec. Granholm, gave a presentation on quantum computing. He opened his presentation with a two-minute video that surveyed the landscape of Sandia's investments in quantum information science and technology over the past 15 years. Read more about Secretary Granholm's visit to Sandia and learn more about how LDRD has helped shape Sandia's quantum information science capabilities.

Labs Director James Peery addressed the workforce during DOE Secretary Jennifer Granholm's visit to Sandia on Feb. 16. During her visit, Granholm received briefings on key Sandia programs and applauded employees for their work and charitable contributions. (Photo by Lonnie Anderson)

SANDIA WINS FIVE 2022 R&D 100 AWARDS, THREE WITH LDRD ROOTS

In 2022, Sandia won five R&D 100 Awards (one in conjunction with Idaho and Pacific Northwest National Laboratories, and Johns Hopkins University Applied Physics Laboratory) and garnered an additional specialty honors award. R&D World Magazine presents the awards to the 100 most revolutionary technologies of the past year. For the nation, these awards indicate that the research and development done here, in support of the mission, is technologically significant and groundbreaking.

R&D 100 Award Winner

ULTRA-STABLE THERMALLY EXCELLENT ADVANCEMENTS IN MATERIAL STRENGTH (USTEAMS).

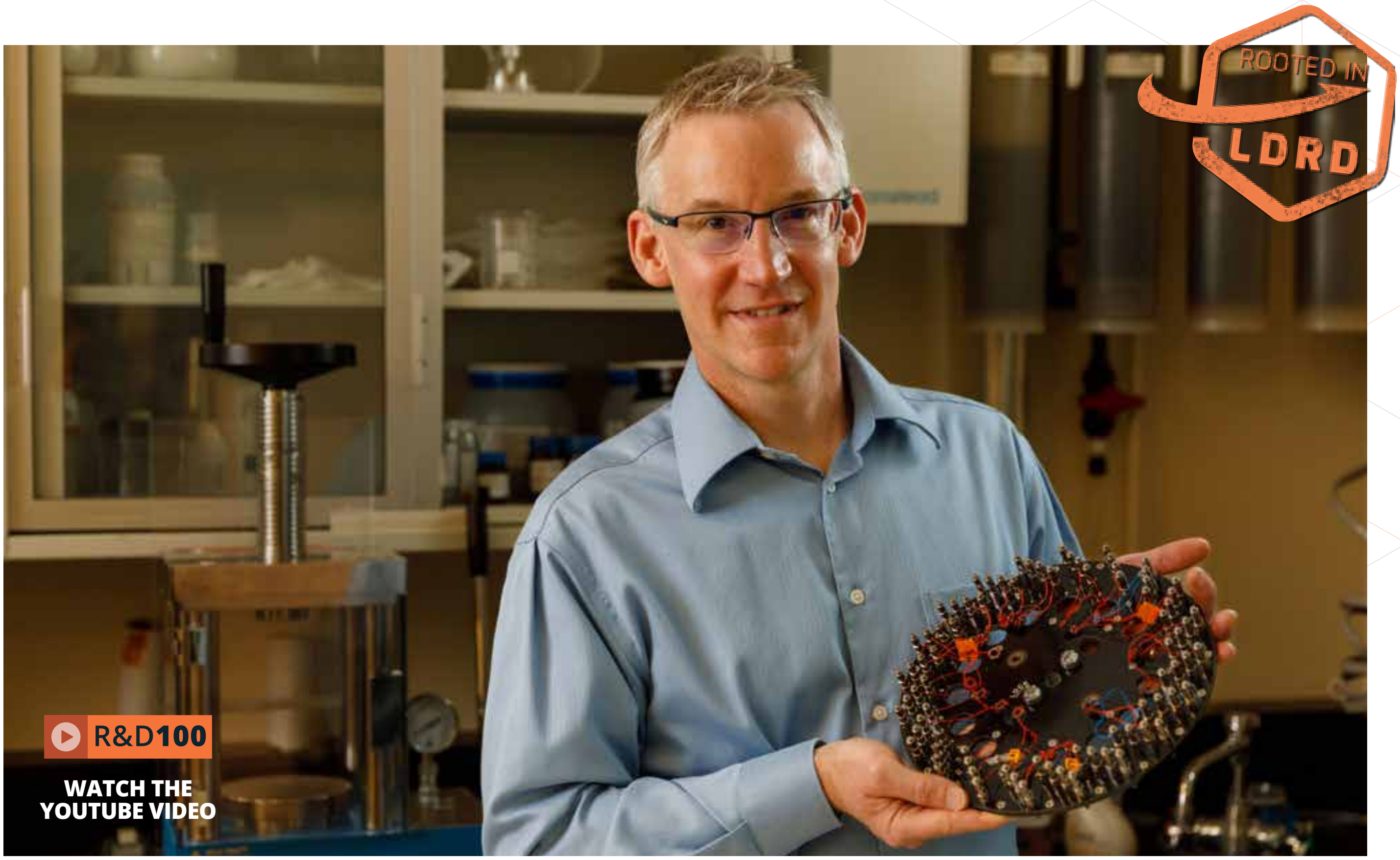
This technology, developed out of the LDRD Assured Survivability and Agility with Pulsed Power Mission Campaign, enables production of new thermally stable and mechanically strong coatings using commonly available and inexpensive materials. The innovative post-coating thermal treatment stimulates chemical crosslinking between silica layer and sugar-derived carbon layer. The coatings reduce cost and eliminate environmental safety and health concerns. These coatings have been demonstrated on the Z machine, one of the harshest radiation test environments, and found to effectively shield the blast wave from the test layer. (PI: Guanping Xu).

USTEAMS PI Guangping Xu, right, with team of researchers, from left, Hongyou Fan, Haley Davis, Chad McCoy, Jens Schwarz and Melissa Mills (Photo courtesy of Guangping Xu)

R&D 100 Award Winner

IRON NITRIDE SOFT MAGNETICS.

Global demand for high-efficiency, green energy technologies and products has placed new challenges on the electrical grid, efficient exploitation of renewable energy resources, and all electric-based solutions for transportation (vehicles, aircraft, and ships). All these applications require ultra-high-voltage power semiconductor devices (to reduce energy loss) with high-frequency ratings (to reduce system size, weight, and volume), and therefore, rely on high performance soft magnetic materials. The Electrochemical Solution Growth of Magnetic Nitrides LDRD project provided seed funding for the initial development of this effort. (PI: Todd Monson).



Todd Monson, PI for the Iron Nitride Soft Magnetics R&D 100 winning project (Photo by Bret Latter)

R&D 100 Award Winner

AUTOMATED THREAT ESTIMATOR FOR NETWORKS AND APPLICATIONS (ATHENA): CYBER ANALYSIS PLATFORM.

ATHENA is an analytic platform that fuses data collected from several disparate sources (e.g., deep packet inspection data, Zeek data, routing tables, device configurations, user asset inventories, organization Information, etc.). The current focus of ATHENA is enterprise network architecture and device configuration data. The platform enables users to quickly access and correlate data describing near-real time network architecture and device configuration. This data includes device inventory, network topology, device description including MAC and IP addresses, manufacturers, operating system details, system subnetting, inventory of connected end-point addresses, situational awareness, and configuration changes. ATHENA is highly extensible in the types and specific data queries it can execute. Elements of ATHENA were derived from the Automated Threat Modeling for Cyber Security Analytics and Emulation LDRD project.
(PI: Vince Urias)

Vince Urias, PI for the Automated Threat Estimator for Networks and Applications R&D 100 winning project (Photo by Randy Montoya)

R&D 100 Award and a Silver Market Disrupter Award for Products Category under Special Recognitions.

PROACTIVE INTRUSION DETECTION AND MITIGATION SYSTEM (PIDMS) FOR DISTRIBUTED ENERGY RESOURCE SYSTEMS.

To address a significant and emerging gap in power systems cybersecurity, a first-of-its-kind proactive intrusion detection and mitigation system was developed to secure grid-edge photovoltaic (PV) smart inverters and other distributed energy resource (DER) equipment in DER systems. The PIDMS is a distributed, flexible bump-in-the-wire solution for protecting PV smart inverter communications. Both cyber (network traffic) and physical (power system measurements) are automatically processed using network deep packet inspection tools and custom machine learning algorithms for performing detection of abnormal events and correlation of cyber-physical events. The PIDMS not only detects abnormal events but also automatically deploys mitigations to limit or eliminate system impact. The PIDMS communicates with peer PIDMSs at different locations using a publisher/subscriber framework for increased situational awareness and alerting. (PI: Shamina Hossain-McKenzie)

Shamina Hossain-McKenzie, PI for PIDMS (Photo by Taylor McKenzie)

R&D 100 Award Winner

MOSAICS: BRINGING THE FUTURE OF INDUSTRIAL CYBERSECURITY INTO FOCUS.

William Waugaman, Sandia acting manager and laboratory technical manager overseeing development and demonstration for the entire project (Photo courtesy of William Waugaman)

More Situational Awareness Industrial Control Systems (MOSAICS), a technology initiated by the DOD, provides the first-ever comprehensive, integrated and automated solution to detect and prevent cyberattacks of industrial control systems. This collaborative project focused on providing scalable evaluation of commercial, off-the-shelf security solutions and test harness for initializing, launching and collecting results from cyber-resilience testing in virtual environments. *Sandia is a partner on the MOSAICS technology with Idaho National Laboratory, Johns Hopkins University Applied Physics Laboratory, and Pacific Northwest National Laboratory.
(Sandia PI: William Waugaman)

National/Federal Awards

2021 ERNEST ORLANDO LAWRENCE AWARD.

On June 21, 2022, U.S. Secretary Energy Jennifer Granholm announced the ten recipients of the 2021 Ernest Orlando Lawrence Award, which included two Sandians. Established in 1959, the Lawrence Award recognizes research contributions from mid-career scientists and engineers that have significantly advanced the state of the art in key missions of DOE and its programs.

"I am thrilled to recognize these researchers and the significant advances they have contributed to society. Scientists like these individuals are the backbone of DOE, and we cannot achieve our mission without them. I'm excited to see what the future holds for them and where they may lead us," said Asmeret Asefaw Berhe, Director of the DOE Office of Science.

Sandia physicist Daniel Sinars won an Ernest Orlando Lawrence Award for helping transform the Z Pulsed Power Facility to record a variety of record-breaking outputs supporting U.S. nuclear security, nuclear fusion energy, and basic science. (Photo courtesy of Sandia)

DAN SINARS is recognized in the National Security and Nonproliferation Category for his "pioneering development of seminal X-ray diagnostics and their innovative application to z-pinch implosions that transformed the experimental capabilities on the Z Pulsed Power Facility and enabled novel, record-breaking platforms supporting our nation's nuclear security." A former LDRD PI, Sinars now oversees Sandia's Pulsed Power Sciences Center, best known for the world's most powerful pulsed-power machine, the Z machine. Under Sinars' tenure, experiments on Z helped quantify stockpile aging effects, led to new insights in our understanding of the science of our universe, and moved us closer to the goal of reaching controlled high-yield fusion. Sinars is the Director Champion of the Assured Survivability and Agility with Pulsed Power LDRD Mission Campaign and the Radiation, Electrical, and High Energy Density Science LDRD Investment Area.

Sandia physicist Andrew Landahl is the first person to receive an Ernest Orlando Lawrence Award in the field of quantum information science. (Photo by Stephanie Blackwell)

ANDREW LANDAHL is recognized in the Computer, Information, and Knowledge Sciences Category for his "groundbreaking contributions to quantum computing, including the invention of transformational quantum error correction protocols and decoding algorithms, for scientific leadership in the development of quantum computing technology and quantum programming languages, and for professional service to the quantum information science community." Landahl was the PI for the AQUARIUS (Adiabatic Quantum Architectures in Ultracold Systems) LDRD Grand Challenge (2011-2013), which played a key role in helping shape Sandia's vibrant program in quantum information science. Also a research professor in the University of New Mexico's Department of Physics and Astronomy, Landahl co-invented a decoding protocol for quantum error correcting codes that can overcome decoherence (the tendency for a quantum computer to revert to digital logic under certain circumstances). Landahl currently leads the software team for Sandia's Quantum Scientific Computing Open User Testbed (QSCOUT) project, which received a 2021 R&D 100 award, and is rooted in LDRD.

Read more about the awardees here.

Defense Programs Award of Excellence

TECH TRANSFER AWARD.

Presented annually by NNSA's deputy administrator for Defense Programs, the award recognizes exceptional and significant achievements in quality, productivity, cost savings, safety, and creativity in support of NNSA's Stockpile Stewardship Program.

ADVANCED TECHNIQUE FOR CHIP-LEVEL AUTHENTICATION AND EVALUATION.

In 2022, a Defense Programs Tech Transfer Award was awarded to the Sandia team behind the advanced technique for chip-level authentication and evaluation. To ensure mission success, NNSA requires all nuclear deterrence electrical components be authenticated. Using the LDRD-developed Power Spectrum Analysis with an unconventional biasing scheme to power microelectronic devices, researchers from Sandia developed a nonintrusive, nondestructive technique to authenticate various microelectronic devices. Understanding the potential benefit of the analysis to the electronics market, but realizing the significant cost factors, Sandia submitted the technology to the NNSA NA10.1-sponsored FedTech program for commercialization. After signing a research license with Sandia through the program, Chiplytics was founded in 2021 with the goal of providing a user-friendly, cost-effective Power Spectrum Analysis testing procedure to the commercial electronics market. The company has the potential to save the electronics industry tens of millions of dollars and ensure the authenticity of microelectronics used within nuclear deterrence and national security programs.

From left, Paiboon Tangyonyong, Edward I. Cole, Jr., and David V. Wick. Not pictured, Stephen DiBartolomeo, Steven Dourmashkin, Guillermo Loubriel, Matthew Skeels, and Brandon Smith

2021 NATIONAL LAB ACCELERATOR PITCH EVENT.

A team of Sandia bioscientists co-won the 2021 National Lab Accelerator Pitch Event, which showcases commercialization-ready technology developed at DOE national laboratories. The team, led by Brooke Harmon, created a platform for discovering, designing, and engineering novel antibody countermeasures for emerging viruses. The process of screening for nanobodies that disable the virus points the way to developing nanobody therapies that protect against COVID-19 and defend against future biological threats.

"Vaccines are very good at preventing infection, but they can take a long time to be developed and move through the regulatory process," Harmon said. "We saw a critical need to create effective therapies that can be rapidly developed and deployed." Once the protein sequence, or genetic coding, of a virus has been identified, Sandia researchers have shown they can produce a nanobody-based countermeasure within 90 days. The method has not yet been tested on humans. Speeding up the discovery of neutralizing antibodies could reduce the impact of future viral outbreaks.

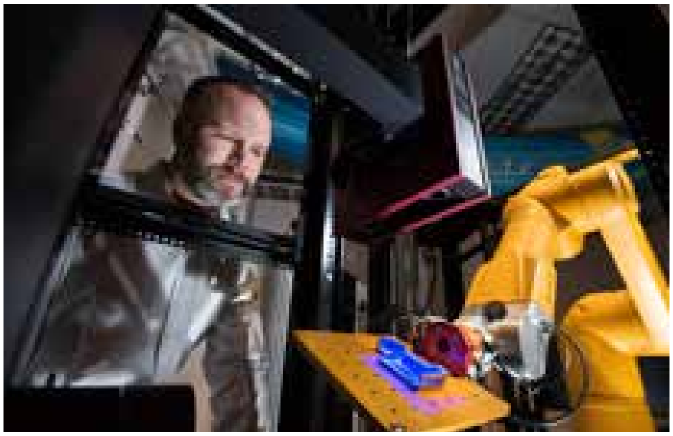
Read more about Sandia's work defending against future pandemics, and check out Harmon's winning pitch.

Sandia bioscience researchers, from left, Christine Thatcher, Jennifer Schwedler, Yooli Kim Light, Peter McIlroy and Brooke Harmon

Prestigious Fellowships, Appointments and Memberships

BRAD BOYCE NAMED VICE PRESIDENT OF THE MINERALS, METALS AND MATERIALS SOCIETY.

Brad Boyce, a materials scientist at Sandia, was elected president of The Minerals, Metals and Materials Society. Boyce became vice president of the society on March 3, 2022, at its annual meeting, and will serve three consecutive one-year terms as vice president, president, and past president. He is the second Sandia employee to be elected to lead the professional society. The professional society, also known as TMS, includes 11,000 materials scientists and engineers from around the world. It fosters the exchange of knowledge and ideas in topics ranging from producing metals from mined ores to advanced applications of materials. Boyce has led numerous LDRD projects; he is currently the PI for the Beyond Fingerprinting Grand Challenge. The project aims to discover new resilient materials and manufacturing processes by taking an artificial-intelligence-guided approach that integrates human-subject-matter expertise with algorithms enriched with physics-based constraints to unearth process-structure-property correlations.

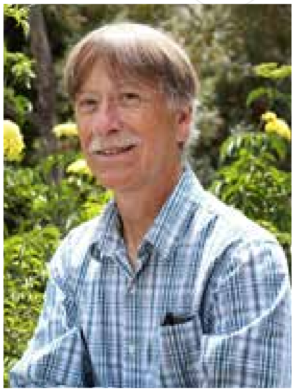


In a 2018 photo, Sandia materials scientist Brad Boyce watches as the Alinstante robotic work cell scans a 3D-printed part to compare what was made to the original design. (Photo by Randy Montoya)

GANESH SUBRAMANIA RECOGNIZED BY SPIE, OPTICAL SOCIETY OF AMERICA.

Ganesh Subramania was named a 2021 Fellow of SPIE, the international Society for Optics and Photonics, and a SPIE community champion. He was also appointed as a senior member of the Optical Society of America. Subramania has led eight LDRD projects and been a collaborator on numerous others and is an expert in light-matter interaction in photonic and plasmonic structures. He has over 15 years of experience in the design, fabrication, and characterization of nanophotonic structures.

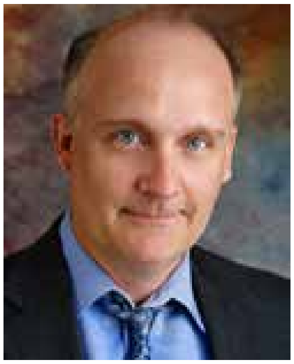
SANDIA RESEARCHER RAY TUMINARO NAMED SIAM FELLOW.



Sandia computational scientist and applied mathematician Ray Tuminaro was named a 2022 Fellow of the Society for Industrial and Applied Mathematics for "contributions in iterative linear-solver algorithms and software that address scientific computing applications on large-scale parallel systems." Tuminaro has been a team member on numerous LDRDs and led a FY22 project developing linear system solves for matrix equations associated with multi-physics partial differential equation systems.

THE FOLLOWING THREE INDIVIDUALS WERE PROFILED IN LDRD PROGRAM VALUE SECTION.

DAVID ADAMS ELECTED AS FELLOW OF AVS: SCIENCE & TECHNOLOGY OF MATERIALS, INTERFACES AND PROCESSING.



DAVID ADAMS was elected as a Fellow of AVS: Science & Technology of Materials, Interfaces and Processing (formerly referred to as the American Vacuum Society). Additionally, Adams was elected to be President of AVS, serving as President-elect in 2023 and President in 2024.

Adams reflects on his experience with the LDRD Program: "Sandia's LDRD program has provided me with several exciting, collaborative scientific and engineering investigations over my career. I am grateful to have worked with different, multi-disciplinary LDRD teams and value our many discoveries and contributions. These collaborative LDRD projects are a key reason that I have remained at Sandia for more than 25 years. I strongly encourage early-career staff to engage in LDRD studies, if interested. LDRD programs span a wide variety of topics, and one can potentially contribute to multiple investment areas over the course of a career while building your own technical expertise. There are also opportunities to collaborate with U.S. universities, via the Sandia University Partnerships Program, which greatly enhance the experience. It is a wonderful program!"

DAVID MOORE ACCEPTED INTO ACADEMIA NONDESTRUCTIVE TESTING INTERNATIONAL SOCIETY.

DAVID G. MOORE was nominated and accepted into the Academia Nondestructive Testing (NDT) International Society during its 13th General Assembly Meeting. The society, with 72 worldwide full members, is focused on promoting science, conducting research, developing new diagnostic tools, and encouraging the application of findings in the field of NDT.

BO SONG DESIGNATED A SOCIETY FOR EXPERIMENTAL MECHANICS FELLOW.

(Photo by Lonnie Anderson)

BO SONG, recently recognized as a 2020 Asian American Engineer of the Year by the DiscoverE Engineering Program, was designated a Society for Experimental Mechanics Fellow as recognition "for his cutting-edge research in Dynamic Behavior of Materials. Dr. Song has established himself as a well-recognized leader of the Experimental Mechanics community."

Early Career Awards and Honors

FOUR SANDIA RESEARCHERS RECEIVE DOE OFFICE OF SCIENCE'S EARLY CAREER RESEARCH AWARDS.

The DOE Office of Science has selected four Sandia researchers to receive Early Career Research Awards this year. Krupa Ramasesha, Pete Bosler, Tim Proctor, and Andy Mounce will receive up to $500,000 per year for five years to advance their research. The program, now in its 13th year, is designed to provide support to researchers during their early career years, when many scientists do their formative work. In 2022, the DOE awarded 83 scientists nationwide, including 27 from national laboratories.

Krupa Ramasesha earned a 2022 DOE Early Career Research Award.

KRUPA RAMASESHA is an experimental physical chemist with expertise in ultrafast laser spectroscopy and chemical dynamics. She has led two LDRDs during her Sandia tenure, most recently a project to detect short-lived intermediates in catalytic transformations using table-top extreme ultraviolet radiation. She will use her award to develop a fundamental understanding of the electronic interactions between molecules and metallic nanoparticles.

Quantum physicist Tim Proctor is a recent recipient of a DOE Early Career Research Award.

TIM PROCTOR, PI of the LDRD project "Capabilities of a Quantum Computer," was awarded was awarded a DOE Advanced Scientific Computing Research Early Career Award project based on his recent research within this LDRD. His Early Career project "Quantum Capability Learning," will (1) measure how well a quantum computer runs a specific program and (2) predict what novel programs it will or will not be able to run. This research will make it possible to understand the capabilities of quantum computing hardware, and to make best use of each particular quantum computer's strengths.

Sandia applied mathematician Pete Bosler moves fluidly with help from very fine data sets. (Photo by Craig Fritz)

PETE BOSLER is an applied mathematician focused on developing numerical methods and software for coupled multi-physics problems. He is currently a team member of the climate focused CLDERA Grand Challenge, investigating computational relationships in the form pathways between climate sources and impacts. With his DOE award, Bosler hopes to improve accuracy of simulations in complex domains like climate and plasmas by developing new algorithms that can resolve a broad range of scales through intelligent heuristic model selection.

Andy Mounce makes microscopic sensors to try to understand quantum materials. He is also a recent recipient of a DOE Early Career Research Award.

ANDY MOUNCE specializes in making microscopic sensors to try to understand the nature of quantum materials and their electrons' behavior. He recently completed an LDRD project focused on establishing the technological foundation for a new class of solid-state, quantum light emitters in III-nitride semiconductors. With his DOE Early Career Award, Mounce hopes to understand the topological phase transitions of quantum materials by levering diamond quantum sensors.

FY22 Hruby and Truman Postdoctoral Fellowships

JILL HRUBY POSTDOCTORAL FELLOWSHIP.

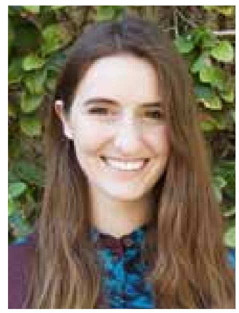
The LDRD-funded Jill Hruby Postdoctoral Fellowship was established in 2017 to encourage outstanding women with PhDs in technical fields to consider leadership in national security. Jill Hruby, the Under Secretary of Energy of the United States, was the first woman to lead a national security laboratory and served as Sandia's director from 2015 to 2017.

SOMMER JOHANSEN – FY22 HRUBY FELLOW.

(Photo by Sommer Johansen)

SOMMER JOHANSEN received her doctorate in physical chemistry from the University of California, Davis, where her thesis involved going backward in time to explore the evolution of prebiotic molecules in the form of cyclic nitrogen compounds; her time machine consisted of combining laboratory spectroscopy and computational chemistry to learn how these molecules formed during the earliest stages of our solar system. Johansen hopes to help improve comprehensive models of the after-effects of burning bio-derived fuels on Earth's planetary ecology. Johansen is working with the gas-phase chemical physics department, studying gas-phase nitrogen chemistry at Sandia's Livermore site.

ALEX DOWNS – FY22 HRUBY FELLOW.



(Photo courtesy of Alex Downs)

ALEX DOWNS completed her doctorate at the University of California, Santa Barbara, in August 2021. Downs hopes to create wearable biosensors that would gather real-time molecular measurements from health markers and lessen the need for patients to visit doctors' offices and labs for evaluations. The recognition element for this type of biosensor are aptamers—strands of DNA that bind specifically to a given target, such as a small molecule or protein. When a reporter is added to an aptamer sequence and put down on a conductive surface, target binding to the sensor can be measured as a change in electrochemical signal. The work fits well with Sandia's biological and chemical sensors team.

HARRY S. TRUMAN POSTDOCTORAL FELLOWSHIP.

Sandia established the Harry S. Truman 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.

GABRIEL SHIPLEY – FY22 TRUMAN FELLOW.

(Photo courtesy of Gabe Shipley)

GABRIEL SHIPLEY received his doctorate in electrical engineering from the University of New Mexico in 2021 and worked at Sandia for eight years as an undergraduate student intern from 2013 and as a graduate student intern since 2015 prior to becoming a Truman Fellow. Shipley broadened the use of a small pulsed power machine called Mykonos in a past internship and is investigating the origins and evolution of 3D instabilities in pulsed-power-driven implosions at Sandia's powerful Z machine. Shipley has authored articles in the journal *Physics of Plasmas* and provided invited talks at the Annual Meeting of the APS Division of Plasma Physics and the 9th Fundamental Science with Pulsed Power: Research Opportunities and User Meeting. His most recent publication in *Physics of Plasmas*, "Design of Dynamic Screw Pinch Experiments for Magnetized Liner Inertial Fusion," represents another attempt to increase Z machine output.

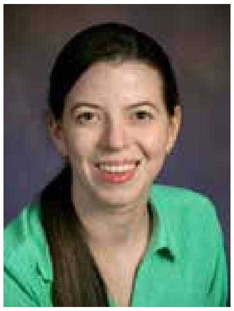
ALICIA MAGANN – FY22 HRUBY FELLOW.

(Photo courtesy of Alicia Magann)

ALICIA MAGANN obtained her PhD from Princeton University and will extend aspects of her doctoral research to help explore the possibilities of quantum control in the era of quantum computing. She is working with Sandia's quantum computer science department to develop algorithms for quantum computers that can be used to study the control of molecular systems. During her doctoral research, Magann was a DOE Computational Science Graduate Fellow and served as a graduate intern in Sandia's extreme-scale data science and analytics department. Her work has been published in various technical journals, including *Quantum, Physical Review A*, *Physical Review Research*, *PRX Quantum*, and *IEEE Transactions on Control Systems Technology*. One of her most recent 2021 publications is "Digital Quantum Simulation of Molecular Dynamics & Control" in *Physical Review Research*.

Professional Society and Conference Awards

AMERICAN PHYSICAL SOCIETY NICHOLAS METROPOLIS AWARD.



(Photo credit American Physical Society)

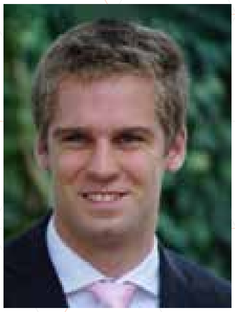
ALINA KONONOV, a postdoc in Sandia's Quantum Computer Science Department and team member of an FY22 LDRD, focused on improving predictive capability in high energy density simulations, was awarded a Nicholas Metropolis Award from the American Physical Society. The award recognizes outstanding doctoral thesis work in computational physics. Kononov was acknowledged "for trailblazing contributions to the computational modeling of materials physics, including largescale simulations of irradiated materials and advances in time-dependent density functional theory." At Sandia, she continues to develop and apply cutting-edge methods to model excited electron dynamics in collaboration with Andrew Baczewski and Stephanie Hansen. Her current projects involve advancing modeling capabilities for warm dense matter and exploring prospects of near-term quantum computing for simulating excited electrons.

AMERICAN NUCLEAR SOCIETY BEST PAPER AWARD.

(Photo credit University of Michigan)

EMILY VU, a University of Michigan PhD candidate, collaborated with Sandia PI Aaron Olson on a project to develop the first-ever Monte Carlo radiation transport in stochastic media model capable of accurately characterizing the effects of real-world random material mixing. The American Nuclear Society acknowledged her paper, an extension of her LDRD work, titled "Amnesia Radius Versions of Conditional Point Sampling for Radiation Transport in 1D Stochastic Media" with a Best Student Paper award, based on the overall quality of presentations from the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering. Vu reflects on her time at Sandia and the mentorship she received, "I believe my accomplishments now are a palimpsest of the skills I gained as a year-round intern at Sandia."

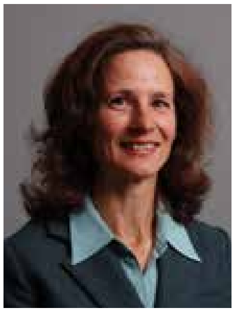
DOE'S HYDROGEN FUEL CELL TECHNOLOGIES OFFICE POSTDOCTORAL RECOGNITION AWARD.



MATTHEW WITMAN, was the co-winner of DOE's Hydrogen Fuel Cell Technologies Office (HFTO) Postdoctoral Recognition Award for "exceptional work in materials-based hydrogen storage, machine learning, and high entropy alloys." Now a staff member in the Energy Nanomaterials Department, Witman's award was supported in part by his research contributions on the LDRD project entitled "Developing Novel Liquid Metal Solution Chemistry that Combines Thermochemical and Electrochemical Processes to Produce Renewable Hydrogen by Water Splitting."

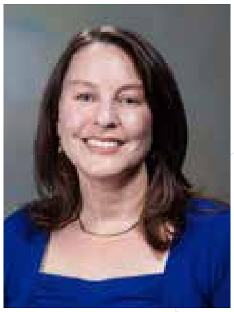
Society of Women Engineers (SWE) Achievement Awards

SWE ACHIEVEMENT AWARD.



TINA NENOFF, Sandia Senior Scientist, received a 2022 SWE Achievement Award, SWE's highest honor, which is reserved for a person "who has made significant and progressive technical contributions." Nenoff, a fellow of both the American Association for the Advancement of Science and the American Chemical Society, uses chemistry to solve worldwide challenges. Her work with metal-organic frameworks and other nanoporous materials has resulted in numerous inventions. A longstanding proponent of collaboration, Nenoff has been PI on 12 different LDRD projects at Sandia and is currently developing a sensor that detects iodine gas, which releases from a nuclear power plant during a meltdown. The sensor could be further developed into an early detection and warning system for plant workers and nearby communities.

SWE PATENT RECOGNITION AWARD.



NEDRA BONAL, Sandia Research Integrity Officer, received an SWE Patent Recognition Award for muon detectors, systems, and methods. Bonal and her co-inventors were awarded a patent last year for an imaging device they created to investigate whether muons, particles similar to an electron but much heavier and shorter lived, could be used to image underground structures like facilities inside mountains. "We needed a different set of hardware than what was available," Bonal said. "Naturally occurring muons mostly travel in a downward direction, but we needed to utilize those traveling from other specific angles. So, we invented a way to determine their direction and isolate the ones of interest, like those traveling horizontally through a mountain." Bonal's work in LDRD helped lead to this patent.

Black Engineer of the Year Awards (BEYA)

BEYA is a program of the national Career Communications Group, an advocate for corporate diversity, and part of its STEM achievement program. The awards annually recognize the nation's best and brightest engineers, scientists, and technology experts.

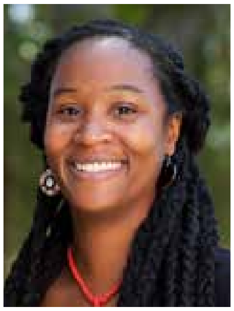
BEYA SCIENCE SPECTRUM TRAILBLAZER.

LA TONYA JENKINS focuses on systems dynamic modeling supporting projects in Sandia's Energy Water Systems Integration department. Her modeling capability supports the department's work with human-engineered and natural systems to support the security of the nation's energy water systems. Jenkins' expertise in modeling is also utilized by multiple organizations across Sandia. As a mentor, she works in developing and advancing youth STEM programs. She has been a team member on three LDRD projects, most recently funded through the National Security Programs Investment Area to study data-driven cognitive modeling.

BEYA MODERN-DAY TECHNOLOGY LEADER.

GERARD BENNETT develops navigation, guidance, and control solutions for aerospace systems. His work focuses on developing aerospace applications and validating them through simulation. He is responsible for developing the technical applications for modeling and simulation of these systems and creating a model for developing algorithms and optimizing trajectories, and most recently served as team member on an LDRD project in the Autonomy for Hypersonics Investment Area.

BEYA MOST PROMISING SCIENTIST IN GOVERNMENT.



KARLA MORRIS, the PI of an Early Career R&D LDRD in 2011, was recently honored with the 2022 BEYA Award for Most Promising Scientist in Government. Morris, who is a mechanical engineer and a computer scientist, joined Sandia in 2011 to develop complex computing codes and models to enable extreme-scale simulations incorporating uncertainty. She is now the formal methods lead for a weapons program.

BEYA RESEARCH LEADERSHIP.

CHRIS JENKINS is a principal cybersecurity research and development staff member in Sandia's Information Operations Center. He leads a team researching innovative ways to protect critical infrastructure and other high-consequence operational technology. His work focuses on three key areas: cyber-physical cybersecurity research, high-performance computing, and cybersecurity expertise outside Sandia. He has led four LDRD projects, including two in the Science and Technology Advancing resilience for Contested Space Mission Campaign.

INTERNATIONAL UNION OF SOIL SCIENCES (IUSS) JEJU AWARD

Sandia soil scientist Umakant Mishra starts his hike to the base camp of Mount Everest. (Photo courtesy of Umakant Mishra)

UMAKANT MISHRA was awarded the 2022 JEJU Award by the IUSS for innovative and outstanding accomplishments in soil sciences. Mishra is the chair of the International Soil Science Award Committee for the Soil Science Society of America, an executive board member of the International Soil Modeling Consortium, and an active editor for multiple journals. He was PI on two LDRDs in 2022 and is also assisting on another LDRD by modeling how soil microbes are contributing to greenhouse gas emissions to reduce the uncertainties in our climate change predictions.

SOCIETY OF ASIAN SCIENTISTS AND ENGINEERS CAREER ACHIEVEMENT AWARD.

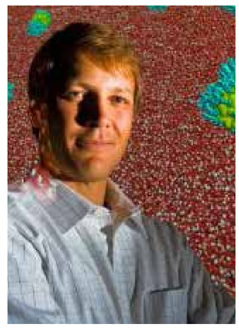
HONGYOU FAN, Sandia nanomaterials researcher, was selected by the Society of Asian Scientists and Engineers to receive its 2022 Career Achievement Award. The strong endorsement is confirmed by Fan's many technical papers, awards and patents, appointment to scientific societies and outreaches to students. During his 25-year career, he has led eight LDRD projects, published 138 papers, and co-founded a startup company based on his inventions, Lunano LLC, to develop disinfectants that kill viruses, bacteria, and fungi, including the virus that causes COVID-19.

HONORS AND DISTINCTIONS.

Chemist Krupa Ramasesha received a competitive award from the Journal of Physical Chemistry after only seven years at Sandia. (Photo by Dino Vournas)

KRUPA RAMASESHA received the American Chemical Society Physical Chemistry Division Lectureship Award from the *Journal of Physical Chemistry* for her major contributions to the field. Ramasesha has been PI on four previous LDRD projects and is leading one in 2023. Her impacts across the spectrum of the *Journal of Physical Chemistry's* research areas include atmospheric chemistry and proton transfer dynamics in molecules, hydrogen-bonding dynamics in liquids and solid-state attosecond dynamics and transfer.

BILIANA PASKALEVA was elected chair of the Center for Advanced Electronics through Machine Learning Industry-University Research Partnership's second phase. This partnership involves Sandia University Partners University of Illinois at Urbana-Champaign, Georgia Tech, and North Carolina State. Paskaleva has led and teamed on numerous LDRD projects, most recently on compact radiation effects modeling and analysis.



Matt Lane (Photo by Randy Montoya)

MATT LANE was elected as treasurer of the Shock Compression of Condensed Matter Topical Group of the American Physical Society in December 2021. He will serve on the Executive Board through the end of 2024. Lane has served as the PI of three LDRD projects, most recently focusing on simulated x-ray diffraction and machine learning techniques to better optimize interpretation of data from Sandia's pulsed power systems.

ADAM DARR and **LUKE STANEK** were the first two James Clerk Maxwell Distinguished Postdoctoral Fellows funded by the LDRD Assured Survivability & Agility with Pulsed-Power Mission Campaign. Darr's research topic is "Power-Flow Model of Behavior, Transitions, and Stability of Five Magnetically Insulated Transmission Line Regimes," and Stanek's is "Multi-fidelity Equation of State and Transport Coefficient Datasets for Pulsed Power Applications." The Fellowship supports exceptional researchers in the domains of pulsed power physics and/or engineering and its application to radiation, electrical, and high energy density sciences.

Matt Eichenfield

MATT EICHENFIELD joined the University of Arizona's Wyant College of Optical Sciences as the inaugural SPIE Endowed Chair in Optical Sciences. Eichenfield, part of Sandia's new Faculty Loan Program for Joint Appointments, has led eight LDRD projects, including "Phononic Memory and Optical Teleportation Using Optomechanics: Hardware Accelerators for Quantum Computers," described here.

LESLIE PHINNEY, Thermal Sciences & Engineering manager, and **TRACY VOGLER**, Distinguished Member of Technical Staff, were inducted into the University of Texas at Austin Department of Aerospace Engineering and Engineering Mechanics Academy of Distinguished Alumni in 2022. Phinney has served as team member on numerous engineering-science focused LDRDs; Vogler, an American Physical Society Fellow and former LDRD PI, is an expert in shock propagation in metals, ceramics, and granular materials.

LaRico Treadwell

LARICO TREADWELL was named to the Executive Board for the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers. Treadwell is a chemist at the Advanced Materials Laboratory, who has led multiple LDRD projects at Sandia. His work covers the materials science spectrum. He was named a Black Engineer of the Year: Most Promising Scientist in 2021.

STEPHEN PERCIVAL was awarded "2022 Excellence in Review" from Industrial & Engineering Chemistry Research (American Chemical Society). Percival is a former Sandia postdoctoral researcher and current staff member leading an LDRD focused on sustainable carbon dioxide capture.

BRAD BOYCE will serve on a panel for the National Academies on Autonomous Materials Science. Boyce is currently leading the Beyond Fingerprinting Grand Challenge LDRD.

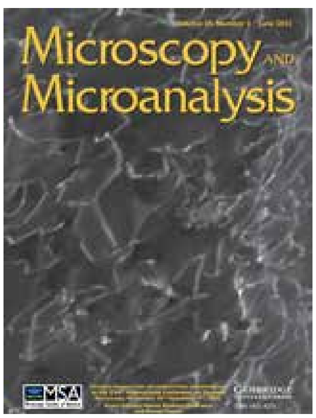
PETER MARLEAU was nominated as the Associate Editor of the *Journal of Nuclear Materials* Management for the Nonproliferation and Arms Control technical division. Marleau is an experienced LDRD PI and team member who has led several arms control-related projects. He is also the chair of two international working groups tasked with understanding and developing verification technologies.

Alec Talin

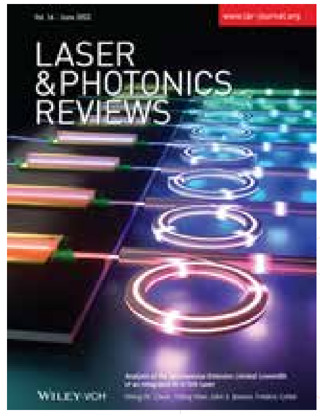
ALEC TALIN was appointed to the *Science Magazine* Board of Reviewing Editors. Talin has led 10 LDRD projects and contributed to many others. He has written over 200 publications and been cited more than 12,000 times. He was elected as Fellow of the American Physical Society in 2018.

Journal Covers

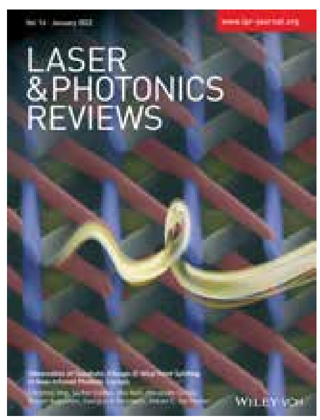
"Inelastic Relaxation in Silica Via Reactive Molecular Dynamics," published in the *Journal of the American Ceramic Society* (April 2022), uses molecular dynamics simulations to explore how silica glass behaves under deformation. The work is part of the LDRD "Stress Intensity Thresholds for Development of Reliable Brittle Materials" led by PI Jessica Rimsza that investigates the conditions that govern when, or if, a material will fail. The cover images illustrate stress distributions at the atomic scale ahead of a crack tip following relaxation at varying temperatures.



"Semi-Automated, Object-Based Tomography of Dislocation Structures," published in *Microscopy and Microanalysis* (June 2022), presents a new method of studying dislocations in materials sciences that reduces the amount of data needed by using prior knowledge of dislocations being line objects. The work is part of the LDRD "Dislocation Cell-Wall Formation in Deformed Structural Metals: Untangling the Theory of Low Energy Dislocation Structures" led by PI Douglas Medlin that investigates the mechanisms governing the formation and stability of dislocation cell walls in minerals. The cover image depicts a raw diffraction-contrast scanning transmission electron microscope image of dislocations.



"Analysis of the Spontaneous Emission Limited Linewidth of an Integrated III–V/SiN Laser," published in *Laser & Photonics Reviews* (June 2022), develops a new approach to reduce the linewidth of a semiconductor laser coupled to a silicon nitride resonator, including potential improvements to optimize device engineering. The work is part of the LDRD "High Performance Heterogeneously Integrated Lasers for RF Photonics and Quantum Sensing" led by PI Michael Gehl that explores the materials, fabrication processes, and physics required to demonstrate a fully heterogeneously integrated laser (<100Hz linewidth, relative intensity noise below -165 DBc/Hz).



"Observation of Quadratic (Charge-2) Weyl Point Splitting in Near-Infrared Photonic Crystals," published in *Laser and Photonics Reviews* (January 2022), experimentally demonstrates (using infrared spectroscopy) splitting of a quadratic Weyl point into two linear Weyl points on a photon crystal, which gives insight into creating topological devices that work in the near infrared. The work is part of the LDRD "Enhancing Photonic Systems Using Topology and Non-Hermiticity" led by PI Alex Cerjan that is discovering new methods and mechanisms for confining light in compact photonic structures using recent discoveries in the fields of topological and non-Hermitian physics.

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

Becky Cox, *Editor*
Vonceil Daniels, *Editor*
Stan Mathews, *Editor*
Sophia Romero, *Editor*
Laura Sowko, *Editor*

LDRD PROGRAM OFFICE

Wahid Hermina
Marie Arrowsmith
Dorean Chaleunphonh
Leigh Cunningham
Ladonna Martin
Jenni Pandazis
Nicole Seay
Amy Treece

CHIEF RESEARCH OFFICE

Susan Seestrom,
Advanced Science & Technology Associate Labs Director & Chief Research Officer

Basil Hassan,
Deputy Chief Research Officer

Issued by Sandia National Laboratories, 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.

Available to DOE and DOE contractors from

U.S. Department of Energy Office of Scientific and Technical Information P.O. Box 62 Oak Ridge, TN 37831

Telephone: (865) 576-8401 | Facsimile: (865) 576-5728
E-Mail: reports@osti.gov
Online ordering: http://www.osti.gov/scitech

Available to the public from

U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312

Telephone: (800) 553-6847 | Facsimile: (703) 605-6900
E-Mail: orders@ntis.gov
Online order: http://www.ntis.gov/search