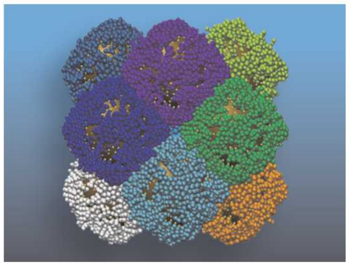
SAND2018-3216R

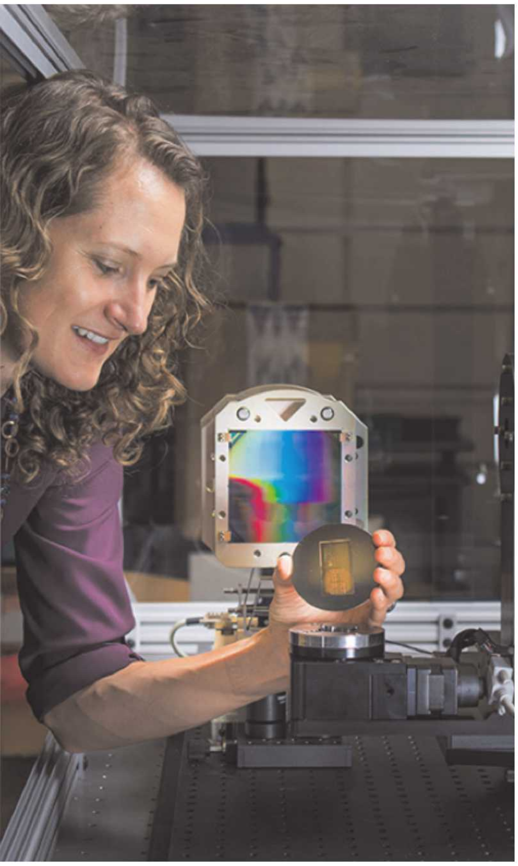
SANDIA NATIONAL LABORATORIES

Exceptional service in the national interest

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2017 ANNUAL REPORT





Sandia National Laboratories

LDRD
Laboratory Directed Research and Development

LDRD

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LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2017 ANNUAL REPORT

March, 2018

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and 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.

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From the Chief Research Officer

Every year, Sandia National Laboratories' LDRD program supports innovations that contribute to national security. The LDRD program also funds projects that have made enormous strides on energy security and reliability, public health, environmental quality, and other disciplines critical to the security of the United States and its citizens.

Within Sandia, the LDRD program is essential to building and maintaining our status as a source of science, technology, and engineering expertise for the nation. LDRD funding ensures that Sandia can advance the frontiers of knowledge in areas relevant to our missions; supports Sandia researchers developing innovative solutions and novel tools; and helps Sandia attract, develop, and retain a world-class technical workforce. This funding also supports Sandia's efforts to develop technology for economic impact and the public good.

Sandia considers proposals from across the Labs, following NNSA and internal processes to select creative projects that align with Sandia strategy and national security impact; demonstrate technical merit and feasibility; and lead to cutting-edge, high-risk R&D. In 2017, Sandia staff submitted 824 short idea proposals, of which 268 were invited to submit long proposals. In the end, 125 new projects received LDRD funding for FY 2017. Over the course of 2017, an additional 42 late start projects were selected. With the FY 2017 additions, the number of active LDRD projects now totals 344.

For FY 2018, watch for several changes to Sandia's LDRD program. Re-engineering LDRD is one of the new Sandia leadership team's top five goals. Since I became Sandia's Chief Research Officer, I have worked closely with my staff to make the LDRD program simpler, more efficient, and better founded on Labs-wide principles and metrics. We also are taking steps to improve the alignment of research with Sandia's missions and strategy. For FY 2018, we already have initiated new approaches for LDRD that are designed to speed the movement of LDRD-funded developments from concept to mission, and to focus an increased portion of LDRD research on future national security challenges. I look forward to reporting our successes on these fronts and on the accomplishments of Sandia's talented R&D staff.

2017

Susan Seestrom

Chief Research Officer
Associate Laboratories Director
Advanced Science and Technology

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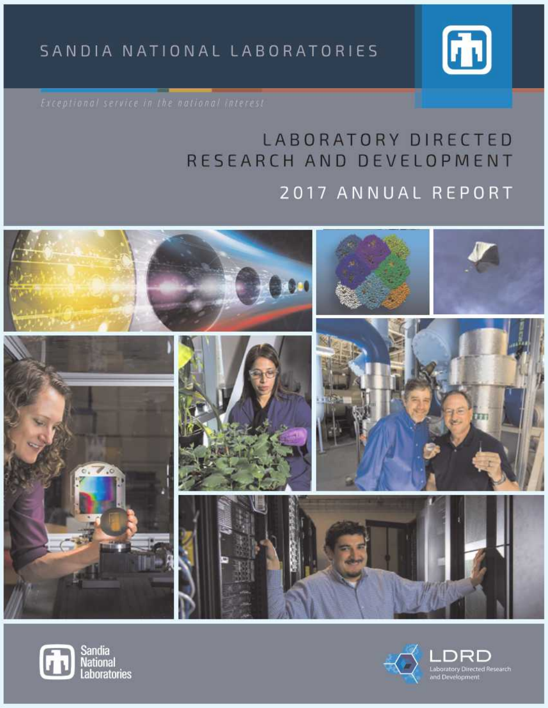


On the Cover

Top Left: This stylized illustration of a quantum bridge shows an array of holes etched in diamond with two silicon atoms placed between the holes.

Top Middle: Coarse-grained model of face-centered cubic array of 6 nm diameter alkanethiol gold nanoparticles.

Top Right: Balloon-borne infrasound microphone system.

Middle: Seema Singh examines a tobacco plant that has been genetically engineered for the easy extraction of important chemicals. (Photo by Dino Vournas)

Middle right: Curtis Mowry, left, and Mike Siegal show nanoporous carbon coated surface acoustic wave sensors. (Photo by Randy Montoya)

Bottom Left: Amber Dagel holds a calibration sample to be loaded into the Labs' x-ray phase contrast imaging machine. (Photo by Randy Montoya)

Bottom Right: Vincent Urias helped develop the HADES program that employs alternative realities to confuse hackers. (Photo by Randy Montoya)

PROGRAM OVERVIEW

Sandia's Laboratory Directed Research and Development Program

Sandia National Laboratories is charged with working on tough technical problems on behalf of the nation. As Sandia's sole discretionary research and development (R&D) program, Laboratory Directed Research and Development (LDRD) funds foundational, leading-edge R&D that nurtures and enhances core science and engineering capabilities, supports national security missions, and creates new capabilities. Sandia's LDRD program is an essential element of the Laboratories' purpose to provide "exceptional service in the national interest."

Enduring LDRD Program Goals

The purpose of the LDRD program is to **enable current and future national security missions by**:

- advancing the frontiers of knowledge in areas relevant to the Labs' missions
- developing innovative solutions and novel tools, and
- attracting, developing, and retaining a world-class technical workforce

Advancing the frontiers of knowledge in areas relevant to Sandia missions

Developing innovative solutions and novel tools

Attracting, developing, and retaining a world-class technical workforce

FY 2017 LDRD Program Statistics

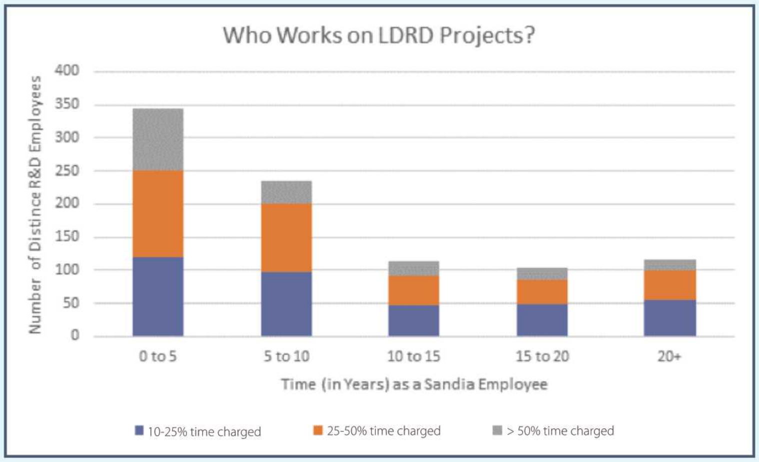
$154.7M Total Program Cost

$343K Median Project Size

344 Total LDRD Projects

165 New Projects in 2017

LDRD Participants



LDRD-Supported Postdocs	**132**	42% of Sandia total
LDRD-Supported Postdoc to Staff Conversions	**22**	47% of Sandia total
Refereed Publications	**291**	27% of Sandia total
Technical Advances	**124**	42% of Sandia total
Patents Issued	**86**	57% of Sandia total
Software Copyrights	**35**	35% of Sandia total
R&D 100 Awards	**3**	60% of Sandia total

Program Structure

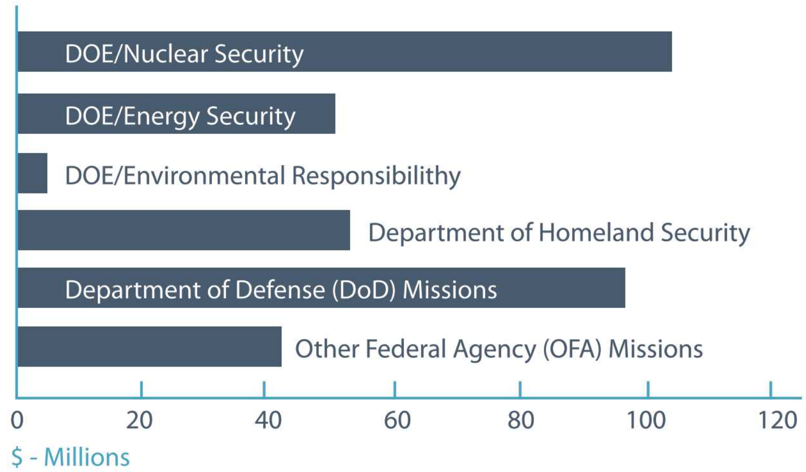
Sandia's research strategy arises from Labs strategy: LDRD investments are based on a strategic and balanced portfolio of funding targets for major elements, known as Program Areas, which are further broken down into Investment Areas (IAs). Each IA is focused on discipline- or mission-based research priorities set by Sandia's leadership. The LDRD program structure and the allocation of funds to the associated IAs are designed to align LDRD investments with Sandia strategy and future mission needs.

LDRD investments provide cutting-edge foundational support for all of Sandia's strategic national security missions (Research Foundations), create and nurture the ability to provide innovative solutions for NNSA, DOE, and other Federal agencies (Mission Foundations), and address major research challenges to develop bold solutions to important national security challenges (Grand Challenges). The Corporate Investments Program Area supports strategic collaborations, special Labs fellowships, and Exploratory Express, an agile mechanism to test and mature novel R&D ideas.

	Investment Area	Mission Impact/Laboratory Capability
RESEARCH FOUNDATIONS	**Bioscience**	Conduct multidimensional, integrated analyses of complex biological samples and communities to reduce national security risks posed by biological threats and US reliance on fossil fuels.
	Computing and Information Sciences	Advance the state of the art in mathematics, information sciences, and computing relevant to Sandia's national security missions.
	Engineering Sciences	Integrate theory, computational simulation, and experimental discovery and validation to understand and predict the behavior of complex physical phenomena and systems.
	Geoscience	Perform world-class R&D in support of Sandia's national security missions focused on the properties, structure, phenomena and processes associated with the earth's geosphere, hydrosphere, and atmosphere and/or address how engineered systems interact with the earth.
	Materials Science	Nurture Sandia's materials science capabilities needed to: (1) enable science-based engineering decisions for Sandia's mission areas, (2) provide the materials discovery, synthesis and processing to underpin current and future Sandia materials applications, (3) respond to emerging national security needs including military, terrorism, cyber, economic and energy, and (4) execute foundational R&D to develop new insights and understanding that are critical to our national security missions.
	Nanodevices and Microsystems	Perform creative, leading edge, and high-impact R&D to discover new phenomena at the nanoscale and microscale; and create or prove new concepts, devices, components, subsystems, and systems.
	Radiation Effects and High Energy Density Sciences	Advance the state of the art in radiation effects sciences, dynamic material properties, high energy density science, inertial confinement fusion, and pulsed power technology to enable stockpile stewardship and national security missions.
	New Ideas	Support pioneering research that may lead to game-changing breakthroughs in science and technology that could eventually impact national security.
MISSION FOUNDATIONS	**Defense Systems and Assessments**	Develop innovative systems, sensors, and advanced science and technology solutions to detect, deter, track, defeat, and defend against threats to our national security.
	Energy and Climate	Develop and create capabilities to contribute to the nation's energy security and resilience, economic viability, and environmental sustainability.
	Global Security	Support innovative science and technology that enhances our abilities to provide effective advice, analyses, technologies, and enterprise-level solutions to manage risks from the world's most dangerous events.
	Nuclear Weapons	Nurture a creative and vibrant science, technology, and engineering base to support a deep scientific understanding of current and future NW products with a focus on affordability, agility and assurance.
Grand Challenges		Address bold science, technology, and engineering challenges requiring large multidisciplinary teams to provide breakthrough solutions to critical national security challenges.
Exploratory Express		Answer key research questions within a relatively short timeframe in an area of current or future strategic importance to Sandia. (Corporate Investments Program Area)

Mission Enabling Research

The LDRD program invests in research to enable mission success. As a multidisciplinary laboratory, Sandia brings researchers from all areas of science and engineering. By working together on LDRD projects, researchers develop leading edge solutions to both current and future challenges. From building foundational science capabilities to applied research to technology development, each LDRD project addresses one or more of the following: DOE/NNSA's missions, as well as the national security missions of the Department of Homeland Security, the Department of Defense, and Other Federal Agencies.

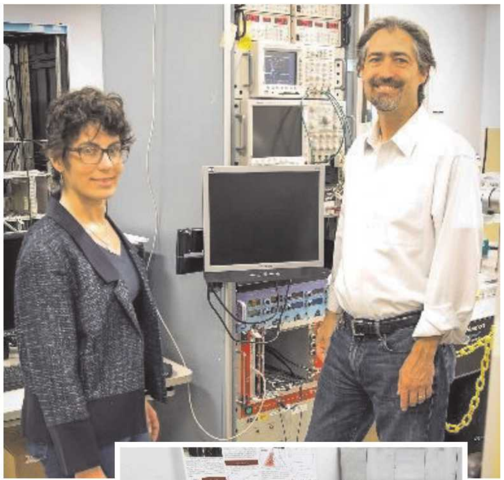


ADVANCING THE FRONTIERS OF SCIENCE AND ENGINEERING

Sandia is a 21st century, broad spectrum national security laboratory, and LDRD research plays an essential role in maintaining the Labs' scientific vitality. As the nation's most diverse national security laboratory, Sandia is uniquely equipped to tackle groundbreaking interdisciplinary research. Sandia researchers work across a broad spectrum of disciplines, collaborating to advance the frontiers of science and engineering in areas that are critical to Sandia's national security mission areas.

HIGHLIGHTS

World's smallest neutrino detector finds big physics fingerprint. A Sandia team was among the COHERENT collaboration of 80 researchers from 19 institutions and four nations that discovered compelling evidence for a neutrino interaction process using the world's smallest neutrino detector. The research, performed at the Oak Ridge National Laboratory (ORNL) Spallation Neutron Source (SNS) and published in the journal, *Science* [1] , provides compelling evidence for a neutrino interaction process predicted by theorists 43 years ago, but never seen. The breakthrough paves the way for additional discoveries in neutrino behavior and the miniaturization of future neutrino detectors. In an Exploratory Express LDRD project in 2013, Sandia made the critical initial measurements in the basement of ORNL's Spallation Neutron Source that established the viability of the experiment.



LDRD Project 173302 Enabling the First Ever Measurement of Coherent Neutrino Scattering through Background Neutron Measurements (FY 2013)

Top: Sandia researchers David Reyna, right, and Belkis Cabrera-Palmer were instrumental in the COHERENT collaboration. (Photo by Michael Padilla) Bottom: Sandia module for neutron monitoring.

[1]D. Akimov *et al., Science* 10.1126/science.aao0990 (2017)

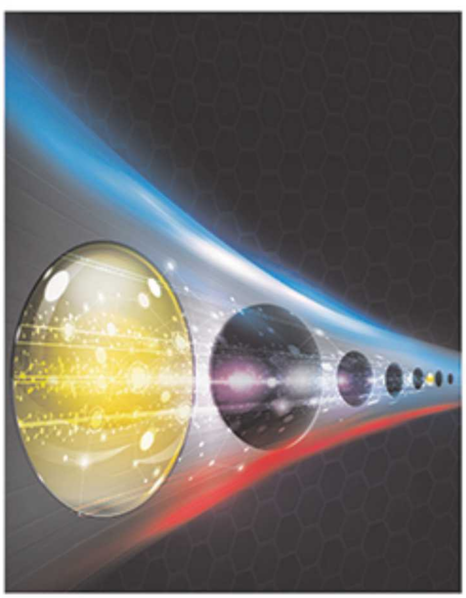
Brain stimulation during training boosts performance. LDRD-funded research from Sandia published in *Neuropsychologia*[2] shows that working memory training combined with a kind of noninvasive brain stimulation can lead to cognitive improvement under certain conditions. Improving working memory or cognitive strategies could be very valuable for training people faster and more efficiently. Using more than 70 volunteers divided into six groups, the researchers used different combinations of working memory training with transcranial direct current stimulation. Then they assessed the volunteers' performance on working memory tests and a test of problem-solving ability. Co-PI Laura Matzen said the research could benefit many national security mission areas "where people must learn complex tools and systems. Reducing training time and improving cognitive performance would have substantial benefits to overall system performance."

LDRD Project 165715 Testing the Effects of Transcranial Direct Current Stimulation on Human Learning (FY 2013)

Cognitive scientist Mike Trumbo adjusts the placement of a transcranial direct current stimulation unit on cognitive scientist Laura Matzen's head. (Photo by Randy Montoya)

Sandia-Harvard team create first ever quantum computer bridge. By forcefully embedding two silicon atoms in a diamond matrix, Sandia LDRD researchers have demonstrated for the first time on a single chip all the components needed to create a quantum bridge to link quantum computers together. "People have already built small quantum computers," says Sandia researcher Ryan Camacho. "Maybe the first useful one will not be a single giant quantum computer but a connected cluster of small ones." Distributing quantum information on a bridge, or network, also could enable novel forms of quantum sensing because quantum correlations allow all the atoms in the network to behave as though they were one single atom. The joint work with Harvard University used a focused ion beam implanter at Sandia's Ion Beam Laboratory designed for blasting single ions into precise locations on a diamond substrate. The work is published in the journal, *Science*[3].

LDRD Project 192701 Optimization of SiV Defect Yield in Diamond Substrates (FY 2016)



This stylized illustration of a quantum bridge shows an array of holes etched in diamond with two silicon atoms placed between the holes.

[2] M. C. Trumbo *et al., Neuropsychologia* 10.1016/j.neuropsychologia.2016.10.011 (2016)
[3] A. Sipahigil *et al., Science* 10.1126/science.aah6875 (2016)

INNOVATIVE TOOLS AND SOLUTIONS

LDRD projects create and enhance capabilities and products that support national security missions through innovative science, technology, and engineering. LDRD has been, and will continue to be, a key contributor to the development of science and engineering capabilities used to secure our nation now and into the future.

Many Sandia LDRD projects include collaborations with industry, academia, and other government agencies. The Labs and its strategic partners gain from collaborative research results. Many technological breakthroughs originating from, or improved through the LDRD program, are transferred to industry, commercialized under licensing agreements, and brought to market for the US public good.

HIGHLIGHTS

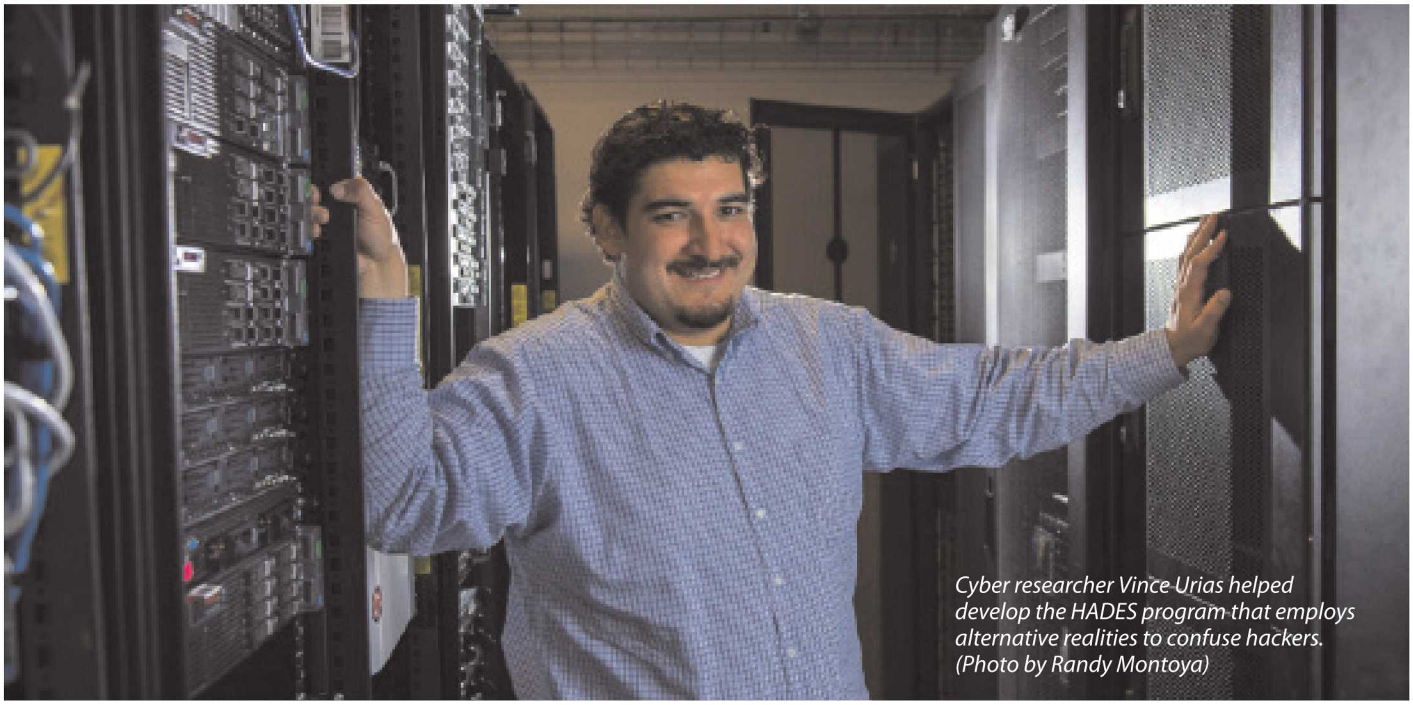
The world's first free flying infrasound sensor array in the lower stratosphere.

In July 2017, a fleet of five solar-powered balloons reached a height of 13 to 15 miles, twice as high as commercial jets, and detected the infrasound from a test explosion. Infrasound is important because it is one of the verification technologies the US and the international community use to monitor explosions, including those caused by nuclear tests. Traditionally, infrasound is detected by ground-based sensor arrays, which do not cover the open ocean and can be muddled by other noises, such as the wind, or even air conditioners. "The stratosphere is much less noisy so you can detect events of interest to science and national security from greater distances," said Daniel Bowman, LDRD principal investigator. The stratosphere is the atmospheric layer from about 5 miles to 31 miles above the ground. This LDRD funded experiment showed that networks of balloon borne infrasound microphones can detect and locate events. Sandia now has the capability of fielding airborne swarms of infrasound microphones over inaccessible or denied areas. This capability offers new opportunities in geophysics, atmospheric science, planetary acoustics, and mission-based operations. This is the next frontier of infrasound, with implications for remote monitoring and source characterization that is difficult to accomplish on the ground.

LDRD Project 206542 Evaluating the Capability of High-Altitude Infrasound Platforms to Cover Gaps in Existing Networks (FY 2017)

Above: Infrasound microphone system post-launch

Right: Geophysicists Danny Bowman, left, and Sarah Albert display an infrasound sensor and the box used to protect the sensors from the extreme temperatures experienced by balloons that take the sensors twice as high as commercial jets fly. (Photo by Randy Montoya)



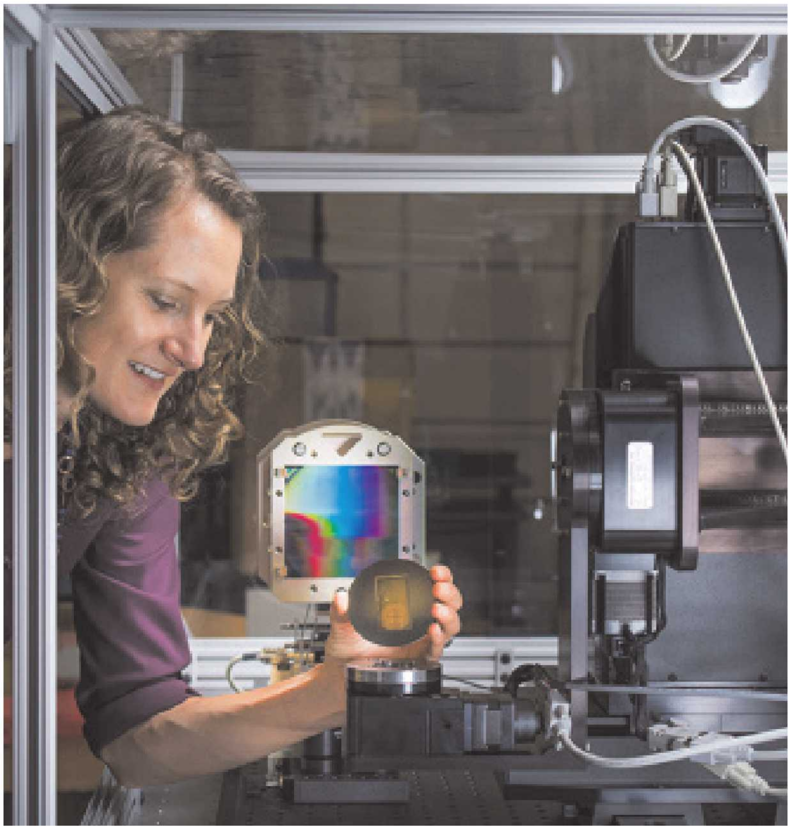
Cyber researcher Vince Urias helped develop the HADES program that employs alternative realities to confuse hackers. (Photo by Randy Montoya)

HADES creates alternate reality to mislead hackers. The rise in sophisticated cyberattacks has prompted businesses and organizations to seek out robust security measures with the ability to detect and respond to an adversary's attacks in real time. Many are using deceptive tools and tactics; however, current deception tools only provide partial solutions to full-spectrum deception. Sandia's High-Fidelity Adaptive Deception and Emulation System (HADES) is a comprehensive cybersecurity platform that utilizes revolutionary advances in deception technologies that allow network defenders to defend and collect information on the adversary in real time. Rather than simply blocking a discovered intruder, HADES feeds a hacker not what he needs to know but what he wants to believe. "Deception is the future of cyber defense," said researcher Vince Urias. "Simply kicking a hacker out is next to useless. The hacker has asymmetry on his side; we have to guard a hundred possible entry points and a hacker only needs to penetrate one to get in." The HADES platform utilizes software defined networks, cloud computing, dynamic deception, and agentless virtual machine introspection. These elements fuse to not only create complex, high-fidelity deception networks, but also provide mechanisms to directly interact with the adversary—something current deception products do not facilitate.

HADES won a 2017 R&D100 award, presented by R&D Magazine, to recognize exceptional innovations in science and technology. The Sandia work began with an LDRD project and was patented in October 2017.

LDRD Project 165547 Computer Network Deception (FY 2013-2015)

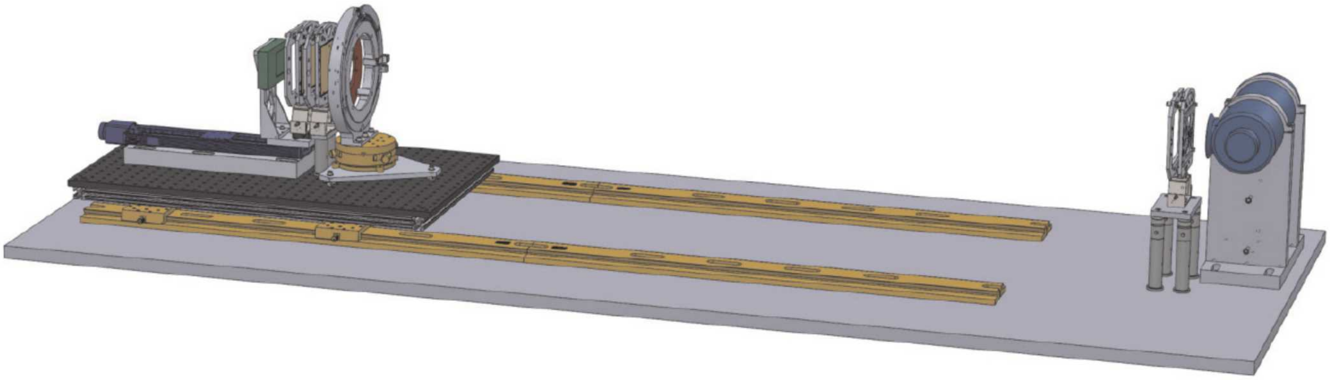
Lighting up the study of low-density materials. It is hard to get an x-ray image of a low-density material like tissue between bones because x-rays just pass right through like sunlight through a window. But what if you need to see the area that is not bone? Sandia studies myriads of low-density materials, from laminate layers in airplane wings to foams and epoxies that cushion parts, and has to be able to spot defects before they cause a high-consequence failure, because materials do not perform well with voids or cracks or if they separate from adjacent surfaces. Sandia borrowed and refined a technique being studied by the medical field, x-ray phase contrast imaging, to look inside the softer side of things without taking them apart. In an LDRD project that ended in 2016, researchers demonstrated that x-ray phase contrast imaging could show details where one material meets another. A new LDRD project seeks to make gratings that operate at higher x-ray energies. Gratings, optical components that look like bunches of upright parallel bars, create interference in the x-ray beam, merging sources of light to create an interference pattern that can be measured. Researcher Amber Dagel believes the technique eventually will have an enormous impact for research and manufacturing. "I think it can be useful in the research phase, when you are trying to understand the distribution of microbeads within an epoxy or how the foam is mating with the canister it is filling up, is there a gap there? Or what defects can I see in my airplane wing laminate?" she said. "I also think it can be used in quality assurance: I know what my part should look like, but I need to make sure there are no cracks, there are no voids."



LDRD Projects 180828 Internal Structure Mapping with X-Ray Phase Contrast Imaging (FY 2016) and 200524 Non-Destructive Evaluation for Encapsulated Component Qualification. (FY 2017-2019)

Amber Dagel holds a calibration sample to be loaded into the Labs' x-ray phase contrast imaging machine. Dagel is principal investigator for the Labs' work into using x-ray phase contrast imaging to study low-density materials. (Photo by Randy Montoya)

Below: Sandia's x-ray phase contrast imaging system fits on a laboratory table. The source grating fits in front of the x-ray tube on the right, creating an array of tiny x-ray sources, which travel to the sample that sits in the ring. Behind the sample are phase and analyzer gratings and the detector.



Overcoming the trust barrier in NW verification measurements. Sandia physicist Peter Marleau has developed a new method for verifying warhead attributes. Called CONFIDANTE, for CONfirmation using a Fast-neutron Imaging Detector with Anti-image Null-positive Time Encoding, the method could help address the problem of conducting verification measurements while simultaneously protecting sensitive design information. It provides middle ground for the warhead owner, or host, who wants to protect sensitive information, and the monitor, who may be seeking to verify that sensitive information to confirm the inspected item is a warhead. "CONFIDANTE is an implementation of a zero-knowledge proof (ZKP) as a way to demonstrate the validity of a claim while providing no further information beyond the claim itself," Marleau says. "Unlike other ZKP confirmation methods, which rely on a measuring instrument that has been pre-loaded with sensitive information, CONFIDANTE allows the monitoring party to conduct the measurement in real time without accessing sensitive design data."

Marleau, along with Patricia Schuster, a University of Michigan postdoctoral fellow, and Rebecca Krentz-Wee, a University of California, Berkeley nuclear engineering graduate student, set out to solve the problem of a ZKP for warhead verification without compromising critical design information. The three explored different concepts that might provide more practical and verifiable ZKP implementations. They identified a promising solution using time-encoded imaging (TEI), a method Sandia developed first under LDRD funding, with further development funded by NNSA's Defense Nuclear Nonproliferation Research and Development program.

BRAIN TRUST — Researchers, left to right, Peter Marleau, Patricia Schuster, and Rebecca Krentz-Wee have developed a new method for verifying warhead attributes. (Photo by Dino Vournas)

TEI is a new approach for indirect detection and localization of special nuclear materials. Sandia developed TEI to overcome the precise calibration and high cost of typical detection, which uses arrays of detectors. TEI uses a single detector within a cylindrical coded mask. As the mask rotates, radiation from the object is modulated by a pattern of apertures and mask elements on the cylinder. Using TEI, a single detector can do the work of multiple detectors in creating an entire two-dimensional image of the object.

"We realized that if we designed the mask such that the pattern on one half of the cylinder is the inverse of the other half, an object on one side of the system will project the inverse image of an object on the opposite side of the system at all times if and only if the two objects are identical. The image and anti-image will effectively cancel each other out and the detector will show a constant unmodulated rate," Peter says. "And we can do it without ever recording potentially sensitive information."

LDRD Project 155299 "Time Encoded Radiation Imaging" (FY 2011)

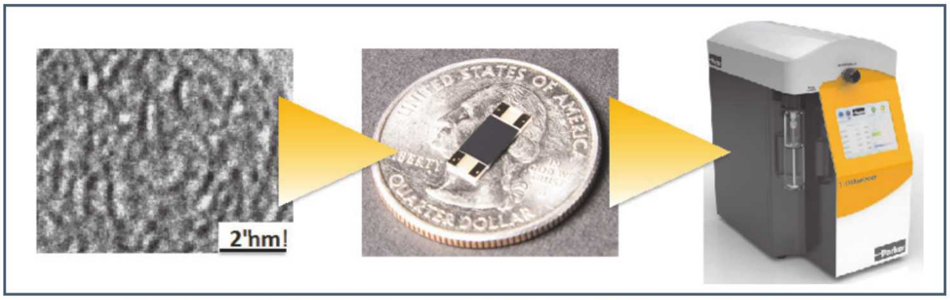
On the trail of a killer. Sandia has developed a safer, easier, faster, and cheaper way to detect anthrax and is working with an Albuquerque company, Aquila, to commercialize the technology. Dubbed BaDx (Bacillus anthracis diagnostics), the credit-card-size device, a mini-laboratory, can detect the anthrax bacteria in places with no power, refrigerated storage, or lab equipment. Initially developed in an LDRD project launched in 2011, it could cost around $5-$7 and requires no specialized tools and minimal or no training. With help from the Labs' technology transfer programs, BaDx is moving closer to market. "This is a wonderful example of where sophisticated technology has enabled a practical solution to a very important problem," says Mary Monson, senior manager of Technology Partnerships and Business Development.

LDRD Project 151375 "CVD Encapsulation of Mammalian Cells for Hazardous Agent Detection" (FY 2011-2013)

The credit-card-size device, a mini-laboratory, can detect the anthrax bacteria in places with no power, refrigerated storage, or lab equipment. (Photo courtesy of Aquila)

PREPARING TO MARKET—The BaDx technology has been licensed to Aquila, a New Mexico company that specializes in the design and manufacture of technologies and services for nuclear security and international safeguards. Aquila is working with Sandia through a Cooperative Research and Development Agreement to complete testing with external partners and begin marketing BaDx. (Photo courtesy of Aquila)

Clean water that is 'just right' with Sandia sensor solution. Working with Parker Hannifin, Sandia combined basic research on an interesting form of carbon with a unique microsensor to make an easy-to-use, table-top tool that quickly and cheaply detects extremely low levels of each trihalomethane: chloroform, bromoform, bromodichloromethane and dibromochloromethane. Enabling work was funded by the LDRD program. "Everybody who has been involved with this project always smiles when they talk about it," says researcher Mike Seigal. "Not only did we see our basic research into what this carbon material was and the physics of how surface acoustic wave (SAW) devices work come together, but we helped develop a successful product that improves public health." Parker-Hannifin has more dedicated trihalomethane analyzers installed in North America than any other company. Recently, Parker Hannifin released an automated online version of the water analyzer for continuous monitoring of trihalomethanes.



LDRD Projects 52595 Real-Time Discriminatory Sensors for Water Contamination Events (FY 2003-2005) and 62269 Nanoporous-Carbon Adsorbers for Chemical Microsensors (FY 2003-2004)

Above: Transmission electron microscopy image of nanoporous carbon, left, "the most controllable carbon in the world, in the terms of its mass density and its total surface area," according to Sandia researcher Mike Siegal. A nanoporous carbon coated surface acoustic wave sensor on a quarter, middle. This sensor is the key component of Parker Hannifin's Trihalomethane Water Analyzer, right.

Right: Curtis Mowry, left, and Mike Siegal show their nanoporous carbon coated surface acoustic wave sensors. Their sensor forms the heart of Parker Hannifin's Trihalomethane Water Analyzer that provides almost-instant feedback on the disinfection byproduct levels of water, before it reaches consumers. (Photo by Randy Montoya)

R&D 100 AWARDS

Since 1976, Sandia has received more than 114 R&D 100 Awards, often referred to as the "Oscars of Invention" or the "Nobel Prizes of Technology." Competing in an international pool of universities, corporations, and government labs, Sandia inventions and co-inventions captured five R&D 100 Awards in 2017; three included developments funded by the LDRD Program. *R&D Magazine* presents the awards each year to researchers who its editors and independent judging panels determine have developed the year's 100 most outstanding advances in applied technologies. The 2017 LDRD Winners are:

2017 LDRD Winners

The SolidSense "Gas Analyzer on a Chip"—Sandia researchers have developed a robust sensor platform that measures all US Environmental Protection Agency-regulated emissions. SolidSense provides exhaust chemistry feedback for engines, turbines, power plants, and other applications improving combustion and fuel efficiency and reducing harmful emissions. The sensor is the first of its kind to operate in hostile high-temperature environments without the need for cooling or filtration. It can be mass produced at low cost. Click here for the video.

Ultra-Wide Bandgap Power Electronic Devices—These devices would replace transformers with transistor based electronics, enabling next-generation power electronics by providing switching speeds 10 times faster than the current state-of-the-art passive components. Ultra-wide bandgap power electronic devices are also smaller, more efficient, and less expensive, and would enable other components in electronic devices to be smaller as well. These devices can also function at higher operating temperatures and in high radiation environments such as space. Click here for the video.

High-fidelity Adaptive Deception and Emulation System (HADES) Platform—HADES radically changes the way cybersecurity defenders protect their networks and gain insight on adversaries. The platform emulates a realistic environment of as many as 10,000 machines, creating a far richer deception than honeypots and other techniques. It encourages adversaries to stay long enough to reveal their intent, tools, and tactics. HADES then automatically sends information on adversaries to defenders. Click here for the video.

ATTRACTING, DEVELOPING, AND RETAINING A WORLD-CLASS TECHNICAL WORKFORCE

Sandia's specialized missions require highly motivated, qualified staff with deep expertise, committed to advancing the frontiers of science and engineering through continual growth and development. The LDRD program supports some of Sandia's most accomplished scientists and engineers, as well as many promising early career researchers. Here are some of the LDRD participants who were recognized for their achievements this year. Additional awards for LDRD projects and researchers are listed in the Awards Section of this report.

Presidential Early Career Award for Scientists and Engineers (PECASE)

Sandia LDRD researchers Stephanie Hansen and Alan Kruizenga received the Presidential Early Career Award for Scientists and Engineers (PECASE) in 2017. The PECASE is the highest honor bestowed by the US government on outstanding scientists and engineers in the early stages of their careers. The awards traditionally are conferred annually at the White House following recommendations from participating US agencies. Stephanie studies the behavior of atoms in extreme environments and is working under a five-year Early Career Award granted by the DOE Office of Science in 2014. Alan's primary area of research focuses on materials degradation and interfacial interactions in molten nitrate salt systems and liquid metal systems for thermal energy storage.

Stephanie Hansen
(Photo by Lonnie Anderson)

Alan Kruizenga
(Photo by Randy Wong)

Society of Women Engineers

Two Sandia LDRD participants have been recognized by the Society of Women Engineers for their support in the enrichment and advancement of women in engineering.

Kelly Hahn received the Emerging Leader Award, which honors individuals "who have been actively engaged in an engineering or technology profession and have demonstrated outstanding technical excellence as an individual resulting in significant accomplishments." As an expert on measuring neutron yield, Hahn was the primary scientist supporting the measurements associated with an LDRD project to develop new physical simulation capabilities to qualify non-nuclear weapons components in radiation environments.

Leslie Phinney received the Prism Award, honoring "a woman who has charted her own path throughout her career, providing leadership in technology fields and professional organizations along the way." Phinney is a thermal analyst working in thermal sciences and engineering, focusing on using thermal analysis to evaluate weapons system response, and has led and participated in LDRD projects.

Minerals, Metals, and Materials Society

Stephen Foiles

The Minerals, Metals, and Materials Society (TMS) honored Stephen Foiles with its 2017 Cyril Stanley Smith Award. The award honors his outstanding contributions to the science and technology of materials structure. Stephen and two Sandia colleagues — Murray Daw, now at Clemson University, and Mike Baskes, now at Mississippi State University — developed what is now the standard formula for how atoms interact in simulations of metals. Stephen's years of work on the structure, thermodynamics, and mechanical properties of grain boundaries have also received recognition. His recent studies of defects in metals and semiconductors focus on the variability of interfacial properties, including external conditions such as temperature and alloy composition. His research has been funded by LDRD, as well as by DOE's Office of Basic Energy Sciences and Advanced Simulation and Computing Program.

Fellows

Below are some of the LDRD researchers honored in 2017 by their professional societies for distinguished contributions in technical leadership.

American Physical Society 2017 Fellows

- **François Léonard:** for fundamental studies of the physics of nanoscale electronic devices.
- **Andrew Landahl:** for outstanding leadership and conscientious service to the quantum information community and pioneering contributions to quantum computing theory, including fault-tolerant quantum computing, quantum error correction, universal adiabatic quantum computing and novel quantum search algorithms.
- **Hongyou Fan:** for pioneering contributions to the development of novel synthesis methods and self-assembly processes to fabricate nanostructured materials for nanoelectronic and nanophotonic applications.
- **Igal Brener:** for contributions to optical phenomena in semiconductors, including their coupling to metasurfaces for passive, tunable and nonlinear metamaterials, and coherent terahertz phenomena and instrumentation.

American Society of Mechanical Engineers

- **Cliff Ho** has led innovations in solar energy, water treatment and nuclear waste management;
- **Hy Tran** works in the Primary Standards Laboratory to develop and maintain precise measurement standards for nuclear weapons components; and
- **Kevin Dowding** has developed advanced standards for computational modeling in nuclear weapon design.

Optical Society

- **Hope Michelsen** for pioneering contributions to the fundamental understanding of laser-radiation interactions with soot particles through laser-induced incandescence, absorption and scattering, and using laser-induced incandescence to assess environmental impacts of carbonaceous particle.

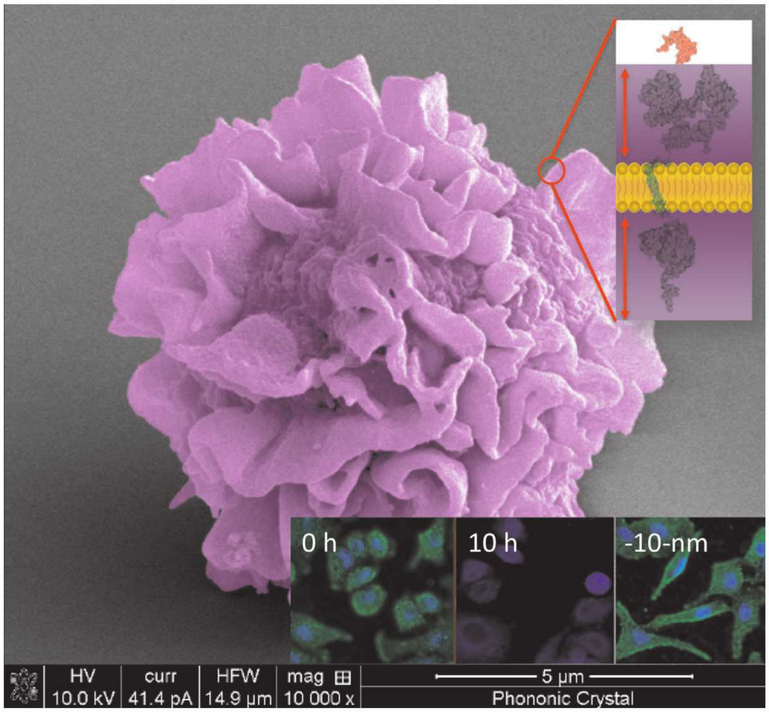
RESEARCH EXCELLENCE IN SERVICE TO THE NATION

LDRD supports Sandia's mission by investing in leading-edge research that advances the frontiers of science and engineering critical to national security. The program also is instrumental in attracting and developing a world-class workforce of scientists and engineers, the people who make it possible for Sandia to achieve its mission and goals.

To learn more, visit www.sandia.gov/ldrd.

BIOSCIENCE

The figure on the right shows examples of silica cell replica—lower inset shows antibody (green) binding to surface receptors before silicification (0 h) and after silica etching (-10-nm); at 10 h of silicification receptors are obscured by silica (as depicted in upper inset). Nucleus stained blue. [Project 190960, Modular Abiotic/ Biotic Systems (MABS) for Understanding and Directing Biological Function]



The overarching goal of the Bioscience Investment Area is to develop new competencies in biological science to address two application areas in Sandia's broad national security mission—biodefense and emerging infectious disease, and sustainable biofuels. The research in biodefense includes developing better ways to detect, characterize, and contain harmful pathogens. The strategy integrates advanced technologies with an understanding of human health and immune response. The goal is to improve the response to disease outbreaks and to limit their spread. The research regarding the nation's reliance on fossil fuels focuses on developing efficient, economical biofuels that can replace or reduce current gasoline, diesel, and aviation fuel consumption. The research includes two sources of energy: lignocellulose, or dry plant matter, and algae. The aim is to find efficient and economical methods to convert lignocellulose (dry plant matter) into fuels and to understand the factors that govern algal pond stability and identify molecular mechanisms that can be used for lipid/fuel production.

PROJECTS

Analyzing and Understanding of Transporters to Control Lignin Transformation into Fuel

190958 | Year 2 of 3

Principal Investigator: J. A. Timlin

Executive Summary:

This project will create an engineered bacterial or fungal host capable of enhanced transport of a specific lignin breakdown product into the cell. In order to accomplish this goal, several lignin analytic tools will be developed. Targeted transport is a critical step to economically upgrade lignin into more valuable products for energy security.

Big Data, Machine Learning and Dynamic Complex System Modeling to Improve Algae Cultivation

199975 | Year 1 of 3

Principal Investigator: R. W. Davis

Executive Summary:

This project will develop new fundamental understanding, experimental validation, and modeling capabilities to identify low cost mechanism for minimizing algae biomass productivity losses based on finite horizon environmental data. Understanding the fundamental interactions of fluid dynamics, microbial communities, and basic raceway management practices in variable environmental regimes will help to maximize algae biomass productivity to impact our nation's biomass resource potential.

Bio-Emulative Metal-Organic-Framework-Based Lignin Degradation Catalysts

180812 | Year 3 of 3

Principal Investigator: M. D. Allendorf

Executive Summary:

Production of lignin byproduct by a growing US biofuels industry could exceed 200 metric tons per year. This project developed catalysts to convert lignin, the most abundant source of renewable aromatics, to value-added chemicals. Efficient lignin conversion will improve the economics of biofuel production, increase energy independence, and improve air quality by making use of a waste product that might otherwise be burned.

Diagnostic Tool for Measuring Early Chemical Signatures of Pond Crash

199974 | Year 1 of 3

Principal Investigator: M. W. Moorman

Executive Summary:

Our research seeks to demonstrate that predation in algal ponds produces detectable chemical signatures. These gas phase chemical biomarkers are identifiable with Sandia's sensor technology and could be used as a diagnostic to reveal the health of the algal community. This may provide a powerful tool for biofuel producers to monitor the health of their ponds and increase yield.

Discovery of Antiviral Inhibitors against the Chikungunya Virus nsP2 Protease Domain

186364 | Year 3 of 3

Principal Investigator: B. N. Harmon

Executive Summary:

We seek to discover Chikungunya virus (CHIKV) therapeutics using our drug discovery pipeline that includes compound screening with novel fluorescence resonance energy transfer (FRET)-based substrate, and validation of selected compounds using mass spectroscopy and cell-based assays to measure safety and efficacy against infection with CHIKV and distant or related viruses. Unique combined expertise in biodefense, modeling/simulation can accomplish these objectives.

Engineering 'Green' Algae: Reducing Metabolic Waste for High Biomass Productivity

190962 | Year 2 of 3

Principal Investigator: A. Ruffing

Executive Summary:

The economic production of algal biofuels is limited by low natural biomass productivities. To improve biomass productivity in an industrially relevant alga, we will engineer mutants that have reduced metabolic waste (i.e., carbon loss). Specifically, we will target photorespiration and dark respiration, which account for carbon losses in the range of 50-70% on a daily basis.

Exploiting the Microbial Achilles Heel for New Broad Spectrum Anti-Microbials (NBSAMs)

190961 | Year 2 of 3

Principal Investigator: S. Rempe

Executive Summary:

Bacteria resist traditional antimicrobials, costing the US $45B/year for drug-resistant infections and lost lives. Recent discovery of the first new class of antimicrobial in 30 years, Teixobactin (TXB), provides a potential game-changing opportunity for biodefense and public health. Using molecular simulation, quantitative binding assays, and state-of-the-art synthetic strategies, we aim to understand how TXB reaches its targets to facilitate development of more potent, broad-spectrum antimicrobials.

Modular Abiotic/Biotic Systems (MABS) for Understanding and Directing Biological Function

190960 | Year 2 of 3

Principal Investigator: C. J. Brinker

Executive Summary:

This project is developing two classes of modular abiotic/biotic systems (MABS): 1) synthetic biological cells constructed of synthetic/abiotic and natural/biotic components and designed to interact with natural cells; and 2) nanoparticle modified cells with retained viability but altered function. MABS are more durable and chemically complex than natural cells and will enable new capabilities in detection, drug delivery, and detoxification for countering emerging chemical and biological warfare threats.

Predictive Pathogen Biology: Genome-Based Prediction of Pathogenic Potential and Countermeasures Targets

180814 | Year 3 of 3

Principal Investigator: J. S. Schoeniger

Executive Summary:

This project pioneered improved methods for assembling bacterial genomic sequences from low cost next-generation sequencing (NGS) data, developing tools to characterize genomic features determining pathogen virulence, including toxin repeats, mobile elements, and genome rearrangements. Tools for identifying mobile elements were validated against the Reference Sequence (RefSeq) database. A clinical series of ninety *Clostridium difficile* isolates were assembled from low-cost NGS data.

Selection of Ribosomes from Infected Mammalian Cells to Identify Viral Pathogens

199973 | Year 1 of 3

Principal Investigator: K. J. Parchert

Executive Summary:

This project aims to improve the detection and identification of viruses by enriching for viral messenger RNA (mRNA) being translated by host ribosomes. Pathogen identification will be accomplished when viruses are emerging and/or early in infection, when identification of viruses is particularly challenging. Accurate identification of viruses is necessary to determine appropriate mitigating responses to natural outbreaks and biosecurity threats.

Signatures of Genome Editing

204977 | Year 1 of 3

Principal Investigator: J. A. Timlin

Executive Summary:

This project will develop biochemical, bioinformatics, and analytical tools, including assays and protocols to quantify the efficiency and accuracy of genome editing. This work addresses the growing need for robust diagnostics and therapeutics in support of the gene editing activities that are rapidly developing for translational medicine, and to mitigate safety and dual use concerns raised by this technology.

Three-Dimensional Multicolor Superresolution Microscopy for Imaging the Machinery of Cells and Capturing Biochemical Interfaces

199972 | Year 1 of 3

Principal Investigator: A. Backer

Executive Summary:

This project aims to enhance and reimagine all facets of bioimaging technology. Using unconventional imaging system designs, we are working to increase the speed and sensitivity with which large datasets can be acquired, and biological pathogens identified. In addition, using novel optical materials, our work seeks to realize lightweight, small form-factor imaging/display devices for use by military personnel.

Unmasking Hidden Compounds within Hyperspectral Images

190959 | Year 2 of 3

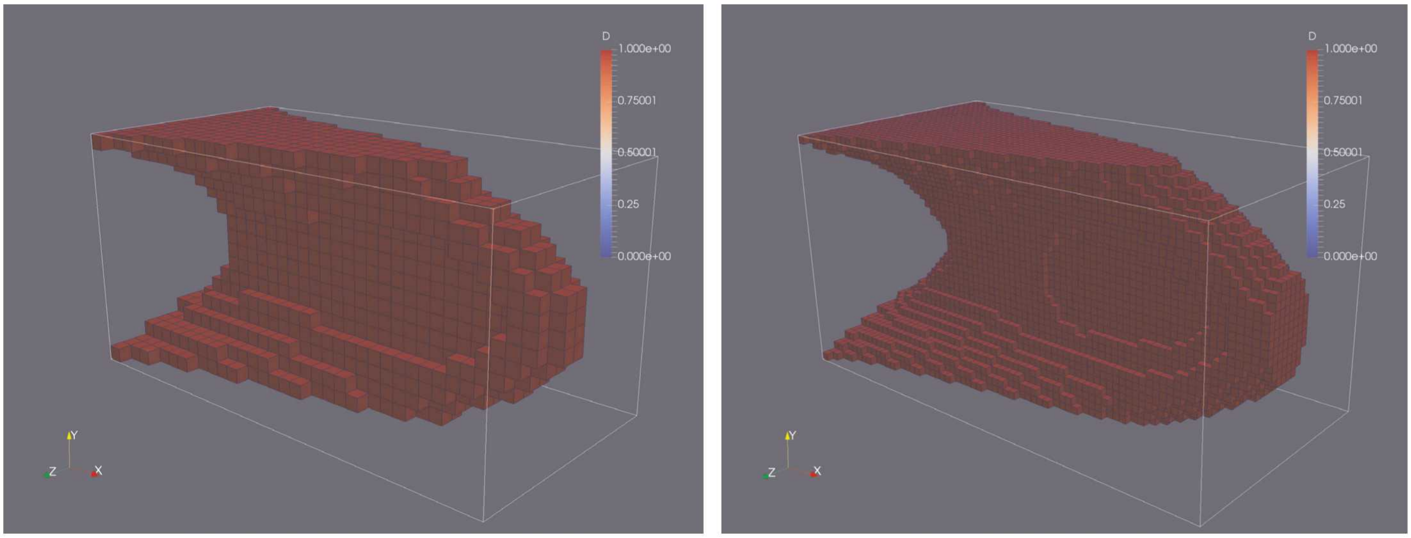
Principal Investigator: S. M. Anthony

Executive Summary:

This project will develop software and hardware to improve detection of weak signals within hyperspectral images. The capabilities developed with the hyperspectral stimulated emission depletion microscope will allow super resolution, spatially resolved detection of pathogenic processes, supporting detection and treatment of infectious disease, and biothreat agents. Software improvements can be more widely applicable to national security applications including remote sensing.

Research Foundations

COMPUTING AND INFORMATION SCIENCES



The figures above show averaged "unfiltered" density optimization variables z for a 32_16_16 mesh (top), and a 64_32_32 mesh (bottom). [Project 180821, Topological Design Optimization of Convolutes in Next Generation Pulsed Power Devices

The Computing and Information Sciences IA champions innovative research and development that advances the state of the art in mathematics, information sciences, and computing relevant to Sandia's national security missions. As these applications continue to technically deepen and broaden, there is an ongoing need to refresh and advance underlying knowledge and capabilities. The scope includes computer and computational science and engineering, information science (including mathematics and cognitive sciences), and aspects of cyber sciences and data sciences.

PROJECTS

PROJECTS (continued)

A Case Study on Neural-Inspired Dynamic Memory Management Strategies for High Performance Computing

194773 | Year 2 of 2

Principal Investigator: C. M. Vineyard

Executive Summary:

This project will investigate whether neural-inspired approaches to multilevel memory management can meaningfully impact high performance computing. The project will explore whether a neurogenesis-inspired algorithmic approach can enable improved resource utilization for increasingly sophisticated high performance computing architectures needed for national security modeling and simulation.

A Disaggregated Memory Architecture for Future High Performance Computing

199977 | Year 1 of 3

Principal Investigator: S. D. Hammond

Executive Summary:

This project will investigate novel approaches to the design of large-scale computing systems in which the storage/memory components of the architecture are placed directly into the high speed interconnection fabric rather than being co-located with processors. The results will demonstrate how, or whether, such an architecture can provide benefit to Sandia's national security mission programs.

A Domain-Specific Language for High-Consequence Control Software

203433 | Year 1 of 3

Principal Investigator: R. C. Armstrong

Executive Summary:

As a joint research project between the Jet Propulsion Laboratory and Sandia in the formal verification of high-consequence controls, Sandia will concentrate research towards high-assurance for time-critical single-threaded controls, using the Statechart language as input allowing interoperability. Sandia's focus is on formal refinement of timed events in controls that will improve the safety, security, and reliability of nuclear weapon controls.

Advanced Data Structures for Improved Cyber Resilience and Awareness in Untrusted Environments

180820 | Year 3 of 3

Principal Investigator: C. A. Phillips

Executive Summary:

This project designed new data structures and algorithms for better assessment of high speed streaming cybersecurity data. Write-optimized data structures (WODS) manage data movement to secondary storage optimally, allowing analysts to store more data. This enables detection of attacks that occur in pieces over time, initially hiding in normal traffic. We also improved disk security, event tracking, and streaming cybersecurity benchmarks.

Adverse Event Prediction using Graph-Augmented Temporal Analysis

190965 | Year 2 of 3

Principal Investigator: R. Brost

Executive Summary:

We seek methods for finding precursors to events of interest in temporal data streams. Our approach employs a combination of temporal analysis and graph analysis. The temporal analysis identifies candidate precursors or temporal anomalies, which are then refined using graph information. Work progresses for evaluating alternative approaches. Successful results would enable improved identification of warning signals for critical events, including counter terrorism, improvised explosive device (IED) detection, and nonproliferation.

An Exascale Computational Simulation Capability for Pervasive Fracture and Failure of Structures

203537 | Year 1 of 3

Principal Investigator: M. W. Heinstein

Executive Summary:

This project will develop the physics models and computational approaches to create a computational simulation approach to answer questions about how structures fail in an explosion, and explore engineering design opportunities to mitigate the effects of a blast. Furthering the science of fracture modeling and simulation is important to our nuclear weapon and other national security programs.

Assembly, Test, and Evaluation of Integrated Complementary Metal Oxide Semiconductor/Silicon Photonics Circuits

199979 | Year 1 of 1

Principal Investigator: A. L. Lentine

Executive Summary:

The goal of the project was to investigate the performance of interface circuits to silicon photonics, primarily to support modeling of the use of optics inside high performance computing (HPC). These circuits are key drivers of energy consumption in optical interconnects. Low energy interface circuits enable low power, high bandwidth optical interconnects that benefit HPC systems as well as embedded systems on military platforms such as avionics and satellites.

Compatible Particle Methods: A New Paradigm for Structure-Preserving Discretization without a Mesh

199981 | Year 1 of 3

Principal Investigator: P. B. Bochev

Executive Summary:

This project will develop new classes of compatible meshless methods, which will provide advanced simulation tools for mission-relevant applications in subsurface, multi-material and atmospheric flows, climate, and energy storage. The project will develop new agile software libraries to support the new methods and to enable their demonstration on exemplar problems motivated by mission applications.

Counter Adversarial Graph Analytics

190966 | Year 2 of 3

Principal Investigator: W. P. Kegelmeyer

Executive Summary:

Graph analysis algorithms are a key part many of national security missions. This project asks: What vulnerabilities lurk in those algorithms? We will discover, study, and quantifiably characterize those vulnerabilities under the assumption that they are being exploited by informed, empowered adversaries. We will also determine whether we can develop remediations for those vulnerabilities that are not, themselves, subject to subversion. Project success will benefit the cybersecurity and counterintelligence communities.

Diffusion Maps: A Unified Framework for Reasoning about Imperfect Data

199984 | Year 1 of 3

Principal Investigator: A. Kumar

Executive Summary:

This project will develop new fundamental techniques for algorithmically extracting structure from and reducing the dimensionality of large, time-dependent, noisy and incomplete datasets. The resulting computational understanding and representation of the structure present in data, as well as the minimal representation of its dynamics, will benefit national security needs for dynamical systems, big data analysis, and defense and space applications.

Fast and Robust Linear Solvers based on Hierarchical Matrices

199983 | Year 1 of 3

Principal Investigator: E. G. Boman

Executive Summary:

This project will explore new mathematical algorithms for large sparse linear systems based on hierarchical low-rank matrices. The goal is to develop new solvers/preconditioners that are both fast and robust for a wide range of problems from Sandia and DOE applications, including ice sheet modeling, circuit modeling, and structural mechanics. We are developing a parallel solver in collaboration with Stanford.

Graph Learning in Knowledge Bases

183780 | Year 3 of 3

Principal Investigator: A. Pinar

Executive Summary:

The amount of text data has been growing exponentially, calling for information extraction methods and ability to manage the uncertainty databases. We introduced pi-CASTLE, a system that optimizes and integrates human and machine computing for prediction problems involving conditional random fields. We used strategies grounded in information theory. Project success will benefit national security missions that rely on signals in big data to determine operational actions.

Heimdallr: Automated Binary Analysis via Symbolic Execution

190964 | Year 2 of 2

Principal Investigator: C. B. Harrison

Executive Summary:

Scalable automated analytics of binary programs is required to solve many national security issues, and developing analyses that can handle obfuscation and encryption is a necessary precondition. To that end, our project focuses on detecting cryptographic functions and making symbolic execution cryptographic-tolerant by decomposing constraints utilized by the encoding functions into independent constraints and then merging them after decoding bypassing encryption.

Identification of Markers of High Reynolds Averaged Navier Strokes Uncertainty for Model Improvement in Engineering Flows

180823 | Year 3 of 3

Principal Investigator: J. Ling

Executive Summary:

This work was conducted as part of a Harry S. Truman Fellowship LDRD project. The goal was to use machine learning methods to provide uncertainty quantification and model improvements for Reynolds Averaged Navier Stokes (RANS) turbulence models. This work demonstrated the potential of machine learning to fundamentally change how turbulent flows are modeled, of interest for applications in energy, safety, and security.

In Situ Compressed Sampling and Reconstruction of Exascale Unstructured Mesh Datasets

180818 | Year 3 of 3

Principal Investigator: M. Salloum

Executive Summary:

This project introduces compressed data computations for faster simulations and more efficient data storage and transfer toward extreme scale. It currently focused on reducing the size of data as it is generated during large scale simulations, and on developing compression algorithms based on tree wavelet to address point cloud data represented on irregular grids. It also explored time series data forecasting models in compressed space.

Modeling Human Comprehension of Data Visualizations

190967 | Year 2 of 2

Principal Investigator: L. E. Matzen

Executive Summary:

This project expanded the scientific understanding of human comprehension of data visualizations and developed new tools to evaluate the effectiveness of visualizations. These advances are critically important for improving human performance in the numerous national security mission areas that rely upon visualizations to support analysis and decision making. This work will improve human and system performance by improving information transfer and comprehension.

Multi-Level Memory Algorithmics for Large, Sparse Problems

199982 | Year 1 of 3

Principal Investigator: J. W. Berry

Executive Summary:

This project explores the problem of computing with multiple levels of memory. The work is motivated by current and future DOE supercomputers, all of which are projected to have this feature. We approach the problem through co-design, which includes: theoretical modeling, design and analysis of algorithms, reference implementations, systems software considerations, and simulation. Our approach builds upon classical external memory algorithmics to significantly impact multiple national security missions.

Optimal Control and Design of Qubits

190970 | Year 2 of 3

Principal Investigator: G. J. Von Winckel

Executive Summary:

This project will deliver novel quantum device characterization capabilities and computational tools for determining optimal voltage schedules to improve fidelity of devices in the presence of process nonidealities. Resolving trapped charge and strain contributions to the potential from capacitance measurements requires imposing numerous nonlinear partial differential equation constraints, however, this project provides efficient, scalable solutions for next-generation quantum computing.

PIMS: Memristor-Based Processing-in-Memory and Storage

180819 | Year 3 of 3

Principal Investigator: J. Cook

Executive Summary:

Contemporary computer central processing units implement the traditional von Neumann architecture, where memory and compute are separated by a bus, requiring performance and energy-degrading data movement to feed computation. This project aims to develop and evaluate a processor-in-memory architecture that implements a dense memory/storage technology for applications relevant to our mission to boost computational performance and energy efficiency.

Parallel Tensor Decompositions for Massive, Heterogeneous, Incomplete Data

199986 | Year 1 of 3

Principal Investigator: T. G. Kolda

Executive Summary:

Our goal is to develop a flexible hybrid parallel framework for tensor factorizations that lays the groundwork for meeting future mission requirements to process ever-larger and more complex data sets. A major goal of this project is to provide sure footing for current and emerging national security data analysis tasks.

Quantum Optimization and Approximation Algorithms

190963 | Year 2 of 3

Principal Investigator: O. D. Parekh

Executive Summary:

This project will develop some of the world's first quantum approximation algorithms (QAAs) and will provide higher-quality solutions to mission-critical optimization problems than possible with classical algorithms. Our QAAs will offer novel uses of scarce quantum resources to guide Sandia's world-class quantum hardware development efforts as well as identify new applications of future large-scale quantum computers. Success provides novel approaches to utilizing quantum resources in solving DOE mission relevant problems.

Stochastic Optimization to Enhance Resiliency and Response Strategies in Critical Infrastructure

199988 | Year 1 of 3

Principal Investigator: J. Watson

Executive Summary:

This project will develop advanced algorithms for representing uncertainty and nonlinearities in critical infrastructure operations and planning models. Addressing uncertainty and nonlinearity is crucial to critical infrastructure resilience, to address unknown impacts of extreme events, and to accurately reflect underlying physics (e.g., of power flow). Critical infrastructure resiliency is a pervasive national security issue, for DOE, DoD, and DHS.

Subsystem Reduced-Order Modeling and Network Uncertainty Quantification for Rapid, Agile, Extreme-Scale Simulation

190968 | Year 2 of 3

Principal Investigator: K. T. Carlberg

Executive Summary:

This project will develop a new methodology that enables rapid, scalable simulation, and uncertainty quantification (UQ) of decomposable systems. The approach: 1) models the system as a network of subsystems, 2) performs rapid uncertainty analysis via reduced-order modeling for each subsystem, and 3) couples subsystem uncertainties via network UQ. This will enable a broad-impact capability across mission-critical applications including gas-transfer systems.

Topological Design Optimization of Convolutes in Next-Generation Pulsed Power Devices

180821 | Year 3 of 3

Principal Investigator: E. C. Cyr

Executive Summary:

The goal of this project is to develop a topology optimization capability that could potentially improve the design of components critical to next-generation pulsed power devices. This ambitious goal could have a direct impact on Sandia's weapons qualification mission. Additionally, advanced optimization algorithms, formulations and software developed in pursuit of this goal, will have direct applicability to other Sandia mission spaces such as additive manufacturing.

Understanding the Hierarchy of Dense Subgraphs in Stationary and Temporally Varying Setting

194774 | Year 2 of 2

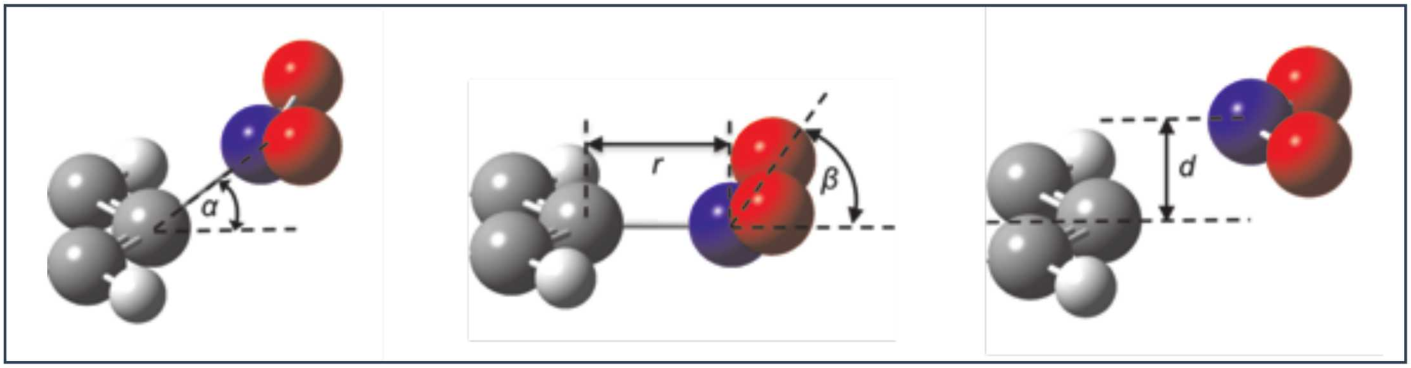
Principal Investigator: A. Pinar

Executive Summary:

This projects aims to develop scalable algorithms to identify dense structures on graphs and the hierarchy among them. These techniques are critical to identify functional units and anomalies in graphs. Our approach is based on using local structures and connectivity among them to compute a unique hierarchy of dense structures. We generalize peeling algorithms to higher-order structures for better solutions. Our results will impact nonproliferation and cyber traffic analysis.

Research Foundations

ENGINEERING SCIENCES



The figures above show molecular deformations NO_2 bend (left), NO_2 wag and C-NO_2 stretch (center), and NO_2 shear (right). [Project 180874, Understanding Hot Spot Initiation Using Electronic Ultrafast Sum Frequency Spectroscopy]

The Engineering Sciences Research Foundation (ESRF) drives understanding and innovation by integrating theory, computational simulation, and experimental discovery and validation to understand and predict the behavior of complex physical phenomena and systems. The ESRF Investment Area supports innovative, leading-edge R&D that: 1) advances the scientific understanding of physical phenomena underlying problems of interest to Sandia, 2) drives innovation and broad usage of state-of-the-art, validated computational modeling and simulation tools, and 3) accelerates the development of experimental diagnostics for discovery, model validation, and enhancement of our test and evaluation capabilities.

PROJECTS

PROJECTS (continued)

Big-Data Multi-Energy Iterative Volumetric Reconstruction Methods for As-Built Validation and Verification Applications

191069 | Year 2 of 3

Principal Investigator: E. S. Jimenez, Jr.

Executive Summary:

This project will develop new interrogation methods in x-ray imaging and new methods to reconstruct the data from the new interrogation method. Multi-energy iterative reconstruction (MEIR) will acquire polychromatic x-ray images using a new energy-resolved detector and iterative reconstruction algorithms. The higher fidelity x-ray data and improved reconstruction will improve detection in 3D reconstruction and will yield richer information for DOE, NNSA, and industrial computed tomography applications.

Design of Acoustic Metamaterials for Shock and Vibration Control in Weapon Systems

200171 | Year 1 of 3

Principal Investigator: T. Walsh

Executive Summary:

This project will develop optimization strategies and design new tailored impedance materials for vibration mitigation applications. The ability to filter and deflect mechanical energy waves, and ultimately shield structural components from harsh vibration environments, will prevent costly overdesign and result in better protection systems for mechanical vibration environments encountered in civil and defense applications.

Developing Strong, Concurrent, Multiphysics, Multiscale Coupling to Understand the Impact of Microstructural Mechanisms on the Structural Scale

180877 | Year 3 of 3

Principal Investigator: J. W. Foulk, III

Executive Summary:

This project developed key capabilities in microscale physics, concurrent multiscale coupling, and a flexible, open source development environment to connect the dominant microstructural mechanisms governing localization to loaded engineering structures. These computational elements of discovery will support multiple Sandia missions which seek to understand and predict the impact of material states on structural performance.

Discovering the Physics of Blast and Fluid Structure Interactions: A Novel Experimental-Computational Approach

200170 | Year 1 of 3

Principal Investigator: J. Wagner

Executive Summary:

The primary goal of the project is to develop new spatially and time-resolved diagnostics to measure blast-structure and fluid-structure interaction. This includes detailed measurements of the shock-induced flow surrounding the structure as well as internal and external structural response. Such capabilities will improve the ability to predict weapons behavior in harsh delivery environments.

Experiments to Elucidate Fundamental Breakup Mechanisms of Molten Components in Shock Driven Flows

180876 | Year 3 of 3

Principal Investigator: D. R. Guildenbecher

Executive Summary:

This project investigated the breakup of liquid metals subjected to strong gas flows. Experimental diagnostics were developed to quantify the size and velocity of secondary particles in 3D space. Comparison with simulations reveals new physical insights. The resulting diagnostics have proven versatile for a wide range of particle fields of relevance to Sandia's national security missions.

High Density Signal Interface Electromagnetic Radiation Prediction for Electromagnetic Compatibility Evaluation

191072 | Year 2 of 2

Principal Investigator: M. Halligan

Executive Summary:

The aim of this project was to develop an approach to address practical challenges in high-density interface, radiated power calculation with incomplete characterization information. The work will enable a predictive radiated emissions capability that can influence commercial and national security product designs early in the design process. This capability will enable designs to better meet radiated emissions requirements.

High Throughput Material Characterization via 6-Degrees of Freedom Loading and Material Parameter Feedback

191068 | Year 2 of 3

Principal Investigator: P. L. Reu

Executive Summary:

This project seeks to change how material models and material properties are determined. The approach includes optimized test specimen design, novel inverse techniques, and full-field measurements. Outcomes of the project will be software to optimize geometry, solve for properties using virtual fields, and an improved understanding of the mathematics of material models. The results will impact our materials science and modeling capabilities for stockpile stewardship and other national security applications.

Illumination of Damage with High-Strength Alloys in Abnormal Mechanical Environments

200174 | Year 1 of 3

Principal Investigator: M. Hudspeth

Executive Summary:

This project will illuminate fundamental failure behavior of both solid and distended media experimentally subjected to extreme states of dynamic loading. This work will provide enhanced understanding of these failure phenomena that will be incorporated into continuum and mesoscale modelling environments utilized in national security applications such as protective armor materials, explosives, and weapon system design.

Magnetic Sensing to Determine Material Flows within Opaque Vessels

180875 | Year 3 of 3

Principal Investigator: M. Nemer

Executive Summary:

The purpose of this project was to develop magnetic field diagnostics to enable insight into flow and temperature in opaque vessels. This concept involves seeding a flow with magnetic particles and observing the time-varying magnetic field outside the vessel using small, low-cost, highly sensitive, commercially available magnetometers. The magnetic field observations can subsequently be matched with numerical predictions through the application of efficient inversion techniques.

Multiscale Now! A Novel Hierarchical Approach for Multiscale Structural Reliability Predictions of Ultra-High Consequence Systems

180878 | Year 3 of 3

Principal Investigator: J. M. Emery

Executive Summary:

The goal of this project is a capability for tractable, multiscale probabilistic predictions of structural failure for high consequence systems. Our approach develops a hierarchical methodology that synthesizes multi-fidelity physics models, leverages stochastic model reduction, and is validated by experiments. This work will strengthen Sandia's science basis supporting ultra-high structural reliability predictions that impact our safety and security mission.

Novel Method to Characterize and Model the Multiaxial Constitutive and Damage Response of Energetic Materials

180883 | Year 3 of 3

Principal Investigator: M. J. Kaneshige

Executive Summary:

This study aims to create an innovative approach to measuring and predicting the mechanical response of energetic materials through the design of new testing methods and using digital image correlation. These new methods will be simpler than conventional techniques and reduce the cost associated with developing predictive models for use in simulations of response to normal and abnormal environments.

Physics of Discharge Initiation from Complex Surfaces

200172 | Year 1 of 3

Principal Investigator: C. H. Moore

Executive Summary:

This project will develop new fundamental mechanistic understanding of electron field emission from real surfaces with contaminant layers. This will be accomplished via comparison of newly developed modeling capabilities to experimental characterization of field emission from surfaces with controlled contaminants. Results will allow us to better understand breakdown initiation which is essential for modeling weapon components.

Pushing Continuum Reactive Capabilities through Novel Sub-Grid and Statistical Methods

200177 | Year 1 of 3

Principal Investigator: C. Yarrington

Executive Summary:

This project will develop statistical and nonlinear physics-based analysis tools that will result in physics-based subgrid models for predicting the observed collective response of dynamic reactive materials. These models will address a critical gap in predictive capability by including the effects of microstructure, and will allow for optimized designs for energetic materials and components important in NNSA missions.

Reduced Order Models of Structures Incorporating Complex Materials

191074 | Year 2 of 3

Principal Investigator: R. J. Kuether

Executive Summary:

This project will develop reduced order modeling strategies for predictive models with nonlinear and time-dependent materials to speed up numerical simulations. These models can be simulated with up to 10,000x reduction in computational cost and permit opportunities to perform uncertainty quantification and optimization analyses for improved characterization of component-level designs in mechanical structures such as weapon systems and aerospace vehicles.

Residual Stress Inversion using Ultrasonic Surface Waves, X-Ray Diffraction, and Sacrificial Material

200175 | Year 1 of 3

Principal Investigator: J. E. Bishop

Executive Summary:

Residual stress in as-manufactured structural components can significantly impact reliability. We are developing new experimental methodologies for estimating the full 3D residual-stress field of as-manufactured components with quantified uncertainty. Our primary experimental technique is semi-destructive relaxation with subsequent inverse modeling to obtain the residual stress field. These new techniques will improve predictive component simulations for current and future weapon systems.

Robust Approaches to Quantification of Margin and Uncertainty for Sparse Data

200173 | Year 1 of 1

Principal Investigator: L. Hund

Executive Summary:

This project developed new ways to quantify and communicate the large, irreducible risk associated with statistical model extrapolation in quantification of margins and uncertainties (QMU) analyses, demonstrating the opportunity for a paradigm shift to improve the way QMU analyses are conducted and utilized for risk-informed decision making in our nuclear weapons mission.

Turbulent Flow Uncertainty Quantification using Machine Learning Techniques

191076 | Year 2 of 3

Principal Investigator: M. F. Barone

Executive Summary:

This project will explore the use of machine learning techniques to develop improved models of near-wall turbulence. The research will specifically target the improved prediction of surface pressure loadings resulting from turbulent flow, which will enable simulation-based specification of design environments for weapon systems, renewable energy systems, and many other engineered systems.

Uncertainty Quantification of Microstructural Material Variability Effects

200176 | Year 1 of 3

Principal Investigator: R. E. Jones

Executive Summary:

This project is developing models of variability and performance to enable robust design and certification. Material variability originating from microstructure has significant effects on component behavior and creates uncertainty in performance. The outcome will be a specific uncertainty quantification (UQ) enabled analysis of material variability effects on performance and a method to evaluate the consequences of microstructural variability in general.

Understanding Hot Spot Initiation using Electronic Ultrafast Sum Frequency Spectroscopy

180874 | Year 3 of 3

Principal Investigator: J. J. Kay

Executive Summary:

Shock-induced reactions in high explosives were investigated using state-of-the-art experimental and theoretical techniques. Experiments yielded new data that indicate reaction on the timescale of tens of picoseconds. The calculations generated important insights on hypothesized reaction mechanisms. The results of this work constitute significant advances in our understanding of the fundamental reaction mechanisms that control explosive sensitivity and initiation of detonation.

Understanding Soot Development and Thermal Stratification in Combustion Engines through Hyperspectral Nonlinear Optical Diagnostics

191060 | Year 2 of 3

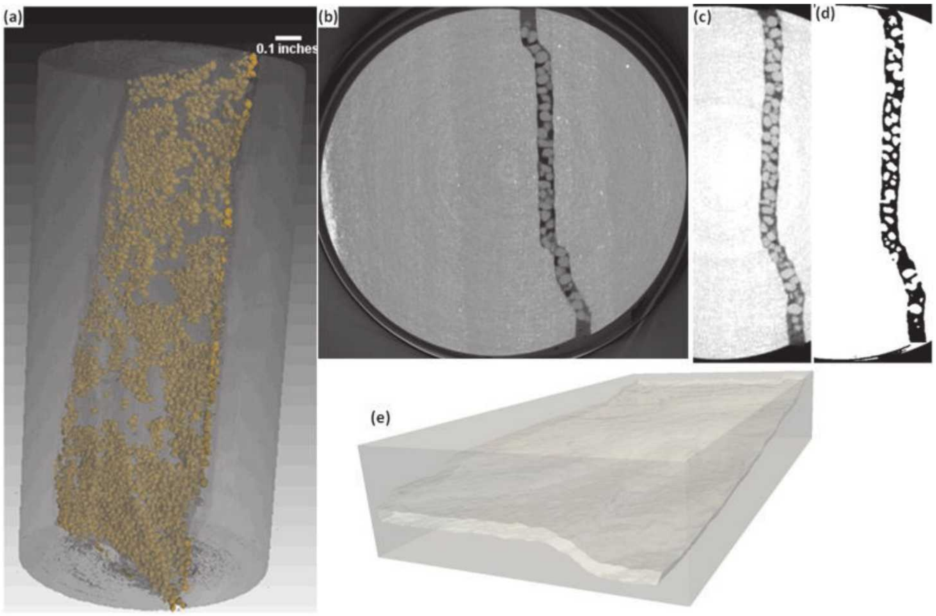
Principal Investigator: C. J. Kliewer

Executive Summary:

This project will develop new laser-based nonlinear optical probes for the study of next-generation combustion energy systems that operate at high pressures with higher efficiency. Previously unobservable processes such as transient thermal stratification and soot formation will be measured. The advanced experimental and theoretical tools developed will yield canonical datasets to serve as feedback to modern predictive combustion simulation tools.

GEOSCIENCE

The figures on the right show digital rock physics and modeling of fractured porous media: (a) 3D view of micro-CT image of a shale core sample filled with proppants (in gold) in a single fracture network (from Ingraham et al., 2015). (b-c) MicroCT image slices. (d) Segmented binary image. (e) A single fracture network digitally reconstructed with segmented binary images. [Project 191129, Digital Rock Physics for Multiscale Experiments and Modeling of Fractured Porous Media



The Geoscience Investment Area seeks to expand the frontiers of knowledge in the following areas: 1) the properties, structure, phenomena and processes associated with the earth's subsurface, surface, and atmosphere and 2) how engineered systems interact with the earth and the earth system. These earth systems and properties impact Sandia's national security missions, including energy security, defense, nonproliferation, disaster response, and climate security.

PROJECTS

Attribution of Methane Emissions in the Arctic and Continental US

200182 | Year 1 of 3

Principal Investigator: R. Bambha

Executive Summary:

This project will develop a novel data analysis approach for quantifying regional methane emissions and estimating the contributions from different methane source types. The project addresses a general problem relevant to national energy, nonproliferation, and defense needs using atmospheric measurements to estimate the emissions of a substance by a collection of sources and including heterogeneous measurements to improve emissions estimates.

Chemical-Mechanical Modeling of Subcritical-to-Critical Fracture in Geomaterials

191133 | Year 2 of 3

Principal Investigator: L. Criscenti

Executive Summary:

This project is developing a fundamental atomistic-level understanding of the chemical-mechanical processes that control subcritical cracks through coarse-graining data from reactive molecular simulations to produce characteristic continuum-scale metrics. This project fills a critical gap in understanding how chemical reaction and stress each contribute to fracture, leading to better control of the subsurface environment. It is important to DOE's Fossil Energy, Nuclear Energy, and Basic Energy Sciences.

Detection of Soluble Ligand-Tuned Molecular Tags for Subterranean Fluid Flow Monitoring using Resonance Raman Spectroscopy

191085 | Year 2 of 2

Principal Investigator: R. Kemp

Executive Summary:

We developed a soluble, ligand metal-based system capable of acting as easily modifiable taggants to track the fluid flows in underground reservoirs, in particular for hydraulically fractured wells. The metal complexes could be soluble in hydrocarbons or water. Molecular dynamics simulations complemented the synthetic work. Implementation of this technology into reservoirs can provide more efficient extraction of energy, and provide information to produce an underground mapping of the reservoir.

Developing Fugitive Emissions Sensor Networks: New Optimization Algorithms for Monitoring, Measurement and Verification

193231 | Year 2 of 3

Principal Investigator: K. A. Klise

Executive Summary:

This project will develop algorithms and software for sensor placement optimization to maximize monitoring effectiveness. While this work is focused on methane emissions, the research can be applied to a wide range of applications, including the placement of surveillance cameras, chemical, and fire detectors. This work aligns with DOE goals to increase the safety and resilience of natural gas infrastructure by improving the way sensors are deployed in the field.

Development of a Downhole Technique for Measuring Enthalpy in Geothermal Reservoirs

191092 | Year 2 of 2

Principal Investigator: A. T. Cashionm, IV

Executive Summary:

Enthalpy is a direct measure of the capacity of a fluid to do work and a critical evaluation criterion in understanding the value of a geothermal energy resource. Enthalpy is often impossible to measure in extreme downhole environments. This project devised a technique for measuring enthalpy in a high-temperature-high-pressure multiphase flowing fluid using a novel electrochemical sensing system. Results suggest it could be of value in subsurface geothermal reservoir analysis.

Digital Rock Physics for Multi-Scale Experiments and Modeling of Fractured Porous Media

191129 | Year 2 of 2

Principal Investigator: M. J. Martinez

Executive Summary:

This project investigated the application of 3D printing for geosciences. The idea was motivated by the recent confluence of high resolution imaging techniques for opaque materials coupled with mesoscale modeling using digital representations of these images. This technology enables the creation/design of reproducible custom/functional porous specimens to discover material response independent of pore structure variability for energy and security applications.

Geomechanics of Induced Seismicity in CO_2 Reservoirs

193418 | Year 2 of 2

Principal Investigator: M. J. Martinez

Executive Summary:

This project assesses the effects of fluid injection into porous sedimentary formations on the stability of nearby faults extending into crystalline basement using coupled (thermo-) poroelastic numerical simulations for single and multiphase fluid systems with boundary conditions applicable to the industrial scale injection of wastewater and anthropogenic CO_2. This research impacts energy security, specifically petroleum recovery and geologic carbon storage.

High Fidelity Hybrid Method for In Situ Borehole Stress Determination

191087 | Year 2 of 3

Principal Investigator: M. D. Ingraham

Executive Summary:

This project aims to improve the accuracy of in situ hydraulic fracture measurements of stress through inclusion of thermo- and chemo-mechanical coupling. Currently, uncertainty is on the order of 50%–we seek to reduce this to 40% or less. In situ stress affects all subsurface activities for energy security, including fossil and geothermal energy, nuclear waste disposal, and geologic storage.

Integrated Geomechanics and Geophysics in Induced Seismicity: Mechanisms and Monitoring

200180 | Year 1 of 3

Principal Investigator: H. Yoon

Executive Summary:

This project will develop new fundamental mechanistic understanding of geomechanical and geophysical processes of fracturing that lead to induced seismicity in fractured systems. This research will lead to the new groundwork for remote characterization of rock failure by identifying the precursors to the induced seismicity in fractured systems, which will significantly impact subsurface resource extraction, waste storage, and energy storage.

Monitoring and Repair of Damaged Cement-Geomaterial Interfaces in High Pressure High Temperature Repository and Borehole Scenarios

200181 | Year 1 of 3

Principal Investigator: E. N. Matteo

Executive Summary:

This project will develop fundamental understanding of chemical and mechanical degradation at cement-geomaterial interfaces via a study that includes novel code development to model coupled reactive transport and solid mechanics codes and state-of-the-art experimental characterization. Understanding from the project is critical to ensure seal integrity (wellbores, nuclear waste repository seals) during subsurface operations that are central to securing our nation's energy future.

Prediction and Inference of Multi-Scale Electrical Properties of Geomaterials

200183 | Year 1 of 3

Principal Investigator: C. J. Weiss

Executive Summary:

This project will develop a computational capability for predictive forward modeling and optimization of electromagnetic geophysical data in situations where fine scale structure—either engineered or naturally occurring—has a profound effect on the data, but is computationally explosive to model with traditional numerical methods. Application spaces include border security, nonproliferation, and energy research. New breakthroughs therein provide a computational ability unmatched elsewhere in the DOE complex.

Real Time Degassing of Rock during Deformation

191137 | Year 2 of 2

Principal Investigator: S. J. Bauer

Executive Summary:

The project developed an experimental system combining triaxial rock deformation and mass spectrometry to measure noble gas flow before, during, and after rock fracture. Geogenic noble gas is released during triaxial deformation (real-time) and related to volume strain and acoustic emissions. The noble gas release thus represents a signal of deformation during its stages of development. This unique capability lays the framework for new tools to monitor subsurface stress/deformation changes.

Self-Tuning Seismic Sensor Data Processing

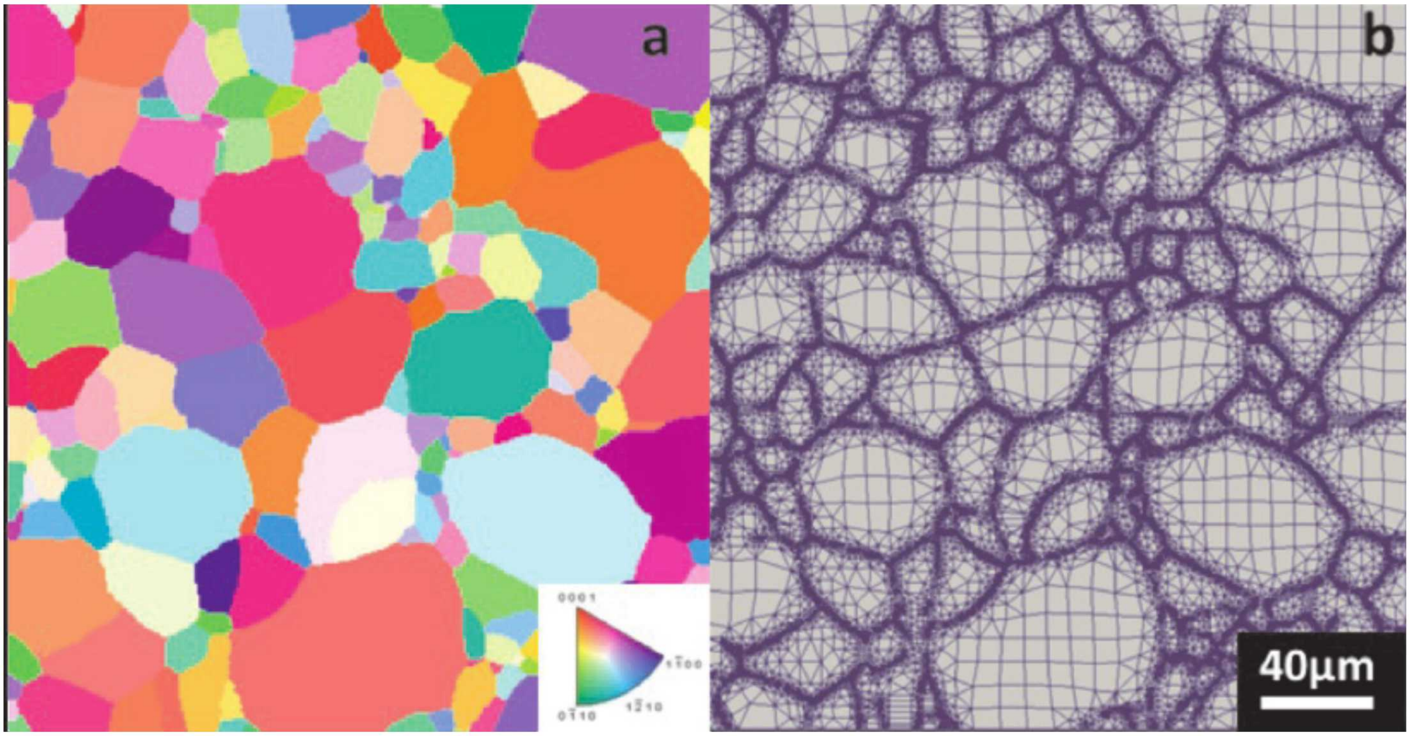
180882 | Year 3 of 3

Principal Investigator: T. J. Draelos

Executive Summary:

This project developed a new adaptive tuning algorithm to adjust the detection thresholds for a network of seismic signal detectors, allowing higher quality (fewer false and fewer missed) signal detections. Adaptive Self-Tuning is applicable to any sensor network that has sensors with overlapping coverage of the environment and a tunable detection parameter. Success may lead to an improved operational seismic monitoring capability useful for nonproliferation assessments and warning.

MATERIALS SCIENCE



The figures above show microstructural modeling of brittle materials: a) Inverse pole figure of alumina used for mesh generation b) mesh generated using OOF2 from microstructure. [Project 195883, Microstructural Modeling of Brittle Materials for Enhanced Performance and Reliability]

R&D sponsored by the Materials Science Investment Area strives to discover new phenomena, to create new classes of materials with novel synthesis techniques and processing approaches, and to understand and control materials' structures and properties. The goal is to foster a bold, vibrant, ground-breaking, materials science base of world-renown, which serves as the foundation for developing the critical and differentiating technical capabilities that will be needed in the future to support our national security missions.

PROJECTS

PROJECTS (continued)

Additive Manufacturing: Predicting the Performance and Reliability of Laser Engineered Materials

180901 | Year 3 of 3

Principal Investigator: J. D. Sugar

Executive Summary:

This project developed multiphysics modeling tools for simulating the Laser Engineered Net Shaping (LENS) process. Thermal models were validated with in situ thermal measurements. Microstructure and mechanical property measurements validated predictions of residual stress and plastic thermal strains. Understanding the processing, microstructure, and property relationships of additively manufactured materials is critical for design of components to be used in long-life, high-consequence environments.

Compliant Nanoepitaxy: The Next Materials Revolution

180899 | Year 3 of 3

Principal Investigator: S. R. Lee

Executive Summary:

The project seeks to develop higher performing indium gallium nitride (InGaN) alloys for solid state lighting (SSL) applications. We will use a novel, nanopattern-based approach to raise the indium composition, lower the defect density, and improve the surface morphology of these semiconductor materials. Scientific understanding of how to make such alloys will significantly improve the energy efficiency of SSL, thereby enhancing the nation's energy security.

Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials

191194 | Year 2 of 3

Principal Investigator: H. Fan

Executive Summary:

This project will develop fundamental understanding of self-assembly of energetic materials and effective control of their morphology. This research proposes to eliminate inconsistent performance of energetic materials by providing a trusted and reproducible method to improve energetic materials for nuclear weapon applications, which will enable significant improvements in design confidence, surveillance approaches, and predictive models of energetic materials reliability.

Electrochemical Model of Humidity-Driven Corrosion

191187 | Year 2 of 3

Principal Investigator: E. J. Schindelholz

Executive Summary:

This work defines the physicochemical characteristics of electrolytes on atmospherically exposed surfaces and their impact on atmospheric corrosion processes. Our approach combines microelectrochemical experiments with modeling to develop linkage between corrosion kinetics and electrolyte properties. The results provide mechanistic insight into a little-understood but primary materials degradation mode in many DOE systems, including the stockpile and spent nuclear fuel canisters.

Enabling Hydrogen Infrastructure through Surface Passivation of Structural Materials

200197 | Year 1 of 3

Principal Investigator: R. Kolasinski

Executive Summary:

This project will develop the science basis for surface passivation as a remediation for hydrogen-assisted fatigue crack growth in pipeline steels. Over-designing pipelines to protect against hydrogen embrittlement presents a significant barrier to the adoption of fuel cell electric vehicles. Our research explores a low cost solution, impacting our nation's ability to field low-carbon, renewable energy sources for transportation.

Engineered Reliability via Intrinsic Thermomechanical Stability of Nanocrystalline Alloys

180900 | Year 3 of 3

Principal Investigator: N. Argibay

Executive Summary:

This project will develop and demonstrate thermally and mechanically optimized nanocrystalline alloys, providing a pathway toward materials with an unprecedented combination of strength, ductility, thermal stability, and manufacturability, while precluding the need for engineering overdesign to account for property degradation under harsh environments. This project represents a breakthrough in metallurgical design, impacting a broad range of aerospace (satellites) and energy systems.

Engineering Next-Generation Zero Thermal Expansion Composite Materials for Additive Manufacturing Technologies

200199 | Year 1 of 3

Principal Investigator: N. C. Burtch

Executive Summary:

This project will develop new fundamental understandings into the promise of negative thermal expansion (NTE) materials that can robustly compensate for positive thermal expansion in additive manufacturing technologies. Positive thermal expansion can lead to high-consequence mechanical failure modes in materials. New NTE material innovations would mitigate such problems and bring significant value to Sandia's materials science and engineering capabilities.

Fluxional Monomers for Enhanced Thermoset Materials

193378 | Year 2 of 2

Principal Investigator: B. H. Jones

Executive Summary:

This project explored the incorporation of organometallic functionalities onto the backbone of polymer thermosets and the consequent impact of organometallic fluxional behavior on stress-related phenomena in such materials. Based on a model epoxy-ferrocene system, we report that fluxional behavior can be exploited to reduce stresses in thermoset materials, which are ubiquitous as encapsulants and adhesives in nuclear weapon components.

High Power Solid State Li-ion Batteries through Interface Engineering

191191 | Year 2 of 3

Principal Investigator: F. El Gabaly Marquez

Executive Summary:

Engineering interfaces can critically improve performance of very small, all solid-state Li-ion batteries that can be integrated with other microelectronics. We focus this project in tailoring the interfacial structure and composition to achieve lower interfacial resistance and high power. Improved solid state rechargeable micro-batteries will impact our nation's ability to field maintenance-free sensors, antennas, and other stealth, but power-hungry microelectronics.

Inkjet Printing Metal Organic Frameworks for Next-Generation Electronics and Optoelectronics

204725 | Year 1 of 2

Principal Investigator: A. L. Benin

Executive Summary:

This project will develop fundamental understanding and methodologies pertaining to the inkjet printing capability of metal organic framework materials onto low-cost substrates. This would support several national security missions including: additive manufacturing and creation of "smart" devices, development of improved nuclear weapon weak-link capacitors, advancements in flexible electronic and photonic devices, and improved energy storage and conversion in thermoelectric devices.

Interfacial Effects on the Microstructure and Morphology of Energetic Materials

191188 | Year 2 of 3

Principal Investigator: E. C. Forrest

Executive Summary:

The microstructure and morphology of energetic materials strongly influences detonation characteristics. We seek to engineer and leverage interfacial characteristics at atomic-to-microscopic length scales to study effects of surface energy and microtopography on properties of explosive films created with physical vapor deposition. Control of explosive performance at length scales of interest represents a paradigm shift in explosive science for national security applications.

Investigating Phase Evolution in Chemical Wavefronts Subject to High Heating Rates (~1e6 K/s)

200204 | Year 1 of 3

Principal Investigator: D. P. Adams

Executive Summary:

This project explores the atomistic mechanisms that underlie propagating wavefront stability in reactive solids. The team is combining dynamic transmission electron microscopy, predictive thermal modeling, molecular dynamics simulations, and advanced material design to research key unknowns of reactive solids that are vital to designing new improved, reliable forms needed for joining, microsystems, and energy applications.

Magnetic Nanocomposites for High Performance Inductor Materials

200203 | Year 1 of 3

Principal Investigator: D. L. Huber

Executive Summary:

This project will develop magnetic nanocomposites for high performance inductor materials. The magnetic nanocomposites will be optimized for specific applications by tuning the particle size and spacing. These new inductors have applications in power electronic circuits for military and civilian applications where size, weight, and power density are of critical importance.

Magneto-Inks: Increasing Materials Reliability in Engineered Devices

205750 | Year 1 of 1

Principal Investigator: L. J. Treadwell

Executive Summary:

This project will develop magnetically robust nanocomposite inks that have the potential to exhibit autonomic restoration to increase the reliability of printed electronics and sensor components.
The formulation of the nanocomposites includes the syntheses of uniform magnetic nanoparticles, followed by equally dispersing them into a polymer so they can be printed to ultimately demonstrate autonomously restoration of mechanical and electrical contacts on printed devices, such as flexible and conformal photovoltaics.

Making Density Functional Theory Work for all Materials

200202 | Year 1 of 3

Principal Investigator: A. Cangi

Executive Summary:

This project develops predictive density functional theory approximations for all materials, including heavier elements such as rare earths, lanthanides, actinides, and transition metal oxides. This work will improve advanced calculations and allow the extension of model-based design and engineering to the unique properties of d- and f-electron materials crucially important to the NNSA national security mission. Potential applications include electronics, computer/communication systems, transportation, health care, and national defense.

Mechanistic Origins of Stochastic Rupture in Metals

200201 | Year 1 of 3

Principal Investigator: B. Boyce

Executive Summary:

The project explores the microstructural conditions that give rise to void nucleation during quasi-static ductile rupture of metals. After inducing progressive damage states through mechanical testing, pedagogical metallic materials are dissected to characterize the local microstructure and defect state. Complementary atomistic and dislocation dynamics models help to explore the critical conditions that give rise to emergent void nucleation. Ductile failure assessment and prevention is relevant to the nuclear weapons mission.

Microstructural Modeling of Brittle Materials for Enhanced Performance and Reliability

195883 | Year 2 of 2

Principal Investigator: M. C. Teague

Executive Summary:

This project will create an experimentally validated microstructure modeling capability to enable failure predictions for brittle materials. A unique combination of finite element modeling and microstructure-scale stress mapping will be used to create the microstructure modeling capability. This effort will contribute to the tools necessary to provide assurance that a brittle component in an application is functional over its intended lifetime, important to the nuclear security mission.

Molecule@MOF: A New Class of Metal Organic Framework Optoelectronic Materials

180898 | Year 3 of 3

Principal Investigator: A. A. Talin

Executive Summary:

We developed electronically conducting metal organic frameworks and evaluated their potential for thermoelectric energy conversion. We explored redox active 'guest' molecules in the pores (guest@MOF), and metal organic graphene analogs (MOGs) with strong electronic overlap between metal ions and its linker groups. Inkjet deposition methods were developed for integration of the guest@MOF and MOG materials into practical thermoelectric energy conversion devices.

Predicting the Friction Behavior of Body-Centered Cubic Metal and Alloys

200200 | Year 1 of 3

Principal Investigator: M. E. Chandross

Executive Summary:

This project aims to develop a model of microstructural evolution in body-centered cubic metals under applied cyclic stress. A quantitative model connecting atomistic processes to macroscale mechanical behavior (friction) would be a paradigm shift in design of mechanical contacts found in nuclear weapons (e.g., stronglinks, accelerometers), power (e.g., electric vehicles, wind turbines) and aerospace, enabling a systematic methodology that greatly improves reliability.

Quantum Nanofabrication: Mechanisms and Fundamental Limits

191196 | Year 2 of 3

Principal Investigator: G. T. Wang

Executive Summary:

This project seeks to provide a detailed understanding of the mechanisms and ultimate limitations of quantum-size controlled photoelectrochemical etching and to explore applicability over a wider range of semiconductor materials. This will enable a capability for the controlled fabrication of epitaxial semiconductor quantum dots, with relevance to numerous mission areas including: high efficiency lasers, single and entangled photon sources and detectors, and radiation-hard devices for space and nuclear weapons applications.

Sequential Design of Experiments for Accelerated Life Testing

195881 | Year 2 of 3

Principal Investigator: C. King

Executive Summary:

This project will develop methodology for optimal accelerated test plans under a limited number of samples. This methodology will allow test planners to best use their limited time and resources to understand product performance so that they can ensure our weapons and other products perform as intended out in the field.

Studying Crystallization Mechanisms to Control Film Growth and Functional Performance

200198 | Year 1 of 1

Principal Investigator: M. P. Siegal

Executive Summary:

This project will determine if surface-specific ultraviolet pulsed-laser-annealing (UV-PLA) can be developed to produce high-quality functional crystalline films with only negligible substrate heating using p-type $(Bi_{0.2}Sb_{0.8})_2Te_3$ thermoelectric films. If ex situ UV-PLA can achieve state-of-the-art properties, then new device architectures can be discovered and implemented. Improving the understanding of thermoelectric materials crystallization with potential impact toward enabling improved additive manufacturing functional materials concepts is important to NNSA's mission.

Topological Quantum Material for Quantum Computation

203429 | Year 1 of 3

Principal Investigator: W. Pan

Executive Summary:

Topological quantum materials (TQMs) are a rapidly emerging field in materials research, with a potential to profoundly impact the nation's information and energy technology applications. Here, we seek to understand the following quantum properties of TQMs that can propel the electronics industry into a whole new topological quantum electronics area: topologically created Majorana fermions, topological superconductivity, and topologically modified photoconductivity.

Understanding Transport and Aging Mechanisms to Optimize Sandia's Ion-Conducting Electrolytes for Energy Applications

191186 | Year 2 of 3

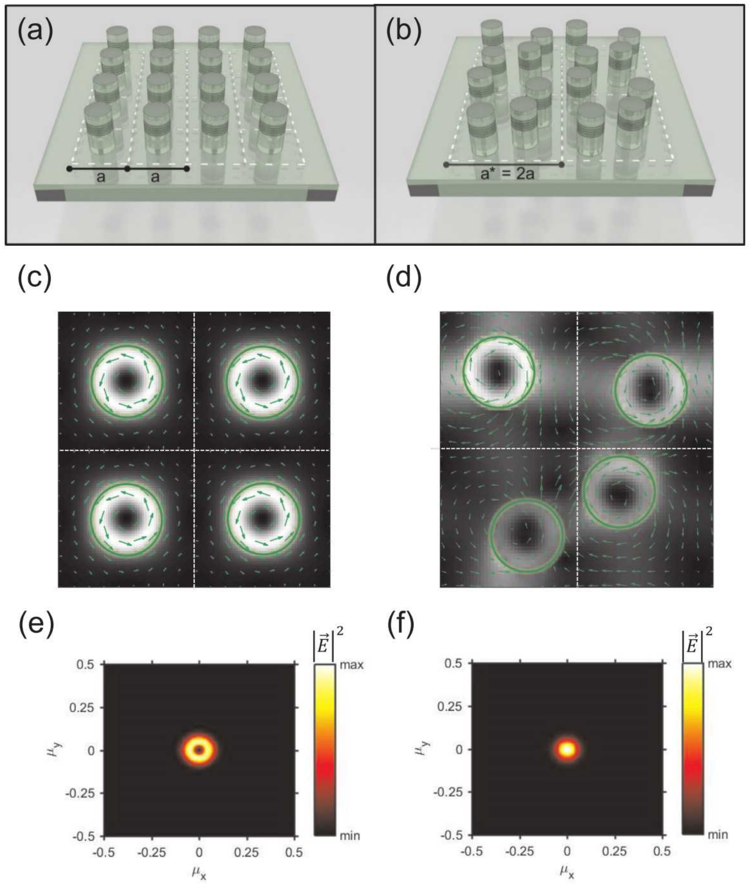
Principal Investigator: A. Frischknecht

Executive Summary:

In this project, we are developing an understanding of the relationships between polymer chemistry, nanoscale to microscale morphology, and macroscale properties, in particular proton conductivity, in a proton-conducting polymer developed at Sandia. This understanding will lead to better design of polymer membranes for use in fuel cells and flow batteries to improve energy storage devices.

NANODEVICES AND MICROSYSTEMS

The figures on the right show visible quantum nanophotonic arrays and plots: a) Schematic of periodic nanowire array. b) quasi-aperiodic array. c) and d) corresponding simulated in -plane electric field plots. e) and f) simulated far-field transmission. [Project 186113, Visible Quantum Nanophotonics]



The Nanodevices and Microsystems Research Foundation supports Sandia's mission by performing creative, leading-edge, and high-impact R&D. This R&D strives to discover new phenomena at the nanoscale and microscale; and create or prove new concepts, devices, components, subsystems, and systems. Its objective is to foster a bold, vibrant, ground-breaking, science and technology base of world-renown to develop the critical and differentiating technical capabilities that are needed in the future to support our national security missions. The Nanodevices and Microsystems Investment Area seeks to: 1) increase our understanding of physical phenomena across the nanoscale to microscale, 2) develop innovative nanoscale and microscale devices, 3) achieve new methods of integration, and 4) realize novel microsystems-based complex systems.

PROJECTS

PROJECTS (continued)

A Compact, Spectrally Tunable Source of Entangled Photon Pairs for Quantum Sensing

192786 | Year 2 of 3

Principal Investigator: I. Brener

Executive Summary:

We propose a new source for generation of entangled photon pairs in the near infrared (~1.5 μm) based on semiconductor heterostructures (III-nitrides) coupled to metamaterials. This combination can create giant, gated, and tunable optical nonlinearities, thereby enabling control of the entangled photons wavelength and the ability to switch photon generation on/off using a bias voltage. Success can lead to significant gains in sensing of trace chemicals and chem/bio weapon threats.

A New Paradigm in Chem/Bio Threat Detection: Evaluating Threats based on Biological Function Rather than Chemical Form

191203 | Year 2 of 3

Principal Investigator: W. F. Paxton

Executive Summary:

This project will develop robust sensors that detect chemical and biological threats, including those that are not yet known, based on their biological function rather than their chemical form. The operating principle is to mimic biological membranes with robust polymer amphiphiles on nanowire field-effect transistors (FETs), and correlate changes in conductivity to exposure to chemical and biological threats.

A Platform for Quantum Information and Large Scale Entanglement with Rydberg Atoms in Programmable Optical Potentials

191211 | Year 2 of 3

Principal Investigator: M. J. Martin

Executive Summary:

This project aims to discover methods for creating large scale quantum entanglement within arrays of neutral atoms coupled to strongly interacting Rydberg states. We will manipulate arrays of atoms using holographically generated traps. This level of control represents a major technological and scientific advance for quantum technologies, with potential for enabling advanced sensors and other quantum capabilities.

A Truly Micro-Scale Low Cost, Size, Weight, and Power Gyroscope based on Optomechanical Oscillation

200231 | Year 1 of 3

Principal Investigator: A. J. Grine

Executive Summary:

We are building a rotation sensor that, through design and scaling breaks, trends in current technologies. Namely, we aim to show that by scaling down to microscale dimensions (goal: 10μm< active radius<100μm), we can simultaneously improve sensitivity while reducing Cost, Size, Weight and Power (CSWaP). The sensor is promising in applications requiring agile navigation, guidance, and control.

Active and Nonreciprocal Radio Frequency Acoustic Microsystems

200229 | Year 1 of 3

Principal Investigator: M. Eichenfield

Executive Summary:

This project will develop novel radio frequency (RF) amplifiers using the acoustoelectric interaction between piezoelectric thin films and semiconductors. Success will allow orders of magnitude reduction in size, weight, and power of RF signal processing units by having active and passive components on one chip. This allows dramatic size, weight, and power reduction for RF devices impacting a broad range of national security and other RF applications.

Atom Traps on a Microfabricated Optical Waveguide Platform for Quantum-Limited Spin-Squeezed Magnetometry and Quantum Information Applications

180919 | Year 3 of 3

Principal Investigator: Y. Jau

Executive Summary:

This project established new technology and new knowledge base that will help the future development of "atom chip," a new cold-atom platform that does not require free-space laser beams for quantum control applications. Developing quantum sensing and quantum information using atom chips will significantly impact our nation's ability to advance navigation precision, remote diagnostics, and security of data transmission.

Beyond Graphene: Boron Nitride-Based Semiconductor Alloys for Next-Generation Optoelectronics

180920 | Year 3 of 3

Principal Investigator: A. A. Allerman

Executive Summary:

This project developed and demonstrated the first ultraviolet (UV) emitters and wavelength-tunable photodetectors employing the B-rich hB(Al,Ga)N alloy system. Solid state emitters and photodetectors operating in the UV spectrum are critical elements to realizing high performance, compact and efficient systems for fluorescence-based biodetection and chemical sensing. Additionally, UV emitters provide a highly flexible optical source for systems targeted for water purification, chemical remediation, and germicidal disinfection of surfaces and air.

Developing a Solid State Technology for Electron Spin Qubits on Liquid Helium

191210 | Year 2 of 3

Principal Investigator: E. A. Shaner

Executive Summary:

The project is exploring electron spin qubits and the foundations of a silicon integrated circuit-based advanced computing technology by integrating electrons on helium with complementary metal-oxide-semiconductor structures and demonstrating spin-to-charge conversion for single spin readout. If this approach is successful, it may be an important building block in eventual advanced quantum information sciences, a key element critical to the US government's national security missions.

Digital Electronics at the Atomic Limit (DEAL)

200232 | Year 1 of 3

Principal Investigator: S. Misra

Executive Summary:

The digital electronics at the atomic limit (DEAL) project seeks to leverage Sandia's atomic-precision fabrication capability to realize the theorized orders-of-magnitude improvement in operating voltage for tunnel field effect transistors (TFETs) compared to complementary metal–oxide–semiconductor (CMOS) transistors. Not only are low-power digital circuits a critical element of many national security systems (e.g., satellites), TFETs can perform circuit functions inaccessible to conventional CMOS electronics (e.g., polymorphism).

Electrochemical Detection of Single Molecules in Nanogap Electrode Fluidic Devices

180907 | Year 3 of 3

Principal Investigator: R. Polsky

Executive Summary:

The project's goal was development of a nanogap fluidic electrode device capable of electrical and optical measurements to measure a single molecule. Orthogonal validation techniques–Total Internal Reflection Fluorescence Microscopy and molecular simulation–were used to clarify the mechanism leading to current build-up due to redox cycling, diffusion, and adsorption of single molecules undergoing redox reactions. Potential national security applications include detection of biological enzymes and battery system components.

Ferroelectric Tunnel Junctions: A Physics-Based Solution to Reliable Resistive Memory

191197 | Year 2 of 2

Principal Investigator: M. D. Henry

Executive Summary:

This work enables scalable resistive memory in a complementary metal–oxide–semiconductor fab-compatible, polycrystalline ferroelectric, halfnium-zirconium oxide. Our solution is the development of ferroelectric-tunnel junctions where the polarization state sets the resistive state of the element and resistance is determined by the quantum-tunneling through the film. This project demonstrated a heretofore-unrealized method to overcome memristor barriers. Potential applications include computing elements for advanced computing, and critical components for counterterrorism and security technologies.

Highly Efficient Solar-Blind Single Photon Detectors

191199 | Year 2 of 3

Principal Investigator: A. Armstrong

Executive Summary:

We propose to demonstrate the first AlGaN-based quantum dot floating gate high electron mobility transistors (HEMTs) for solar-blind detection with >40% single photon detection efficiency. Low voltage and 297 K operation of AlGaN FG-HEMT photodetectors simplifies systems integration compared to high voltage and cryogenic commercial options. A variety of national security applications require high sensitivity ultraviolet photo detection in the solar-blind spectrum, including non-line-of-sight communication and fluorescence-based bioagent sensing.

Magnetic Josephson Junction Memory and 3D Integration for Scalable, High Performance, Low Power Computing

180906 | Year 3 of 3

Principal Investigator: N. A. Missert

Executive Summary:

This project developed a next-generation technology path for superconducting electronics by demonstrating ambient temperature, wafer-scale, and tunable Josephson junctions based on nitrides. The thermal stability of nitrides, relative to the Al-AlOx barriers employed in current state-of-the-art technology, offers the potential for both large-scale integration and 3D scaling in order to realize the goal of ultra-low power, high-performance computing for national security.

MilliKelvin High Electron-Mobility Transistor Amplifiers for Low Noise, High Bandwidth Measurement of Quantum Devices

200233 | Year 1 of 2

Principal Investigator: L. A. Tracy

Executive Summary:

This project will develop ultra-low power cryogenic amplifiers for improving measurement of quantum devices. The low power consumption (a few microWatts) will allow the amplifier to be located near the device, at the coldest cryostat stage, typically less than 100 milliKelvin. Developing the technology for fast, accurate measurement of quantum devices is of importance for quantum computing applications.

Nanoengineering of Detector Surfaces to offer Unprecedented Imager Sensitivity to Soft X-Rays and Low Energy Electrons

203202 | Year 1 of 3

Principal Investigator: M. O. Sanchez

Executive Summary:

In a collaborative effort with NASA's Jet Propulsion Laboratory (JPL), this project will explore how to maximize the sensitivity of a silicon detector surface to shallowly absorbed radiation by using electric field shaping techniques and surface passivation with JPL's Delta Doping process. This will provide insight on how to create silicon detectors that respond to low energy radiation with high efficiency.

Near Infrared Nanophotonics through Dynamic Control of Carrier Density in Conducting Ceramics

200228 | Year 1 of 3

Principal Investigator: D. K. Serkland

Executive Summary:

The goal of this project is to realize a new class of high-speed nanophotonics through active control of carrier densities in unconventional plasmonic materials. If successful, we will develop nanophotonics devices with size, weight, and power performance far superior to existing III-V/silicon photonics, enabling a new generation of optical communications technologies relevant to high performance computing platforms that will impact multiple national security applications.

Optimization of Sputtered Aluminum Nitride for the Seeding of Metal Organic Chemical Vapor Deposition Gallium Nitride Films

191204 | Year 2 of 3

Principal Investigator: K. Knisely

Executive Summary:

This project will develop GaN on Si capabilities at Sandia's MesaFab facility. GaN on Si combines the electrical benefits of GaN, a wide bandgap material, with the cost and scaling advantages of Si wafer processing. GaN on Si technology can be leveraged by a number of projects working in DOE mission areas, including power and radio frequency electronics, photonics, and LEDs/emitters.

Rad Hard Devices Science using Quasi-Electric Fields

200226 | Year 1 of 3

Principal Investigator: G. A. Vawter

Executive Summary:

This project explores new semiconductor devices for harsh radiation environments by creating "rad-hard by band-structure" design concepts for transistors and diodes. The core concept is to use graded bandgap engineering to establish quasi-electric fields in compound semiconductors, which act differently on majority and minority carriers, to push excess populations of minority carriers in the same direction as majority carriers so that no undesired current flows in these graded layers.

Scandium Aluminum Nitride for Advanced Piezoelectric Sensors, Actuators, and Filters

191198 | Year 2 of 3

Principal Investigator: B. Griffin

Executive Summary:

This project will investigate alloying of aluminum nitride piezoelectric films to enhance the piezoelectric properties of the film. Improvement in piezoelectric material properties will impact our nation's ability to field advanced radio frequency systems, ultrasonic imagers, sensors for extreme environments, and near zero power wakeup devices.

Understanding the Physics of Silicon-Germanium Heterojunction Bipolar Transistors for Cutting-Edge Electronics at Deep Cryogenic Temperatures

193422 | Year 2 of 3

Principal Investigator: T. D. England

Executive Summary:

The purpose of this project is to discover new device physics and to create cutting-edge analog and radio frequency circuits with silicon germanium heterojunction bipolar transistors operating at 4 Kelvin. The circuits will have the potential to quickly impact applications and place Sandia at the forefront of 4 Kelvin electronics. Project success relates to DOE Strategic Objective 5 by the creation of cutting-edge technology.

Vertically Injected Ultraviolet Laser Diodes

188288 | Year 3 of 4

Principal Investigator: M. H. Crawford

Executive Summary:

This project seeks to overcome major materials roadblocks to extending laser diodes into the deep-ultraviolet region. Roadblocks include the lack of low-defect, electrically-conductive semiconductor substrates and lack of understanding of contributing factors to optical loss. Ultraviolet laser diodes would provide compact, robust solutions for applications including fluorescence-based bioagent sensing, atomic clocks, and technologies in the solar-blind region (< 280 nm). These technologies support a secure and resilient US energy infrastructure.

Visible Quantum Nanophotonics

186113 | Year 3 of 3

Principal Investigator: G. S. Subramania

Executive Summary:

The goal of this project is to develop a quantum nanophotonics capability that will allow practical control over electron (hole) and photon confinement in more than one dimension. Electron (hole) confinement will be achieved using photo-electrochemically etched InGaN quantum dots while photonic crystal structures are fabricated using nanopatterning to provide control over photons. This work provides capability for future photonic quantum information science, important for future light sources and displays.

What is Happening in Narrow Bandgap Devices? Radiation-Induced Defects and Recombination

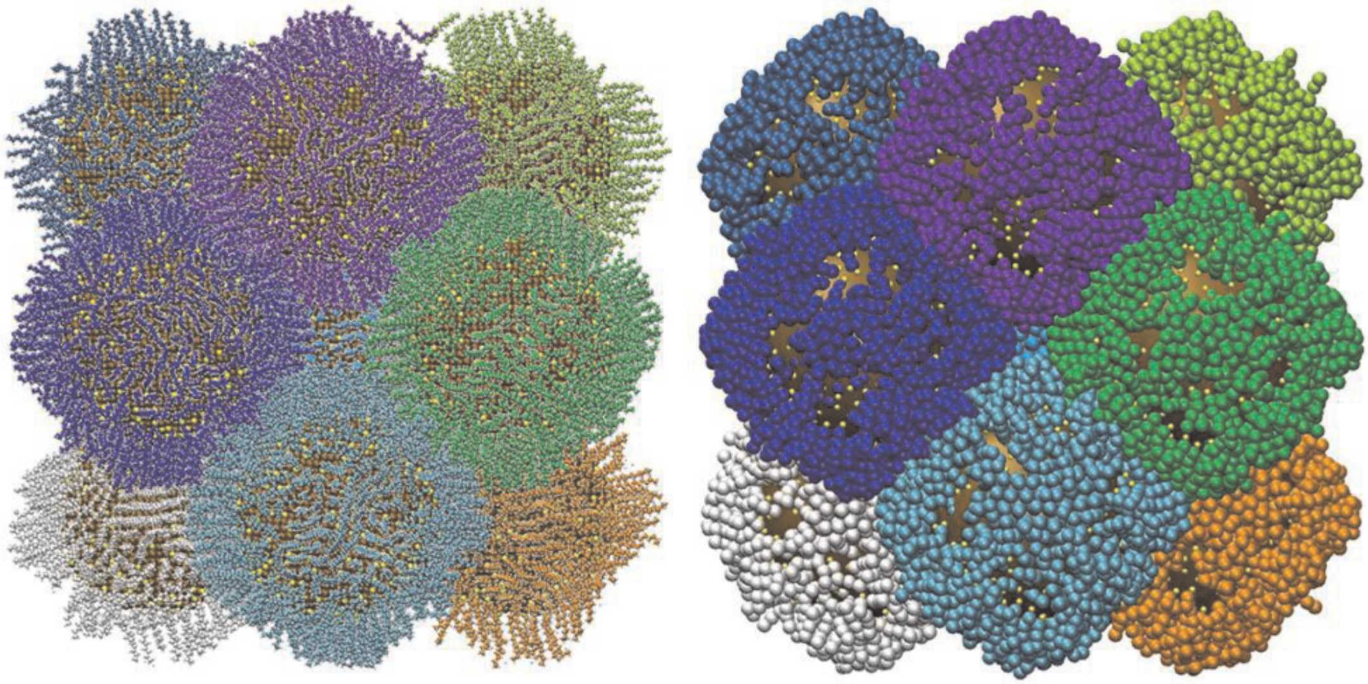
200230 | Year 1 of 2

Principal Investigator: P. A. Schultz

Executive Summary:

The goal of this project is to develop a fundamental understanding of radiation sensitivities in InAs/InAsSb-based superlattice devices. This project will develop new experimental techniques and modeling methods to probe and characterize radiation-induced defects in narrow bandgap systems such as InAs(Sb), capabilities that will impact the ability of the nation to qualify and deploy new technologies in space applications (e.g., focal plane arrays).

NEW IDEAS



The figures above show two face-centered cubic arrays of 6 nm diameter alkanethiold gold nanoparticles with ligands of length 12 carbons for fully atomistic (left) and coarse-grained model with λ=2 (right). [Project 180922, Controlling Nanoparticle Assembly to Engineer New Materials]

The New Ideas Investment Area aims to position Sandia to anticipate and respond to national security challenges (both now and in the future) by supporting high risk new ideas that have the potential to be transformational; for example, those with long time horizons, potentially high, yet uncertain mission impacts, or nascent research in a new field that may in the future become transformational for our mission. It is intended to support leading-edge research that is outside Sandia's current research focus areas, but that may lead to breakthroughs in science and technology that could profoundly impact our national security mission.

PROJECTS

A New All-Dielectric Nanolaser

191223 | Year 2 of 3

Principal Investigator: M. B. Sinclair

Executive Summary:

Recent developments at Sandia provide a path for improving dielectric resonator (DR) performance by: greatly increasing the resonator quality factor (Q), and thereby greatly narrowing the spectral bandwidth; and fabricating DRs from active materials such as GaAs/InGaAs. This project will capitalize on these two breakthroughs to develop tunable, narrow-band nanolasers with no metals in the cavity. Sensing and imaging devices based upon these lasers could benefit DoD and DHS missions.

Controlling Nanoparticle Assembly to Engineer New Materials

180922 | Year 3 of 3

Principal Investigator: G. S. Grest

Executive Summary:

To expedite computational pathways to design nanomaterials while accounting for chemical information critical to their integration and function, we have determined the length scale that atomistic information must be retained while coarse graining polymer. We developed a highly accurate hierarchal coarse grained model that accounts for their physics and chemistry to accelerate computations of nanoparticle assembly. This could impact design of structured materials for applications such as capturing solar energy.

Developing Thermally Activated Acid Release Agents

200236 | Year 1 of 2

Principal Investigator: T. N. Lambert

Executive Summary:

This project will develop molecular control and a new fundamental understanding of chemical bonding concepts that allow for the development of compounds that can release a variety of protic substances upon thermal exposure. Such thermally activated compounds could find use in several applications including molecular switches and in lithography.

Electro-Optical Control over SiV Center Emission in Diamond

200240 | Year 1 of 2

Principal Investigator: E. S. Bielejec

Executive Summary:

The project goal is to develop and characterize silicon vacancy (SiV) defect centers in diamond substrates. We will develop a microfabricated integrated structure for electrical control of both the emission and the charge state of the SiV. The ability to electrically control both the optical emission and the charge state of the defect centers in diamond opens up a wide range of potential applications into cybersecurity and quantum information processing.

Emergent Phenomena in Oxide Nanostructures

180923 | Year 3 of 3

Principal Investigator: W. Pan

Executive Summary:

This project aims to discover novel electronic devices for our nation's next-generation secure information applications. One of the candidates is magnetoresistive random access memory (MRAM) for information storage. An urgent need in developing MRAM is to identify a material system that is suitable for downscaling and is compatible with low-power logic applications. Self-assembled, vertically-aligned $La_{2/3}Sr_{1/3}MnO_3$:ZnO nanocomposites can offer new MRAM applications by combining their superior electric, magnetic, and optical properties.

Engineering Spin-Orbit Interaction in Si

200238 | Year 1 of 2

Principal Investigator: T. Lu

Executive Summary:

This project will engineer a new quantum material using silicon, which has weak spin-orbit coupling, and nanoscale magnets. The newly developed material will possess an energy-momentum dispersion that currently only exists in materials with strong spin-orbit coupling. When coupled to a conventional superconductor, this material can host so-called Majorana fermions, which can be used for fault-tolerant topological quantum computing.

Mediated Flow Batteries

191225 | Year 2 of 2

Principal Investigator: T. M. Anderson

Executive Summary:

The project goal was to build a higher energy density redox flow battery for grid scale energy storage and increased renewables penetration. We identified high energy density metal-oxide clusters and electrochemically compatible mediators and paired them together in a laboratory-scale redox flow battery for testing and optimization. Successful battery design, materials synthesis, and characterization will mitigate concerns involving both performance and safety that are aligned with NNSA and DHS missions.

Sandia's Rotary Vapor Compression Cycle Technology: A Pathway to Ultrahigh Efficiency Building Air Conditioning, Heating, and Refrigeration

180924 | Year 3 of 3

Principal Investigator: H. A. Kariya

Executive Summary:

This project is the first step in developing the rotating vapor compression cycle (RVCC) for improving the efficiency of air conditioning, heating, and refrigeration systems. This project developed fundamental understanding of two-phase flow in the rotating frame. The RVCC has the potential to cut electricity consumption, reduce total energy demand growth, and also reduce the amplitude of heat-wave-induced load spikes, thus improving the stability of the electrical grid.

Topological Photonics: The Quest for Ultimate Photon Control

191221 | Year 2 of 3

Principal Investigator: G. S. Subramania

Executive Summary:

Topological photonics can enable ultimate photon control such as a scatter free propagation and non-reciprocity enabled by topological protection for quantum light control and information. This is an emerging area with mostly theoretical work and few experimental demonstrations. This project leverages Sandia's established strength in nanophotonics to achieve fundamental understanding, positioning us strongly for future mission needs such as fault-tolerant quantum computing and quantum communications vital for national security.

Understanding Si-Decorated Nanoporous-Carbon Anodes for High Performance Li-Ion Energy Storage

200237 | Year 1 of 3

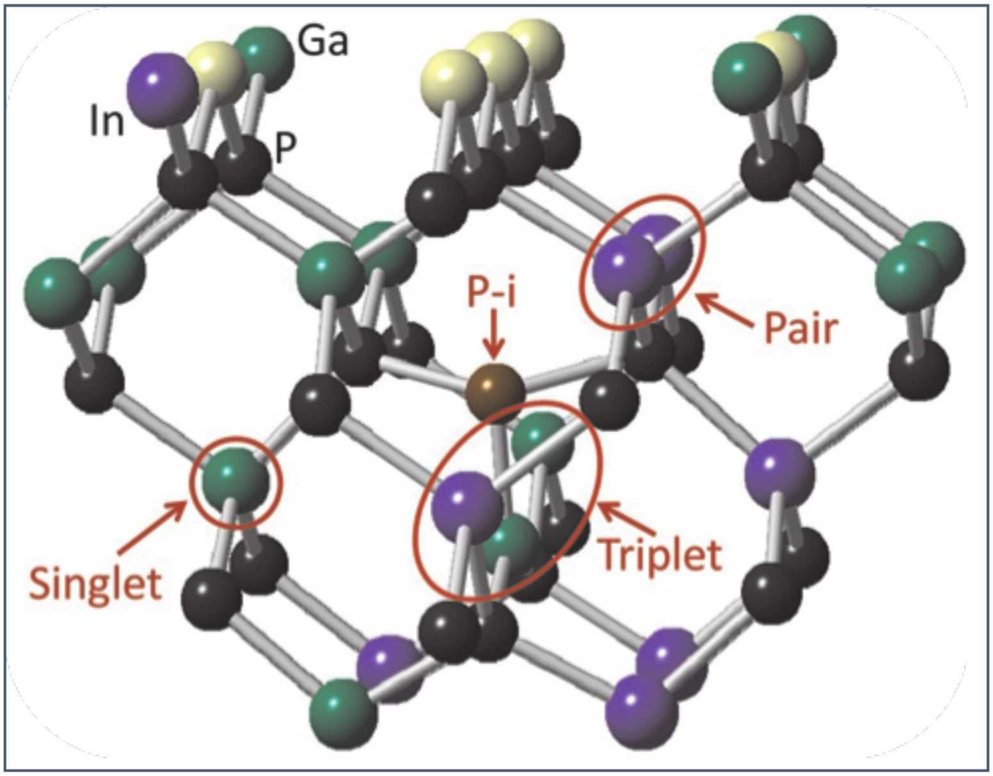
Principal Investigator: K. L. Harrison

Executive Summary:

This project will develop composite anode materials for lithium-ion batteries consisting of silicon and a Sandia-invented form of carbon (nanoporous carbon). These composite materials are expected to perform better than traditional silicon-carbon composites. In addition to improving lithium-ion batteries, synthesis of these materials is amenable to thin-film battery fabrication, which is of particular interest for energy security applications.

Radiation Effects and High Energy Density Sciences

The figure on the right shows compact modeling for defect diffusivity in semiconductor alloys. The group-III nearfield lattice sites for the ground state of +1 C1h p001m IP in InGaP. Green and violet balls denote Ga and In group-III sites within the defect's nearfield; white balls denote other close-by group-III sites identified as having less influence on the +1 IP formation energy that are thus designated to be in the defect's far-field; all of the more-distant group-III sites (not shown) also reside in the defined far-field. [Project 180932, Compact Models for Defect Diffusivity in Semiconductor Alloys}



The Radiation Effects and High Energy Density Sciences Investment Area seeks to advance science and engineering in the areas of radiation effects sciences, dynamic material properties, high energy density science, and pulsed power science. The goal of the radiation effects sciences area is to ensure that engineered systems can operate as intended in radiation environments they encounter, with interest in developing pulsed power technologies, innovative experimental techniques, and novel diagnostics that could scale to higher energy drivers.

PROJECTS

PROJECTS (continued)

Application of Enhanced Photocurrent Models and Single Event Effects

181198 | Year 3 of 3

Principal Investigator: D. A. Black

Executive Summary:

This project will develop fundamental mechanistic understanding, experimental characterization, and modeling capability to explain single event transient behavior and photocurrent response on commercial bulk complementary metal–oxide–semiconductor (CMOS) devices and Sandia's CMOS7 silicon-on-insulator devices. Understanding layout variations for CMOS7 devices under a dose rate environment improves the ability to mitigate the effects and will significantly impact our nation's ability to field advanced technology for Application Specific Integrated Circuits (ASICs) in munitions.

Benchmarking 3D-Magnetohydrodynamic Simulations of Electrothermal Instability Growth by Studying Z-Pinches with Engineered Defects

200269 | Year 1 of 3

Principal Investigator: T. J. Awe

Executive Summary:

This project will generate new data on the nonuniform heating of conductors driven with intense current. Data will constrain 3D-magnetohydrodynamic simulations, accelerating the development of an advanced computational model of instability growth on magnetically driven implosions relevant to radiation effects science and inertial confinement fusion experiments. The research will identify the type of resistivity perturbation that most aggressively drives nonuniform heating—knowledge vital for mitigating magneto-Rayleigh-Taylor instability growth.

Compact Models for Defect Diffusivity in Semiconductor Alloys

180932 | Year 3 of 3

Principal Investigator: A. F. Wright

Executive Summary:

This project developed new capabilities to accurately simulate point-defect diffusion in semiconductor alloys and to extract compact models from the simulation results that can be used in Sandia computer codes to model transient effects in radiation-hard electronic devices following exposure to short-pulse neutron irradiation. The project is relevant to DOE's nuclear security mission.

Correlating the Structural and Electrical Performance of Microelectronics during a Radiation Event

191240 | Year 2 of 3

Principal Investigator: K. M. Hattar

Executive Summary:

Radiation damage affects performance and reduces lifetimes of microelectronics used in space electronics, nuclear reactors, and weapons. After the cascade is done (picoseconds), the resulting defects will diffuse and interact over timescales from nanoseconds to the life time of the device, affecting the material properties and reliability. Our project will provide fundamental understanding of the initial creation, fast reaction, and long-term evolution of collision cascades in materials.

Coupled Electron-Photon Monte Carlo Radiation Transport for Next-Generation Computing Systems

195880 | Year 2 of 3

Principal Investigator: K. Bossler

Executive Summary:

This project will explore alternative algorithms for coupled electron-photon Monte Carlo radiation transport better suited to the single instruction, multiple data (SIMD) paradigm of upcoming exascale computing systems. Exploring these alternative algorithms over traditional methods is essential for maintaining our ability to provide accurate radiation transport results, which helps drive both engineering design and qualification of the nuclear weapon stockpile.

Current Loss in 0.1 - 100 Terawatt Vacuum Transmission Lines: Next-Generation Experiments and Physics-Based Simulations

191237 | Year 2 of 3

Principal Investigator: B. T. Hutsel

Executive Summary:

This project will develop new understanding of electrical power flow in high power density magnetically insulated transmission lines (MITLs). The project will conduct pulsed power experiments and develop next-generation physics-based theoretical models of the experiments. The goal is to develop predictive circuit and fully electromagnetic, fully relativistic, 3D particle-in-cell models of a MITL system. Success could aid in the design of powerful next-generation pulsed power accelerators relevant to DOE missions.

Development of Fast-Pulse Intense Neutron Generation Capability by Beam-Target Interaction on Hermes-III for Radiation Effects Testing

200267 | Year 1 of 3

Principal Investigator: T. J. Renk

Executive Summary:

This project, if successful, will result in an key addition to radiation effects testing, a source of high energy pulsed neutrons. Understanding circuit effects resulting from such a pulsed neutron flux should result in increased reliability of the US nuclear stockpile to respond to adversary threats.

Development of a 200-kV, Low-Inductance, Low-Jitter, Low-Prefire-Rate Spark-Gap Switch

191238 | Year 2 of 2

Principal Investigator: M. L. Wisher

Executive Summary:

Fast, reliable switching is the basis of all pulsed power systems. A switch is needed which can meet all requirements for a next-generation pulsed power accelerator which uses brick-based pulsed power. The switch design resulting from this project could potentially address needs for next-generation pulsed power accelerators. As such, the project was a success in developing a suitable switch for this target application.

High-Energy X-Ray Detectors using Fast, High-Z Semiconductors

200271 | Year 1 of 3

Principal Investigator: D. K. Serkland

Executive Summary:

This project combines radiation physics theory, materials science studies, and electro optic device engineering to develop high-speed compound-semiconductor high-energy x-ray detectors. These new x-ray detectors will benefit national security by enabling high fidelity measurements of time-dependent photon spatial distributions and power history for radiation effects science and inertial confinement fusion experiments.

Measuring Plasma Formation, Field Strength, and Current Loss in Pulsed Power Diodes

180935 | Year 3 of 3

Principal Investigator: M. D. Johnston

Executive Summary:

The purpose of this project is to use visible spectroscopy to measure electrode plasma formation, electromagnetic fields, and current distributions in pulsed power diodes. Experiments were conducted on the RITS-6 accelerator and the Z Machine. The results are important for understanding the role of plasmas in these devices, which is needed to support stockpile stewardship, high-yield fusion, and to inform next-generation pulsed power science.

Polynomial Chaos Methods in Xyce for Embedded Uncertainty Quantification Circuit Analysis

200265 | Year 1 of 3

Principal Investigator: E. R. Keiter

Executive Summary:

This project will develop embedded uncertainty quantification approaches based on intrusive polynomial chaos expansions in the Xyce circuit simulator. These nonsampling-based approaches will allow for a more scalable, verifiable, accurate, and computationally efficient uncertainty quantification analysis for circuit simulation. This will improve confidence in Xyce qualification evidence and will benefit various nuclear weapon programs.

Prediction and Design of Nonlinear Systems and their Emergent Behavior

200275 | Year 1 of 3

Principal Investigator: M. E. Glinsky

Executive Summary:

This project will develop models of turbulent mix and self organization (through the novel application of a state-of-the-art mathematical transformation) to more confidently model the evolution of complex, nonlinear systems. The project will also revolutionize data analysis and code verification, providing quantitative metrics to compare both simulated and experimental images of complex multiscale systems, impacting the design and computational verification of our nation's nuclear stockpile.

Single Event Effects in Sandia's Semiconductor Devices and Acceptance Testing in Integrated Circuits

200264 | Year 1 of 3

Principal Investigator: L. Musson

Executive Summary:

The Single Event Effect (SEE) project advanced in FY 2017 a modeling capability coupled with experimental validation to evaluate critical semiconductor device sensitivity to single event ionizing radiation. The modeling is done employing Sandia's own Charon technical computer aided design (TCAD) tool and collaborating with Vanderbilt University to use their Monte Carlo Radiative Energy Deposition (MRED) code to evaluate soft error (recoverable) rates given a single ionizing particle strike.

Stochastic Shock in Advanced Materials

200268 | Year 1 of 3

Principal Investigator: N. W. Moore

Executive Summary:

This project will develop new fundamental mechanistic understanding, experimental characterization, and modeling capabilities to explain shock generation, propagation, and failure in stochastic media (e.g., flame-sprayed metal films) that are porous and highly anisotropic, enabling tailored design and science-based qualification of these and potentially other new additively manufactured materials with properties optimized for a wide range of defense applications.

Time-Resolved X-Ray Diffraction Measurements on Laser-Compressed Polycrystalline Samples using a Multi-Pulse, Short-Pulse Laser-Generated X-Ray Source

191235 | Year 2 of 3

Principal Investigator: M. Schollmeier

Executive Summary:

This project investigates whether material properties are different in nanosecond-scale compression compared to static compression. Two laser pulses are used to dynamically compress samples and to generate an x-ray source for x-ray diffraction measurements on these samples. These measurements provide data to benchmark atomic-scale modeling of dynamic phase transitions, which is a key contribution to the advancement of predictive capability. Success could benefit the NNSA's nuclear security mission.

Towards Multi-Fluid Multi-Physics Continuum Plasma Simulation for Modeling Magnetically Driven Experiments on Z

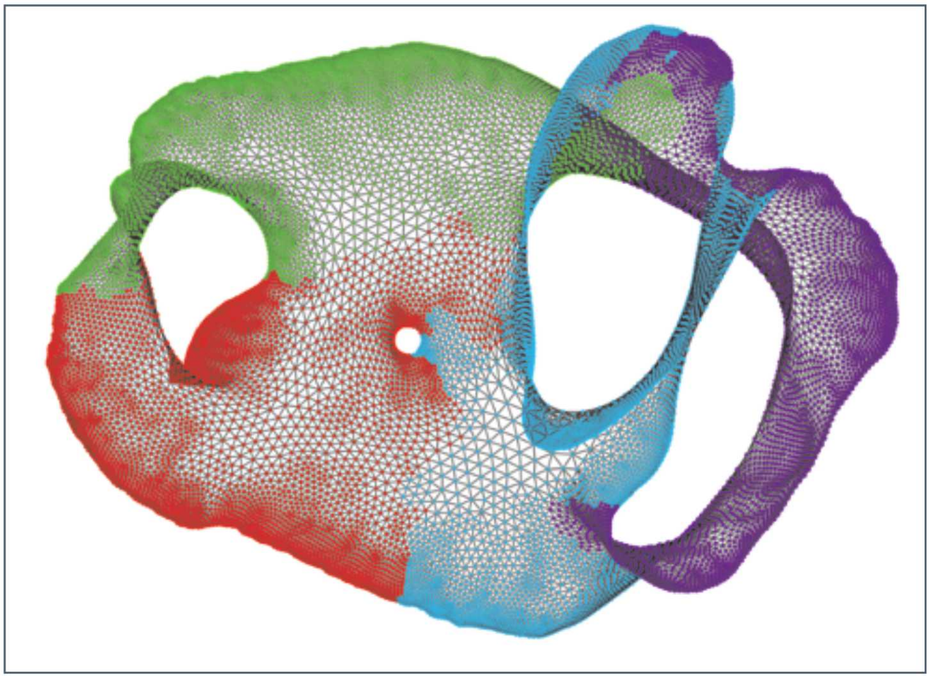
200276 | Year 1 of 3

Principal Investigator: J. N. Shadid

Executive Summary:

Our goal is the development of a unique, robust, and accurate implicit/explicit computational approach for continuum multifluid multiphysics shock-hydro electromagnetic plasma modeling for fast waves and moderate-to-high density enabling longer-time-scale simulations for pulsed power applications. This capability is not only critical as a continuum model, but is also foundational for multiscale kinetic-continuum models for coupling of small (kinetic) and large (continuum) scales.

DEFENSE SYSTEMS AND ASSESSMENTS



This figure is a graph showing partitioning methods for wireless networks done with PuLP. PuLP is a multi-objective, multi-constraint graph practitioner that uses label propagation to compute the partitions. [Project 190979, High Fidelity Simulations of Large-Scale Wireless Networks]

The Defense Systems and Assessments Investment Area delivers advanced science and technology solutions to deter, detect, track, defeat, and defend against threats to our national security. The work includes the development of innovative systems, sensors, and technologies for the nation's defense communities. This IA seeks to draw upon Sandia's state-of-the-art ST&E capabilities through focused investments in four strategic program areas: Cyberspace, Global Nuclear Assurance and Security (GNAS), National Security Space Systems (NSSI), and Synergistic Defense Products (SDP). Cyber delivers science and engineering based cyber technologies to continuously advance national security missions. GNAS enables the US government to confidently anticipate, assess, and address nuclear risks worldwide using advanced systems and technologies, expertise, and situational awareness systems/tools. NSSI develops and exploits innovative space sensing systems to address critical National Security challenges. SDP is focused on developing leading edge technologies and capabilities to respond to emergent national security challenges and is synergistic with NW mission.

PROJECTS

PROJECTS (continued)

PROJECTS (continued)

"Proof-of-Work" for Securing the Internet-of-Things (IoT) Networks

206870 | Year 1 of 1

Principal Investigator: C. Chan

Executive Summary:

"Proof-of-Work" (PoW) protocols may help automatically and dynamically manage trust in distributed systems. This project identified characteristics of embedded devices, cryptographic algorithms, and proof protocols that make lightweight systems equally competetive in terms of computation, memory, or energy when compared to higher resourced devices. Tying devices to physically measurable quantities enforces identity and improves security in critical distributed systems.

A 1V, 1W, 100 GHz Electro-Optic Modulator on Silicon for Space Applications

200134 | Year 1 of 3

Principal Investigator: A. L. Lentine

Executive Summary:

The goal is to develop and demonstrate the world's highest performance optical modulator using electro-optic materials on silicon. Challenges include optical and semiconductor modeling, optimization of the design, and microsystems fabrication to make devices with repeatable performance predicted from the models. This project provides a solution to a rapidly growing big data national security/DOE mission problem and addresses a technology gap that is not being addressed by industrial vendors.

A Novel Joint Hierarchical Model for Hyper-Spectral Target Prediction

200098 | Year 1 of 2

Principal Investigator: D. Z. Anderson

Executive Summary:

This project will develop new optimization algorithms and software for supervised tensor factorization to better detect and classify hyperspectral signatures. Incorporation of supervisory information into model formulation will boost predictive power, facilitating the use of hyperspectral imagery for a wide range of national security mission applications from target detection to treaty monitoring and verification.

Accurate Characterization of Real Networks from Inaccurate Measurements

191009 | Year 2 of 2

Principal Investigator: A. Pinar

Executive Summary:

Our nation's dependence on information networks makes it vital to anticipate disruptions or find weaknesses in these networks. Networks like the Internet are vast, distributed without a mechanism to completely collect their structure. We developed network inference methods by adopting sublinear graph sampling techniques to provide a systematic, rigorous, and scientific approach to understand the structure of information networks. This is important for protecting our information networks for national security.

Additively Manufactured, Athermal, Broadband, and Lightweight Optical Telescope

200063 | Year 1 of 3

Principal Investigator: J. Choi

Executive Summary:

This project will pioneer development of materials and new processes to additively manufacture lightweight reflective optical components using ceramic materials. This project has the potential to reduce weight, fabrication time, and integration time of reflective optical systems, enabling more agile and resilient optical systems for DOE/NNSA national security missions.

Advanced Synthetic Aperture Radar Exploitation

200022 | Year 1 of 3

Principal Investigator: R. D. West

Executive Summary:

We introduce a mathematical framework for discriminating between different types of change within a coherent change detection (CCD) image. We utilize the extra degrees-of-freedom provided by the elementary scattering physics information from polarimetric synthetic aperture radar (PolSAR) data and PolSAR processing techniques to demonstrate change-type discrimination in CCD images. Many intelligence, surveillance, and reconnaissance missions could benefit from successful completion of this research, which is highly relevant to DOE/DoD missions.

Alternate Focal Plane Array Architectures

190995 | Year 2 of 2

Principal Investigator: E. R. Olson

Executive Summary:

This work presents architectural concepts that combine wider dynamic range, higher sample rates, and lower power consumption for next-generation focal plane arrays. A design is demonstrated that operates in three different modes, with the ability to automatically change within a faction of a scan, allowing for extended dynamic range, and higher effective sample rates beyond the sensor's baseline scan rate. Potential DOE/national security benefits: more accurate information with less risk/cost.

Avalanche Photodiode Arrays for High Dynamic Range Infrared Detection

200137 | Year 1 of 3

Principal Investigator: D. K. Serkland

Executive Summary:

This project seeks to develop low-noise avalanche photodiodes using novel compound semiconductor materials. If successful, this work will eventually lead to focal plane arrays with improved performance for remote sensing missions and other DOE applications.

Biologically Enabled Remote Sensing for Real-Time Detection and Threat Response

180842 | Year 3 of 3

Principal Investigator: A. Ruffing

Executive Summary:

Monitoring of chemicals in the environment, such as heavy metal pollutants, can be challenging. Biological sensors can enable the detection of specific chemical signatures, producing an optical output in response to chemical exposure. This project constructed biological sensors for the detection of gold, analyzed various optical biological signals, and tested for natural stress responses of plants to heavy metal exposure.

Broadband Extremely Low-Profile Antennas

200067 | Year 1 of 3

Principal Investigator: G. D. Wainwright

Executive Summary:

This effort researches the development of an extremely low profile ultra wideband antenna to support NNSA national security missions. Development of this antenna will have a positive impact on our nation's ability to communicate on low frequencies in situations where physically large antennas commonly associated with low radio frequency (RF) communications are impractical or undesirable.

Characterizing the Relationship between Side-Channel Leakage and Temperature

199991 | Year 1 of 1

Principal Investigator: R. Helinski

Executive Summary:

This project produced test platforms and conducted experiments to try establishing the effect of operating temperature on side-channel information leakage in microelectronics. This is important because it helps us better understand potential vulnerabilities in the nation's microelectronics security systems; this benefits our NNSA national security missions.

Compact Low-Power Chemical Detector

200114 | Year 1 of 3

Principal Investigator: M. P. Siegal

Executive Summary:

This project will develop/demonstrate a method to indicate the presence of nuclear production activities via a miniaturized, low-power, high-fidelity passive sensor technology for specific byproduct fission gas detection by combining Sandia-developed US-patented nanoarray electrochemical sensors with highly selective porous materials that preconcentrate specific ions/gases to yield part-per-billion level highly selective detections. This proposed technology represents a nuclear materials detection breakthrough for sensitivity and minimization of false positives.

Confidence in Cyber Modeling and Simulation

180830 | Year 3 of 3

Principal Investigator: S. T. Jones

Executive Summary:

We study how to evaluate uses of emulation-based models of distributed computing, communications, and control systems. For predictive uses, where a model is expected to tell something true about the world, traditional validation is the appropriate approach. For uses like idea generation, demonstrations, or training, alternative approaches are preferred. If Sandia creates a meaningful verification and validation process, it can build appropriate credibility and mitigate risk for DOE missions.

Creating an Interprocedural Analyst-Oriented Data Flow Representation for Binary Program Analysis

200071 | Year 1 of 2

Principal Investigator: M. A. Leger

Executive Summary:

This research aims to combine program understanding, human factors, and visualization expertise to develop a comprehensible, intuitive data flow representation that organizes, scales, or filters currently overwhelming data flow information. This representation should address DOE and national security missions to protect our information systems by dramatically increasing the efficacy of binary analysts trying to understand data flow in a program.

Cryogenic Ingress and Egress of Optical Signals for Cyber

200145 | Year 1 of 2

Principal Investigator: C. DeRose

Executive Summary:

This project will develop a new understanding of optoelectronic device physics of low energy ingress and egress of optical signals in a cryogenic environment. New multiphysics models will be developed and validated by experimental characterization of silicon photonic modulators and detectors at cryogenic temperatures.

Diversity for Microelectronics Lifecycle Security

200147 | Year 1 of 2

Principal Investigator: J. Hamlet

Executive Summary:

In this project, we craft novel security and trust architectures that integrate diversity and resiliency to measurably impact and mitigate trust and security concerns for government microelectronic systems by exposing would-be attackers to significant levels of uncertainty and risk of failure when attempting to manipulate systems. This will improve our nation's ability to develop and deploy trustworthy critical systems.

Donor Quantum-Dot Four-Qubit Assessment Platform

200143 | Year 1 of 2

Principal Investigator: M. S. Carroll

Executive Summary:

This project will develop new quantum bits in a form which is compatible with metal oxide semiconductor transistors. The ability to integrate quantum information systems with classical silicon electronics has the potential for significant impacts to quantum information processing, quantum sensing, and cybersecurity.

Efficient-Track-before-Detect with Minimal Prior Knowledge

195968 | Year 2 of 2

Principal Investigator: K. Merry

Executive Summary:

This project developed a new, highly efficient approach to detection and tracking for low signal-to-noise ratio targets in large, fast-framing wide-area motion imagery (WAMI) datasets. The approach has demonstrated state-of-the-art tracking performance against targets of national security interest. It is also uniquely suited to embedded implementation, enabling it to process full-bandwidth WAMI data onboard a sensor.

Enabling Novel, Game-Changing Radar Sensing via Ultra-Wideband Polarimetry

200060 | Year 1 of 3

Principal Investigator: B. H. Strassner, II

Executive Summary:

The goal is to design a planar, lightweight, dual-polarized antenna array. The array should provide 3 GHz of instantaneous bandwidth in Ku-band, cross-polarization levels of about 30 dB, and port-to-port isolations at around 30 dB. The polarimetric antenna will provide radiation characteristics that will enable novel modalities such as maritime imaging, coherent change detection in high-clutter environments, and foliage-penetration algorithm development relevant to DoD defense and DOE energy security missions.

Engineering Efficient Human-System Interaction in Defense Systems of Systems

180856 | Year 3 of 3

Principal Investigator: M. J. Hoffman

Executive Summary:

This project is the first known attempt at incorporating human performance and human technology interactive effects in the larger context of a system of systems (SoS) model. Most SoS are actually sociotechnical systems where human technology interactions are critical to mission success and contribute to a high percentage of failures, so our framework for understanding human effects on SoS performance is vital.

Enhanced Single-Frame Closely Spaced Object Processing

200014 | Year 1 of 2

Principal Investigator: D. P. Woodbury

Executive Summary:

This project will develop a robust algorithm that provides a state-of-the-art capability in the extraction of objects to beyond the resolution limit of a sensor system from a single image. The resulting algorithm impacts a variety of electro optical and/or infrared sensing systems, including those used for DOE national security mission areas.

Entity Resolution at Large Scale: Benchmarking and Algorithmics

200105 | Year 1 of 2

Principal Investigator: J. W. Berry

Executive Summary:

This project concerns "Entity Resolution," a collection of problems shared by many data analysis problems at DOE and its customers. References (such as names, electronic addresses, etc.) to entities such as people, computers, concepts) in mission data are observed, and these references must be mapped to the underlying entities before analysis can proceed. We work with top academics to develop unclassified algorithms, software, and benchmarks for entity resolution.

Event Correlation using Spatio-Temporal Point Processes

196390 | Year 2 of 3

Principal Investigator: J. D. Tucker

Executive Summary:

This project will develop new theoretical statistical modeling in spatio-temporal point processes in which the observations contain missing data. Extending spatio-temporal point process methodologies to develop inferences about the correlation of events in both space and time will provide a more complete and nuanced picture to the analyst in near-real time for intelligence and surveillance applications.

Exploitation of Optical Polarimetry for Remote Sensing

180840 | Year 3 of 3

Principal Investigator: J. M. Craven

Executive Summary:

The objective of this project is to develop a capability for predicting the utility for polarimetric data for a variety of national security missions. This is being achieved through investments in modeling and simulation, phenomenology characterization, and sensor engineering and data exploitation. By laying the foundation for polarimetric data measurement and exploitation, this project advances the state of the art and impacts national security missions in nuclear nonproliferation/other mission areas.

Exploiting Social Media Sensor Networks through Novel Data Fusion Techniques

191004 | Year 2 of 2

Principal Investigator: T. M. Kouri

Executive Summary:

This project will develop algorithms and software for hard (e.g., sensor) and soft (e.g., human generated text) data fusion. This project will explore using soft data to predict events. The new algorithms will be able to efficiently integrate and fuse data from multiple sources, detect misinformation in sources, and exploit the resulting information. This project is relevant to DOE/DoD space/ground situation assessments by generating situational knowledge from fused multi-source data.

Exploring the Effects of Silicon Ultrathinning on Integrated Circuit Behavior

200016 | Year 1 of 2

Principal Investigator: C. R. Friedman

Executive Summary:

Silicon ultrathinning is an emerging capability that has the potential to enhance spatial resolution of laser-based failure analysis techniques. This project will build an understanding of the effects of ultrathinning on circuit behavior that is necessary for the success of the failure analysis approaches. This supports our nation's cross-cutting microelectronics work in both research and fielded technologies for DOE/NNSA missions.

Extreme Power Radio Frequency Amplifiers

200138 | Year 1 of 3

Principal Investigator: P. D. Coleman

Executive Summary:

The fundamental goal of this work is to demonstrate the feasibility of gigawatt class high-power amplifiers capable of radiating complex "smart" waveforms. Successful demonstration of this new amplifier capability would greatly expand the options available for reducing global nuclear security threats and securing cyberspace. This will position Sandia as a leader in providing revolutionary high-powered electromagnetic capability to the nation.

Field Programmable Gate Array Trust and Vulnerability Assessment Guided by Network Criticality Metrics

191011 | Year 2 of 2

Principal Investigator: V. G. Kammler

Executive Summary:

Our microelectronics designs heavily rely on intellectual property provided as logical netlists that are not sufficiently analyzed with existing capabilities. To assist assessment of potential vulnerabilities, we focus on identifying and prioritizing tamper targets within these netlists. We define network criticality metrics, apply them to hardware trojan benchmarks, and present methods to approximate and scale computation to more complex designs. Results will support missions across defense and nuclear weapon communities.

Geospatially Aware System-of-Systems Decision Capability

200140 | Year 1 of 3

Principal Investigator: H. D. Le

Executive Summary:

This project will develop a new capability to integrate discrete event stochastic simulation with geospatial information system databases to aid military decision makers. These hybrid simulations will allow assessments of locations, logistics, and national security missions while streamlining the model-building process by using existing databases to pre-populate key data and eliminate the need to convert spatial information into time-based representations.

High Fidelity Simulations of Large-Scale Wireless Networks

190979 | Year 2 of 2

Principal Investigator: U. Onunkwo

Executive Summary:

This project demonstrates a provable ability to simulate wireless networks at scales much larger than today's simulators can. Our solution is easily extensible to existing solutions and shows orders of magnitude improvement over state-of-the-art simulators. The success of this work can be applied to cyber problems of national interest related to the security and usability of large scale wireless networks.

Hybrid Classifiers using Statistics and Machine Learning

190988 | Year 2 of 2

Principal Investigator: K. M. Simonson

Executive Summary:

While modern machine learning techniques have performed impressively in some data analytic challenges, their "black box" nature and tendency to over-fit training data have limited their use in applications related to critical decision support. We studied new ways of combining neural and statistical approaches to develop classifiers that are robust to operational variability and provide rigorous measures of classification uncertainty. The resulting classifiers will be applicable across many mission challenges.

Implementing Neural Adaptive Filtering in Detection Systems

190993 | Year 2 of 3

Principal Investigator: F. S. Chance

Executive Summary:

This project will develop novel neural-inspired adaptive algorithms, guided by the neural circuitry of the retina, to adaptively filter information at the sensor level. The developed algorithms will enhance the performance of detection systems by allowing them to filter a range of distractor signals, potentially at the sensor-hardware location, leaving more bandwidth for transmitting signals-of-interest. Successful outcomes will apply to DOE/national security remote sensing systems limited by size/weight/power restrictions.

Improved Mobile Device Positioning via Contextual Awareness

200020 | Year 1 of 3

Principal Investigator: A. J. Patterson

Executive Summary:

Given a relative trajectory with associated activities, we aim to establish an absolute geolocation by matching features extracted from the trajectory with those in a contextual database (e.g., OpenStreetMaps, light detection and ranging (LiDAR), building floor plans). This will provide a new analysis technique that will provide enhanced situational awareness in support of US nuclear (NNSA) and national security (DoD/ intelligence community) missions.

Inferential and Feature Selection Methods for Video Imaging

190980 | Year 2 of 2

Principal Investigator: M. G. Chen

Executive Summary:

This project will develop novel methods for fast, unsupervised feature detection methods in video data, as well as mathematically principled novel hypothesis testing methods for dependent imaging data. Features of interest and significant differences will be quickly identified with little to no knowledge. These methods will enhance the efficiency and accuracy of video analysis in many application areas, such as surveillance. Improved algorithms will provide timely information to national security missions.

Latent, Passive, Low-Energy X-Ray Exposure Indicator

199992 | Year 1 of 2

Principal Investigator: L. Biedermann

Executive Summary:

This project develops unique optical sensing capabilities based on coupled optical and chemical amplification to indicate if an object has been x-ray interrogated. We developed polymer systems that exhibited permanent physical changes and optical reflectance shifts upon absorption of few eV photons. We optimized surface energies to allow for assembly into optically amplifying polymeric Bragg crystals. In FY 2018, we will add additional optical amplification to increase x-ray sensitivity.

Measurement of the Optical Opacity of Warm Dense Gas Mixtures to Support High Fidelity Modeling and Interpretation of the Optical and Thermal Emission from Conventional and Nuclear Fireballs

191001 | Year 2 of 2

Principal Investigator: P. L. Dreike

Executive Summary:

We developed a technique to shock, heat, and compress air to temperatures above 6000K and densities of 0.1-10 times standard density and measured the spectrally resolved optical emission. A novel optimization technique was developed for determining shock temperature from the emission spectra. Analyses to determine the chemical equilibration time of the shocked air showed that the experiment is valid. Confident signal interpretation supports national security decisions if events were detected.

Microsystems-Enabled Passive Radio Frequency Signal Processing

190996 | Year 2 of 2

Principal Investigator: C. Nordquist

Executive Summary:

This project explored resonant microsystem technologies for ultra low power radio frequency (RF) receivers. Miniature impedance transformers perform RF filtering and passive voltage gain for improved impedance matching. Resonant switches provide energy build-up specific to the modulation frequency for switch closure with high on/off ratio. These components offer detection of low-power pulse-modulated RF signals with sub-nanowatt quiescent power consumption. Exploring novel microsystem technology and applications will benefit DOE/national security missions.

Mitigating Charge Carrier Generation in Silicon to Enhance Backside Laser Failure Analysis

203539 | Year 1 of 2

Principal Investigator: C. R. Friedman

Executive Summary:

This project will enhance failure analysis capabilities by minimizing the impact of undesired electrical signals. The expected outcome is an improved ability to detect opens and other types of failures. If successful, this work will benefit a broad set of national security sponsors by expanding cyber hardware capabilities and developing critical technical understanding in the emerging fields of backside silicon ultra-thinning and backside visible light probing.

Mitigation of Cyber Proliferation

200113 | Year 1 of 2

Principal Investigator: K. G. Gabert

Executive Summary:

This project will develop technologies to understand the size, scope, and content of darknets and enable mitigation of cyber weapon proliferation in this space. The tools and techniques developed will enable DOE/NNSA and other government agencies to curb the proliferation of malicious cyber tools and exploits.

Motion and Trajectory Algorithms for Visual Information Foraging in Intelligence Analysis Workflows

193424 | Year 2 of 3

Principal Investigator: L. A. McNamara

Executive Summary:

Today's eye tracking systems have practical application across a wide range of domains. However, they are not designed for capturing data about how people interact with information in real-world environments. We are developing a software environment and algorithms to calculate gaze events in relation with image content, while users are interacting dynamically and unpredictably with the image stimulus. DOE/DoD rely on such exquisite sensing systems to support national security missions.

Multilayered Solid State Neutron Detector for Nonproliferation Applications

200136 | Year 1 of 2

Principal Investigator: W. C. Rice

Executive Summary:

This project will develop a solid state neutron sensor that uses a stacked multilayer to achieve high efficiencies within a small volume. This sensor will provide an advanced neutron detection capability for a variety of applications such as radiation dose monitoring and control for safety, as well as nuclear material detection in nonproliferation applications for national security.

Multimodal Data Integration under Uncertainty

190991 | Year 2 of 3

Principal Investigator: D. J. Stracuzzi

Executive Summary:

This project develops methods for integrating data from multiple sources into a single analysis while also evaluating the uncertainty in the measured observations, model structure, and the model inferences and predictions. Successful results will benefit many national security mission spaces, including defense, intelligence, homeland security, and the nuclear weapons life cycle. We have identified several specific applications in these spaces.

Multitarget-Multisensor Tracking

190999 | Year 2 of 2

Principal Investigator: K. Legrand

Executive Summary:

This project's goal is to develop finite-set statistics (FISST) multitarget recursive Bayes filter design methodologies well suited for space mission and remote sensing (SMRS) mission areas. The most prevalent application of FISST to multisensor-multitarget tracking is the delta-generalized labeled multi-Bernoulli (δ-GLMB) filter. The effort will benefit the Department of Energy (DOE) mission "Strategic Partnerships to Address Broad National Security Requirements."

Neural-Inspired Computation Remote Sensing Platform

200106 | Year 1 of 3

Principal Investigator: C. M. Vineyard

Executive Summary:

This project will explore using neural-inspired computation to evaluate, filter, and process remote sensing data at the sensor rather than downstream where the costs (system cost, system volume, system weight, power consumption, and response time) are much higher. Understanding what computational advantages neural-inspired computing can afford for remote sensing will impact our nation's ability to monitor and maintain national security.

Novel Approach for Uniform, Localized Die Thinning

200066 | Year 1 of 2

Principal Investigator: D. P. Adams

Executive Summary:

This project will utilize predictive finite element thermal model simulations, experimental studies of laser-solid interactions, and advanced microstructure characterization to identify novel laser etching methods that uniformly thin semiconductor substrates. The developed techniques should greatly improve failure analysis of integrated circuits important for national security missions.

Persistent Tracking of Dismounts by Multichannel Radar

200065 | Year 1 of 3

Principal Investigator: D. L. Bickel

Executive Summary:

The purpose of this project is to develop a capability to track high value dismounts in all-weather conditions using a radar system. This work extends previous work done for tracking high value vehicles. Successful completion of this research will lead to an important capability relevant to DOE intelligence, surveillance, and reconnaissance-related activities.

Pinned Photodiode Pixel Development Enabling High Performance Visible Focal Plane Arrays

180841 | Year 3 of 3

Principal Investigator: R. R. Kay

Executive Summary:

This work has developed pinned photodiode focal plane array technology for Sandia's CMOS7 microelectronics process. Detailed device simulation, design, and test have been completed. A unique pixel architecture enables wide dynamic range. This research provides a key capability for developing low noise, high sensitivity, radiation hardened imagers in support of DOE national security missions via remote sensing programs.

RF Enabled Cyber: Incorporating Radio Frequency Channel Effects in Modeling of Wireless Networked Information Systems

190992 | Year 2 of 2

Principal Investigator: B. P. Van Leuwen

Executive Summary:

This project will develop an analysis capability to assess effectiveness of security approaches and implementations used for wireless networks. A capability to analyze the lower-layer protocol (i.e., link and physical layers) implementations without need for radio frequency (RF) emissions is necessary. Such a capability to enable cyber analysis of DOE/national security systems that depend on wireless communications will strengthen these systems against cyber attack.

Rapid Abstraction in Confined Environments (RACE)

200070 | Year 1 of 3

Principal Investigator: S. Buerger

Executive Summary:

This project will develop a perception capability to rapidly produce abstract representations of sensed objects, described both geometrically and semantically, to facilitate autonomous mission execution by unmanned systems in confined environments. This work will develop new multiphysics classification methods for perception with sparse training data; it will pioneer the active control of sensors to "close the loop" around classification uncertainty and provide key future technology to support NNSA missions.

Realistic Internet of Things (IoT) Signal Control

190978 | Year 2 of 2

Principal Investigator: I. Zedalis

Executive Summary:

The central purpose of the Realistic Internet of Things (IoT) Signal Control project was to create better defenses for networks containing IoT devices. The project explored a combination of analog and digital Wi-Fi radio signal analysis techniques. Ultimately, the project discovered a way to detect attacks on IoT devices even when the underlying Wi-Fi network is fully encrypted.

Realizing the Power of Near-Term Quantum Technologies

191313 | Year 2 of 2

Principal Investigator: J. E. Moussa

Executive Summary:

This project was tasked with laying a theoretical foundation and computational framework for quantum simulation on quantum devices. The unifying theme of the project has been the desire to delineate more clearly the interface between existent classical computing resources that are vast and reliable and emerging quantum computing resources that will be scarce and unreliable for the foreseeable future. The proposed infrastructure will be applied to quantum devices at Sandia.

Reconfigurable Structure Coupler for Antenna Mode Excitation

180861 | Year 3 of 3

Principal Investigator: N. J. Smith

Executive Summary:

This project developed the theory behind radio frequency (RF) excitation of arbitrary metallic objects. Antenna mode excitation couplers (AMEC) and placement are studied to facilitate the required current distribution for radiation. Antenna design is rethought to include any existing metallic structure, as such, "antennas of opportunity" can be used for field expedient communication systems.

Resilience Analytics for Space Assets and Supporting Infrastructure

200142 | Year 1 of 3

Principal Investigator: M. S. Aamir

Executive Summary:

This project will develop scientifically grounded resilience analytics metrics and techniques to evaluate the ability of proposed space architectures to withstand, adapt, and respond to disruption prior to investment. Our models will be able to better evaluate the performance effects that specific technologies could have on space systems when subject to hazards. In threat environments, greater understanding of these issues could avoid adverse impacts to DOE mission and costs.

Scalable, Targeted Code Analysis using Application Programming Interface Abstraction

200059 | Year 1 of 2

Principal Investigator: D. Bueno

Executive Summary:

This project investigates abstraction as a means for proving that software behaves safely. Reduced-fidelity (abstracted) models of software enable faster and more scalable algorithms. The goal of the project is to increase the speed of tasks, such as automated interface analysis and network protocol analysis through a novel approach to reasoning about computer programs. Automated software analysis is a critical component of cybersecurity and software assurance research for DOE missions.

Social Media Account Resolution and Verification

190990 | Year 2 of 2

Principal Investigator: T. R. Brounstein

Executive Summary:

This project developed algorithms to identify accounts being used for nefarious purposes and aid in determining authorship. We demonstrated that combining post content, social and interaction graph, and temporal activity into one analysis, we can find deceptive users that would be missed by any one-feature analysis. We developed and tested our techniques with publicly available social media data.

Spectral Dominance: Expanding Radio Frequency Antenna Bands into the Optical Regime

206985 | Year 1 of 1

Principal Investigator: J. B. Wright

Executive Summary:

The goal of this project was to explore technology to expand the sensing spectrum of the traditional radio frequency antenna to the optical regime; toward spectral dominance. We modeled optical scale antennas to numerically predict feasibility and quantify performance of an optical antenna, using real material parameters and dimensions.

Spiking/Processing Array (SPARR) for Wide Dynamic Range and High Resolution Photonic Sensing

200135 | Year 1 of 3

Principal Investigator: P. Hays

Executive Summary:

This project will improve national security by strengthening key technologies for remote sensing, detection, and signal processing. Spike-based signal processing embedded in the microelectronic architecture of focal plane arrays will improve sensor dynamic range and effective sample rates while reducing power consumption. The spike-based signal representations connect seamlessly to modern low-power neural inspired processing and allow low total power systems useful in DOE missions.

Synthetic Aperture Radar Targeting for Prompt Global Strike Missions

192870 | Year 2 of 2

Principal Investigator: S. P. Hollister

Executive Summary:

Sandia will develop algorithms that will process forward-squinted synthetic aperture radar (SAR) imagery that would be collected by a prompt global strike (PGS) vehicle prior to pulldown. These algorithms will analyze the imagery, detect, and identify the correct target in the scene. Relevant to DoD/NNSA national security missions, this real-time process will take place during the hypersonic-glide portion of the PGS mission, providing adequate time to perform terminal guidance correction.

The Chemical Composition of Vaporized Ground Materials

200015 | Year 1 of 2

Principal Investigator: J. W. Greenwald

Executive Summary:

We generated a data- and theory-derived equation of state model covering a wide range of temperatures and pressures for a type of ubiquitous volcanic rock. In FY 2018, additional higher fidelity data will be gathered through a series of shock experiments. This model will provide enhanced material and condensation simulation capabilities for US nuclear detection systems and nuclear forensics missions.

Tools and Techniques for PRESTIGE (PRactical Evaluation and Synthesis of Trust In Government systEms)

201939 | Year 1 of 3

Principal Investigator: B. K. Eames

Executive Summary:

This project will develop a practical approach to evaluate risk of development-time manipulation of microelectronics-based systems. The approach incorporates visual modeling of development processes and potential attacks against system development, coupled with a game theoretic analysis of attack viability. This quantitative risk assessment will facilitate making informed engineering tradeoff decisions, and reduce attack risk for multiple government programs.

Trusted Materials using Orthogonal Testing

180857 | Year 3 of 3

Principal Investigator: M. A. Rodriguez

Executive Summary:

We have demonstrated that with the use of a limited number of nondestructive diagnostic tests, coupled with multivariate statistical analysis methods, we can discriminate between various similar steel samples. Our results indicate that our approach is a viable route for materials assurance with regard to suspect counterfeit and adulterated materials.

Ultra-Low Level Security Introspection of Computer Operating Systems

200069 | Year 1 of 3

Principal Investigator: R. E. Bell

Executive Summary:

This project will develop new tools to introspect low level x86 security features. This project will use these tools to explore the inner working of these features as well as interactions between distinct features. Understanding the fundamentals of x86 security allows the Nation to better secure its computer systems, and may enable the identification and understanding of future threats.

Waveform-Agile Multi-Channel Cognitive Digital Radar for Multi-Mission Intelligence Surveillance and Reconnaissance and Radio-Frequency-Enabled Cyber

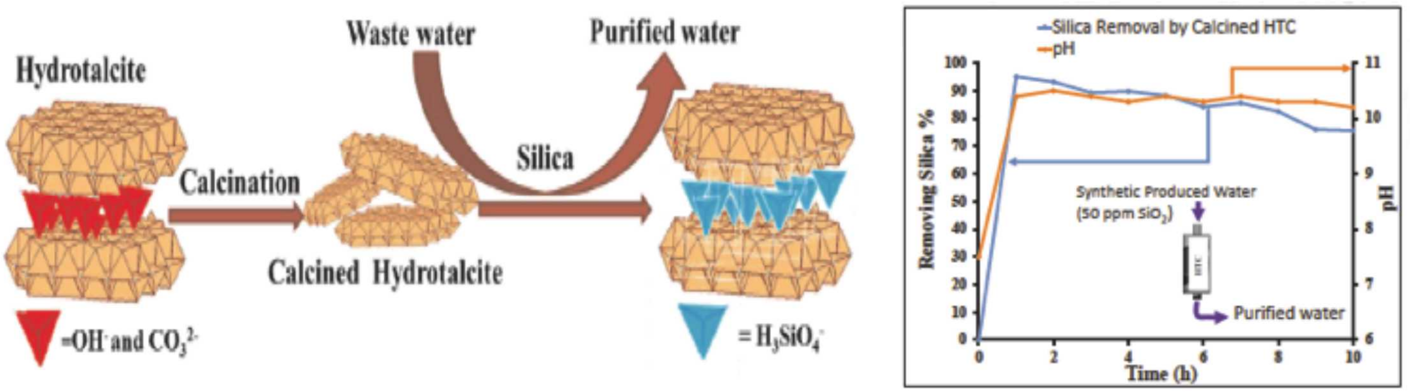
200133 | Year 1 of 3

Principal Investigator: H. Loui

Executive Summary:

This project will develop a multi-mission digital radar architecture that simplifies and modularizes a radar's radio frequency (RF) frontend by replacing application-specific analog sensing with flexible and programmable digital processing. It enables advanced real-time chameleon-like sensors that can send/receive/process arbitrary signals with large instantaneous bandwidth using multiple channels. Radars with these capabilities enable smarter sense, analyze, and respond cycles for DOE national security multi-mission applications.

ENERGY AND CLIMATE



The figure above is a graphical representation of Hydrotalcites. HTCs have high silica selectivity under ambient conditions and are readily recyclable. Silica selectivity remains high even in the presence of competing cations. [Project 191018, Waste Water for Power Generation via Energy Efficient Selective Silica Separations]

The Energy and Climate IA is focused on research and development that advances the state of knowledge and overcomes barriers to deployment of energy technologies for both supply and demand. The investment area seeks R&D that leverages Sandia's differentiating capabilities to create opportunities that can be transformational relative to current technologies or approaches, and encourages building directly on the results of fundamental research to provide real solutions to the most pressing mission challenges.

PROJECTS

ENERGY AND CLIMATE

PROJECTS (continued)

A Fundamental Study on the Physicochemical Process of Soot Particle Inception

191017 | Year 2 of 3

Principal Investigator: S. A. Skeen

Executive Summary:

This project attempts to identify the large hydrocarbons (macromolecules) associated with incipient soot in combustion environments at low, moderate, and high (i.e., engine-relevant) pressures. The goal is to provide kinetic mechanism developers with fundamental knowledge leading to an accurate representation of soot inception in models used for the design and optimization of next-generation engines. The project is relevant to the DOE's energy security mission.

A New Method to Contain Molten Corium in Catastrophic Nuclear Reactor Accidents

200165 | Year 1 of 3

Principal Investigator: D. Louie

Executive Summary:

This project will develop an injectable new granular sacrificial material system to cool and contain molten corium from release to the environment during a catastrophic nuclear reactor accident. The understanding of the interactions of the new granular sacrificial material and corium surrogate will enable us to develop a new safety feature for both existing and future nuclear reactor plants for the national energy security and sustainability.

Advanced Fuel Injection System for Rapid Control of High-Efficiency Low-Temperature Combustion Engines using Gasoline and other Gasoline-Like Fuels, Including Biofuels

180862 | Year 3 of 3

Principal Investigator: J. E. Dec

Executive Summary:

This project will develop a rapid, robust combustion-timing control system for low-temperature gasoline combustion (LTGC) engines, providing the technology needed to make these very high-efficiency engines commercially viable. Engines using LTGC can provide efficiencies above those of diesel engines, improving fuel economy by 30 to 40% over current gasoline engines, greatly improving energy security and mitigating carbon dioxide emissions.

Aggregating Distributed Energy Resources as Secure Virtual Power Plants

180867 | Year 3 of 3

Principal Investigator: J. T. Johnson

Executive Summary:

The Virtual Power Plant project investigated a future vision of the smart grid with far-reaching implications for electric grid distribution-level controls, optimization, forecasting, and cybersecurity. The team created a software platform capable of providing ancillary grid services to power system operators using distributed energy resources, as opposed to traditional thermal generators.

Bio-Inspired Ion-Selective Electrodialysis Membranes

200167 | Year 1 of 3

Principal Investigator: S. Rempe

Executive Summary:

This project will use biological inspiration to design advanced ion-selective membranes for water purification via electrodialysis. Lessons learned from modeling biological systems will be leveraged to design nanostructured synthetic membranes using a variety of materials chemistry, electrochemistry, and chemical vapor deposition techniques. Superior electrodialysis membranes will enable cost competitive water purification from produced and inland brackish water supplies.

Co-Optimization to Integrate Power System Reliability Decisions with Resiliency Decisions

191057 | Year 2 of 3

Principal Investigator: B. J. Pierre

Executive Summary:

The main goal of this project is to develop new models, algorithms, and supporting software tools for selection of electrical infrastructure improvements that simultaneously co-optimize reliability and resilience. The proposed project will ultimately provide a tool to inform utilities and their stakeholders, DHS, DOE, and policy makers of the best decisions available to simultaneously improve power system reliability and resilience.

Deciphering Atmospheric Ice Nucleation using Molecular-Scale Microscopy

200149 | Year 1 of 3

Principal Investigator: K. Thurmer

Executive Summary:

This project develops and applies nanoscale-microscopy procedures to provide a realistic understanding of ice nucleation in Earth's atmosphere, which affects the climate via precipitation and cloud albedo. This novel insight into key steps of ice nucleation under atmospheric conditions informs an improved parametrization of a global climate model (Energy Exascale Earth System Model/E3SM, formerly Accelerated Climate Modeling for Energy/ACME), advancing our nation's capability to predict the evolution of Earth's atmosphere.

Developing Process-Microstructure-Property Correlation of Radiation-Tolerant Nanoporous and Nanostructured Materials for High Irradiation Environments

200150 | Year 1 of 3

Principal Investigator: R. P. Dingreville

Executive Summary:

This project will develop a novel integrated capability to design and engineer novel radiation-tolerant and thermally stable materials operating in irradiated and high temperature environments. Optimization of microstructural features to improve their tolerance to radiation effects will be informed through an iterative process combining multiscale modeling and a corresponding suite of experimental techniques to characterize their thermo-mechanical properties under irradiation.

Development of Detection and Mitigation Algorithms for False Data Injection Cyberattacks against Nuclear Facilities

193419 | Year 2 of 3

Principal Investigator: L.A. Dawson

Executive Summary:

In false data injection attack, adversaries manipulate the control system sensor data. This project will use physics simulation to quantify normal range sensor behavior and identify anomalies. To date, we have developed a commercial reactor model. We generated model validation data and then applied linear dimensionality reduction to determine data signatures. When mature, these techniques could help defend US critical infrastructure against cyberattack.

Enhancing Power Plant Safety through Coupling Plant Simulators to Cyber Digital Architecture Model

200152 | Year 1 of 2

Principal Investigator: P. L. Turner

Executive Summary:

This project seeks to understand how nuclear power plant (NPP) operators would respond to a cyber attack on the digital controls within the plant. The team is building a cyber emulated environment for the plant and coupling it to a NPP training simulator. Experiments will be conducted with licensed operators to understand their perceptions and response to the attacks.

Exploring Fundamental Limitations of Manganese Oxide Cathodes for Reversible Zn/MnO2 Batteries

200168 | Year 1 of 3

Principal Investigator: T. N. Lambert

Executive Summary:

This project will develop new fundamental mechanistic understanding, experimental synthesis, characterization, and computer modeling capabilities in order to understand the chemical and physical changes that occur when cycling zinc-manganese oxide batteries in alkaline electrolyte. Additionally, we will develop new materials with improved performance such that high capacity batteries relevant to grid storage and mobile applications can be realized.

Fundamentals of Pellet-Clad Debonding

191056 | Year 2 of 3

Principal Investigator: R. P. Dingreville

Executive Summary:

This project will enable a new fundamental mechanistic understanding of the complex degradation mechanisms associated with Pellet/Clad Debonding (PCD) through the use of a unique suite of in situ nanoscale experiments on surrogate interfaces, multi-modeling, and characterization of decommissioned commercial spent fuel. Understanding metal/ceramic interfaces' degradation will significantly impact the technical basis related to the safety of high burn-up fuel, a problem of interest to DOE.

High-Resolution Modeling and Measurements in the Arctic

191055 | Year 2 of 3

Principal Investigator: E. L. Roesler

Executive Summary:

This project closes the uncertainty gap between atmospheric in situ measurements of Arctic boundary-layer clouds via sensors strung on a tethered balloon system and atmospheric models by testing different model configurations and resolutions. These prevalent clouds play an important role in the Arctic climate, and improving their representation in climate models will inevitably reduce uncertainty in the Arctic's climate projections, potentially benefitting DOE's energy security mission.

Improved Industrial Control Systems Resilience through Automated Detection and Response

206861 | Year 1 of 3

Principal Investigator: J. M. Henry

Executive Summary:

This project will advance industrial control system (ICS) resilience by developing novel field control device (FCD) indicators for evidence of adversary action that is widely applicable for all FCDs. Complementary work will also identify cyber reaction capabilities that are executed in an autonomous fashion to enable the attenuation of effects from cyber attack on ICS at machine speed. Increased ICS resilience impacts key infrastructure such as the electric grid.

In-Cylinder Diagnostics to Overcome Efficiency Barriers in Natural Gas Engines

200166 | Year 1 of 2

Principal Investigator: M. P. Musculus

Executive Summary:

This project will modify an existing optical diesel engine facility for natural gas (NG) fueling with spark ignition. The goal is to gain missing scientific understanding of end-gas autoignition, or knock, which is critical to the NG engine research and development community for improving fuel efficiency. This understanding will also be useful in developing more advanced NG engine combustion concepts.

Investigating the Chemistry, Physics, Wear and Aging in Rolling Electrical Contact

191053 | Year 2 of 3

Principal Investigator: W. L. Staats, Jr.

Executive Summary:

Twistact technology comprises a novel rotary electrical contact to eliminate the need for rare earth magnets in wind turbines, making wind energy more competitive and directly contributing to US energy independence. To demonstrate that Twistact technology provides the required longevity for wind turbine applications, this project is developing a mechanistic understanding of the electro-tribo-chemistry of extended rolling electrical contact.

Investigation of Novel Glass/Ceramic Composite Electrode Structure for Alkali Ion Batteries

206817 | Year 1 of 1

Principal Investigator: J. P. Koplow

Executive Summary:

The goal of this project is to study two critical aspects of a proposed benign-failure-mode sodium electrode for grid storage batteries: 1) fabrication of a novel ceramic/metal composite electrode structure that ensures benign failure in the event of electrode damage and 2) the feasibility of depositing superionically conductive Na+ ion anti-perovskite amorphous glass (Na2.99Ba0.005ClO) onto a porous ceramic substrate that does not have a matched coefficient of thermal expansion (CTE).

Lithium Oxysilicate Compounds as Stable Analogs for Understanding Li-P-S High Rate Li-Ion Separators: Moving Solid Electrolytes into High Rate Applications

181205 | Year 3 of 3

Principal Investigator: C. A. Apblett

Executive Summary:

This project developed the basis for forming and characterizing Li-Si-O thin films deposited by physical vapor deposition. These films were analyzed after exposure to Si anode electrolytes and electrochemical cycling to understand the effect of starting film on interface evolution. Understanding the interfacial film formation, how model starting films can affect that formation, and time evolution of the film composition and structure may enable a higher energy density battery.

Multiobjective Optimization of Solar-Driven, Hollow-Fiber Membrane Distillation Systems

180872 | Year 3 of 3

Principal Investigator: T. M. Nenoff

Executive Summary:

The purpose of this project was to develop a scalable predictive performance model for solar-driven, hollow-fiber membrane distillation (SHFMD) systems that can be used to simulate system operation and optimize selection of component size, capacity, and operational characteristics for minimization of the unit cost of water produced, subject to production and performance targets. Project success supports the energy security mission in the areas of climate science and environmental challenges.

Multiscale Multiphysics for Subsurface Science and Engineering of Shale

180869 | Year 3 of 3

Principal Investigator: H. Yoon

Executive Summary:

This project will develop new fundamental mechanistic understanding, experimental characterization, and modeling capabilities to explain poromechanical and flow responses of low permeability rocks with compositional, physical, and chemical heterogeneity. Understanding and predicting fluid-rock interactions in nanoporous geomaterials will significantly impact our nation's ability to sustain subsurface energy security for unconventional resources recovery, geothermal energy recovery, and nuclear waste disposal.

Nanocomposite Barrier Films for Enhanced Thin Film Photovoltaic Stability

180865 | Year 3 of 3

Principal Investigator: E. D. Spoerke

Executive Summary:

Novel polymer-clay nanocomposite thin film photovoltaic (PV) encapsulants offer potentially high rewards, promising improvements in PV reliability, stability, and safety, all critical issues plaguing PV integration into the national electrical energy infrastructure. This project explores the feasibility of this approach, employing scientific study to inform system optimization and address risks associated with using these untested materials.

Novel Microelectromechanical-System-Enabled Nanofracking of Subsurface Minerals

192762 | Year 2 of 3

Principal Investigator: K. L. Jungjohann

Executive Summary:

This project is pioneering the development of unique instrumentation to study the mechanisms of chemical-mechanical fracture in materials by using atomic-scale imaging within an environmental cell. Experimental testing from atomic scale to bulk of chemo-mechanical properties of materials in liquid environments provides useful design rules for enhancing fracture in shale minerals for hydraulic fracturing, and combating stress-corrosion cracking in steel pipes. This research is relevant to DOE's energy security mission.

Novel Zoned Wasteforms for High Priority Radionuclide Waste Streams

200151 | Year 1 of 3

Principal Investigator: C. R. Bryan

Executive Summary:

This project will develop innovative zoned wasteforms, based on a rare class of substances (zirconium tungstates, ZrW2O8, and related materials) that shrink upon amorphization, with radionuclide-rich cores and barren shells that isolate the radionuclide even when core amorphization due to radiation damage occurs. These wasteforms will provide a critical disposal option for hard-to-handle radioactive waste streams containing technetium or weapons-grade plutonium.

Nuclear Power Plant Cybersecurity Discrete Dynamic Event Tree Analysis

191054 | Year 2 of 2

Principal Investigator: T. A. Wheeler

Executive Summary:

This project developed a dynamic cyber risk tool to analyze cyber failure modes and time sequencing of cyber faults, malicious and nonmalicious, and impose those cyber exploits and faults onto a nuclear power plant accident sequence simulator to assess how cyber exploits and faults could interact with a plant's digital instrumentation and control (DI&C) systems. The project enhances nuclear power safety and global security by threat mitigation on network systems.

Optimizing Microgrid Energy Delivery Under High Uncertainty

181202 | Year 3 of 3

Principal Investigator: A. Ellis

Executive Summary:

This project will explore new concepts related to the energy delivery paradigm, whereby large power plants provide only blocks of energy, while distributed energy resources (DER) provide balancing and other ancillary services. The research involves distributed optimization to determine the optimal schedule for distributed energy resources under high uncertainty. This requires advanced stochastic optimization applied to DER unit commitment. Project success is relevant to the energy security mission.

Passive Magnetoelastic Smart Sensors for a Resilient Energy Infrastructure

200169 | Year 1 of 3

Principal Investigator: T. Monson

Executive Summary:

We are developing a novel passive, autonomous microsensor for indirect detection of microamp (μA) currents (< $10/sensor, installed). These wireless magnetoelastic smart sensors (MagSens) can be integrated in close proximity to current carrying conductors and are capable of detecting small changes in their magnetic field via frequency shifts. MagSensors can be used for detection of leakage currents, faults, and asset monitoring to enhance the resilience of energy infrastructure.

Physics of Impinging Water Droplets on Inclined Glass Surfaces

206818 | Year 1 of 1

Principal Investigator: C. K. Ho

Executive Summary:

This project will develop computational models and improved understanding of water droplet dynamics that can improve methods for self-cleaning of photovoltaic modules and mirrors, which will increase overall performance and reduce levelized costs of these renewable energy systems. This will allow greater penetration of renewables for increased sustainability, reliability, and security of our nation's energy infrastructure.

System-of-System Model Development for Evaluating EMP Resilient Grid Mitigation Strategies

206338 | Year 1 of 1

Principal Investigator: J. P. Eddy

Executive Summary:

This project will create a value model for analysis of electromagnetic pulse (EMP) impacts to the electric grid and related infrastructures suitable for use in resilience optimization problems. The ability to optimize EMP mitigation strategies in terms of planning, enduring, and recovering from an EMP event is critical to national security.

Validating Hydrogen Concentration Fields at Crack Tips

186839 | Year 3 of 3

Principal Investigator: J. A. Ronevich

Executive Summary:

This project developed capabilities to examine changes in stress and hydrogen concentrations ahead of loaded crack tips through use of kelvin probe force microscopy. The purpose of measuring hydrogen concentrations near crack tips with high fidelity is to provide data for hydrogen assisted fracture model calibration and validation ultimately improving reliability in structural materials. The project supports missions in nuclear and energy security.

Waste Water for Power Generation via Energy Efficient Selective Silica Separations

191018 | Year 2 of 2

Principal Investigator: T. M. Nenoff

Executive Summary:

Thermoelectric power generation is the largest user of fresh water in the US, at ~500 billion gallons/day which is almost half of all water withdrawn daily. Dissolved silica is ubiquitous in impaired waters, resistant to existing anti-scalants, and difficult to remove from power plant feedwaters. This project developed silica getter materials for bench and scaled-up testing. This research addresses national security missions of domestic energy production, efficiency, and water desalination.

Water Treatment System for Resilient Energy Production

191051 | Year 2 of 3

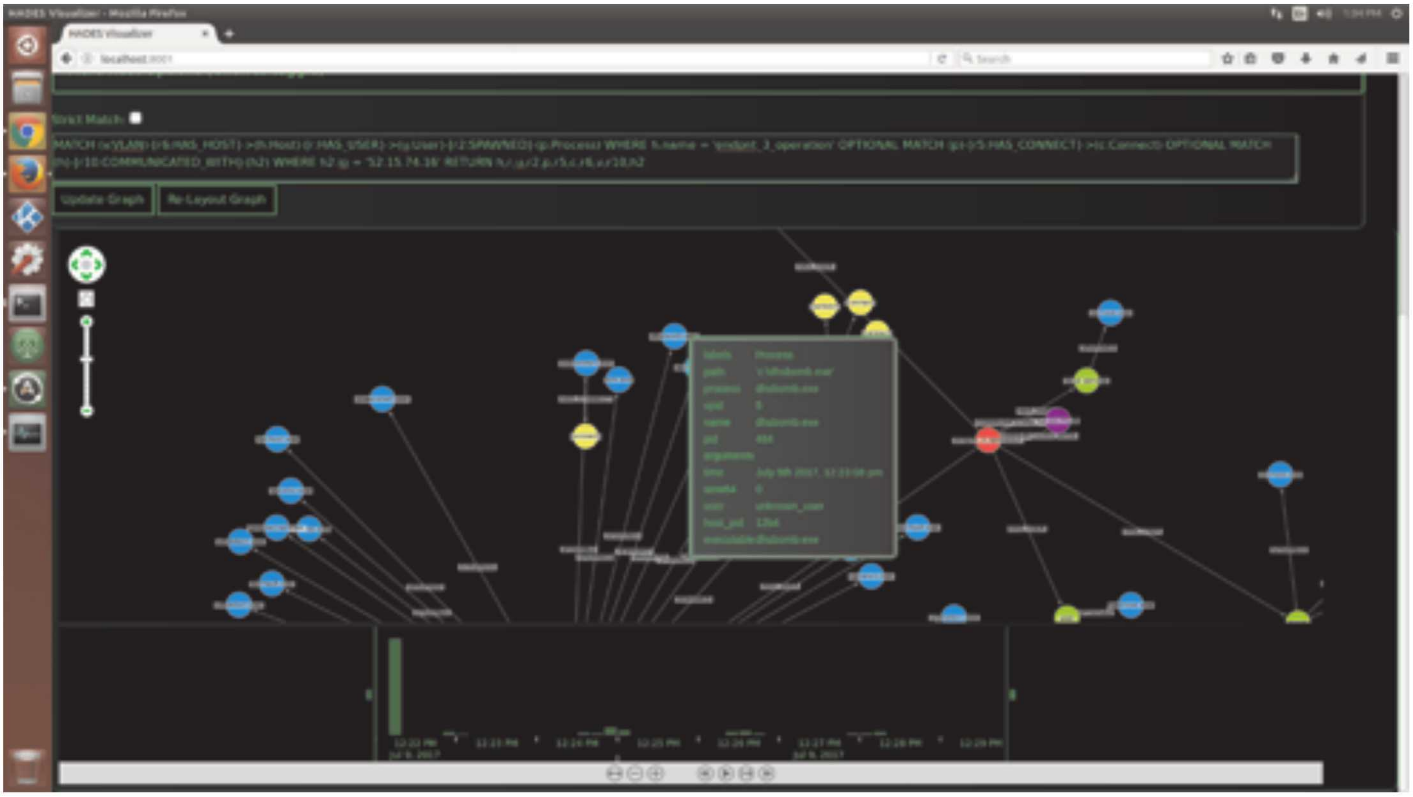
Principal Investigator: L. Biedermann

Executive Summary:

This project will develop chlorine-tolerant, fouling-resistant graphene oxide (GO)/polymer desalination membranes that will reduce the system-level energy cost of desalination and water reuse. This project addresses "What materials ensure robust, scalable membranes" and "How is permeation through laminar GO optimized." Water reuse technologies may potentially be used to support forward deployed warfighters worldwide. Additionally, investing in the research and development of clean water technologies could ultimately improve global stability.

Mission Foundations

GLOBAL SECURITY



Granular data capture, analysis and visualization are key to understanding experimental effects on hosts, networks, and relationships. [Project 191165, Instrumentation Infrastructure for Cyber Emulations]

A vital US national security concern is that various adversaries who want to acquire power, support, and legitimacy are attracted to weapons based on nuclear, radiological, chemical, biological, cyber and explosives threats, or some combination of these threats. As the threat becomes more sophisticated and creative, we must identify effective solutions that mitigate current and future risks. The Global Security IA invests in research that enables creative solutions in international and domestic risk reduction against these threats.

PROJECTS

PROJECTS (continued)

A Novel Approach to Foot and Mouth Disease Early Detection, Epizootic Surveillance, and Differentiating Infection from Vaccination Status

200193 | Year 1 of 3

Principal Investigator: B. Carson

Executive Summary:

This project will develop a new method of quickly developing and producing diagnostic reagents for infectious diseases. Specifically, we will identify antibody targets in bovines that allow diagnosis of foot-and-mouth disease virus infection and vaccination status that are specific to virus serotype. We will adapt the reagents we develop to an inexpensive and readily field-deployable test. If successful, this work will benefit the Department of Homeland Security biosecurity mission.

Airborne Defense against the Small Unmanned Aircraft Systems (UAS) Threat

191152 | Year 2 of 2

Principal Investigator: D. K. Novick

Executive Summary:

The enabling technology, speed, size, and availability of small UAS (sUAS) makes them a rapidly evolving serious threat to national security and critical high security facilities. By moving sensors and precision defense systems airborne, results of our project indicated that we can increase the range and decrease the effect of ground interference, improving detection, tracking, and neutralization of threat UAS while decreasing collateral damage.

Applying Biological Immune-System Concepts to Improve Electronic Biosurveillance System Performance

191183 | Year 2 of 3

Principal Investigator: P. D. Finley

Executive Summary:

This project will improve the ability of national-scale electronic biosurveillance systems to rapidly identify bio-attacks and emerging disease outbreaks. By developing and testing state-of-the-art complex systems and artificial intelligence data analytics methods, this project has documented possibly game-changing improvements in timeliness and specificity of initial alerts for possible bio-weapon events or deadly infectious disease outbreaks.

Arming and Firing System Charge State Determination using Unintended Radiated Electromagnetic Emissions (URE)

191150 | Year 2 of 3

Principal Investigator: J.T. Williams

Executive Summary:

This project is a fundamental investigation into electromagnetic Unintended Radiated Emissions from capacitive discharge firing systems whose results are meant to inform the future development of radiofrequency diagnostic tools for remotely identifying the instantaneous charging state of a firing system. The project may potentially dramatically improve our ability to remotely assess weapons of mass destruction threats and critically inform stabilization, render safe, and consequence management operations performed by DOE, DOJ, and DoD assets.

Automated Generation of Tailored Malware Execution Environments

191162 | Year 2 of 2

Principal Investigator: E. G. Tobac

Executive Summary:

This project's objective was to develop a novel system for quickly and automatically discovering the target environment for a given malware executable, based upon virtual machine introspection (VMI). For cyber defenders dealing with an explosion in the number of new samples of malware, automating the understanding of the behavior of said malware is critical. This work is a first step towards this goal.

Cognitive Information Environments for International Safeguards Inspections

200188 | Year 1 of 3

Principal Investigator: Z. N. Gastelum

Executive Summary:

This project will test how diverse cognitive information environments impact human performance on international nuclear safeguards-like tasks. The project will test accuracy, timeliness, and situational awareness of human subjects in a variety of information environments to further the field of cognitive science and make recommendations about information provision for safeguards inspectors working in the field.

Compressive Optical Physical Unclonable Function for Secure Communication

191185 | Year 2 of 2

Principal Investigator: G. C. Birch

Executive Summary:

The goal of this project is to create a new type of physical unclonable function (PUF) using lensless computational imaging systems. We investigate the design, simulation, and prototyping of such a device. Success would lead to a new type of PUF that is both simple to create and composed of low-cost components. Potential national security applications include sending high consequence commands securely, or integration into trusted systems.

Controlling the Activity of Gene Editing Tools

200186 | Year 1 of 3

Principal Investigator: B. N. Harmon

Executive Summary:

This project will leverage Sandia's experience in computational biology, high-throughput screening and gene editing to meet the need of developing medical countermeasures to new and emerging threats. The innovative screening technology developed can be extended and used for new natural or synthetic threats, which will significantly advance our capability to detect and mitigate chemical and biological dangers.

Dual-Particle Imaging System with Neutron Spectroscopy for Safeguard Applications

180897 | Year 3 of 3

Principal Investigator: T. M. Weber

Executive Summary:

A dual-particle imager (DPI) has been designed that is capable of detecting gamma-ray and neutron signatures from shielded special nuclear material (SNM). The application of stochastic origin ensembles (SOE) to the DPI is presented. This project extends the SOE algorithm to produce spatially dependent spectra and presents experimental results. The DPI is also an effective tool for localizing and characterizing highly enriched uranium.

Efficient and Scalable Modeling of Nontraditional Devices for Emulytics

200189 | Year 1 of 3

Principal Investigator: D. J. Fritz

Executive Summary:

This project will expand the state of the art in emulytics by creating a novel Internet-of-Things description, modeling, and emulation capability. The primary focus will be on providing a scalable non-information technology (IT) communication framework that can support millions of devices communicating with the physical world and IT infrastructure. Successful project completion relates to DOE/NNSA missions in national cyber strategy and could benefit DHS, DoD, and the intelligence community.

Electromagnetic (Optical/Radio Frequency) Signatures Associated with Atmospheric Discharges and Plasma Generation in Explosive Events

195868 | Year 2 of 3

Principal Investigator: R. Tang

Executive Summary:

This project seeks to develop experimental plasma generation and diagnostics methods to increase our understanding of electromagnetic phenomena associated with plasma events from explosive and/or nonproliferation processes and the potential ability to detect these events remotely using plasma-related signatures. It will advance our understanding of explosive characteristics (e.g., how dusty plasma alter signatures) and help mature modeling capabilities through investigation of underlying physics mechanisms.

Enabling Explosives and Contraband Detection with Neutron Resonant Attenuation

186363 | Year 3 of 3

Principal Investigator: M. Sweany

Executive Summary:

This is a high-risk effort focused on detector development leading to better energy resolution and reconstruction errors. This work seeks to enable applications that require precise elemental characterization of materials, such as chemical munitions remediation, offering the potential to close current detection gaps. This work is related to the Department of Homeland Security's Strategic Plan: prevent the unauthorized acquisition or use of chemical, biological, radiological, and nuclear materials and capabilities.

Engineered Materials for Deactivation of Chemical Agents in Non-Aqueous, Non-Corrosive Environments

200196 | Year 1 of 3

Principal Investigator: D. F. Sava Gallis

Executive Summary:

This projects aims to develop chemistries to degrade organophosphates in water-free environments via an iterative feedback loop between materials synthesis and characterization, with molecular modeling and analytical testing. The fundamental understanding of the relationship between materials structural properties and decontamination activity will improve technology for decontaminating sensitive electronics.

Eyes on the Ground: Visual Verification for On-Site Inspection

191161 | Year 2 of 3

Principal Investigator: R. Brost

Executive Summary:

This project seeks to develop tools to assist an International Atomic Energy Agency inspector when visiting a facility. The envisioned tool(s) would take measurements of facility equipment, and then infer semantic information from the measurements. The semantic information would then be used to help answer the inspector's questions of interest. If successful, this work would increase inspector efficiency and could increase safeguards assurance.

Highly Sensitive Atomic Electrometry for Noninvasively Detecting and Diagnosing Electronics

200194 | Year 1 of 3

Principal Investigator: Y. Jau

Executive Summary:

This project aims to understand the foundations for realizing ultrasensitive atomic electrometry to improve electric-field sensing technology, which is highly significant for nuclear security missions. We propose to develop atomic electrometry especially for low-frequency electric-field sensing to greatly improve the accuracy and sensitivity beyond any existing technology that has been reported. This proposed work will also help develop the ultimate detection and diagnostics for completely shielded electronics.

Improved Analytics for Dynamic 3D Security Systems

191160 | Year 2 of 2

Principal Investigator: D. E. Small

Executive Summary:

The current state of implementing physical security systems (PSSs) is problematic, largely due to the high cost of implementing static, fixed sensors within a Perimeter Intrusion Detection and Assessment System. This project developed new computational, volumetric methodologies for evaluating new PSSs designed with autonomous mobile sensing elements having the potential to significantly reduce costs of future PSSs. The project outcomes could benefit efforts in nuclear security and nonproliferation.

Improving Render-Safe Capabilities for National Security from Chemical and Biological Dissemination Devices

191151 | Year 2 of 3

Principal Investigator: A. L. Sanchez

Executive Summary:

This project addresses informational gaps in chemical/biological dissemination devices, specifically, source term data and render safe procedures used by modelers and first responders. Project outcomes will advance experimental data for improved plume modelling performance and render safe techniques, which will enable better predictions for decision makers, decrease time for first responders, and improve consequence management following a release of weapons of mass destruction.

Inferring Proliferation from Supply Chain Signals

200185 | Year 1 of 3

Principal Investigator: N. J. Brown

Executive Summary:

This research will advance ideas from supply chain modeling and social network analysis to develop modeling methods that use sparse and uncertain signals to characterize and understand proliferation networks. In year one, significant progress was made on social network modeling. If successful, the resulting research could benefit the State Department and DOE in support of arms control verification and nonproliferation.

Information Extraction and Logical Reasoning for Derivative Classification Assistance

200187 | Year 1 of 1

Principal Investigator: A. X. Garcia

Executive Summary:

This project aims to address the human-intensive task of derivatively classifying text through research into methods and techniques from areas of natural language processing, logical reasoning, and ontological engineering. Success can lead to impacting the effectiveness and efficiency by which sensitive information is shared across government agencies responsible for national security.

Instrumentation Infrastructure for Cyber Emulations

191165 | Year 2 of 2

Principal Investigator: V. Urias

Executive Summary:

Sandia developed the Emulytics™ analysis to deploy cyber experiments. In order to provide empirical results, there is an exigent need to develop better data gathering (i.e., instrumentation) understanding and techniques to ingest the data. The research will advance cyber analysis-platform modeling technology and provide a novel capability for the analysis of cyber impacts on modeled networks.

Modeling Metal/Metal Compound Combustion for Energetic Material Enhancement

191176 | Year 2 of 2

Principal Investigator: D. J. Allen

Executive Summary:

This project will develop modeling capability for metal enhanced energetic deterrent systems. The development of a predictive modelling capability will significantly reduce the testing burden of new system development and aid in the requirement validation of future research and development systems. Furthermore, modelling can be used to predict effects in environments that are impractical for testing validation, useful in design for both counter terrorism and counter proliferation efforts.

Polarimetry for Extended Persistence and Range in Fog for Infrastructure Protection

191184 | Year 2 of 3

Principal Investigator: J. B. Wright

Executive Summary:

This research will demonstrate that tailored wavelength and polarization selection can provide substantially increased performance in foggy conditions compared to traditional intensity-based techniques. This will involve designing, building, and validating new experimental setups at different wavelengths in Sandia's fog tunnels, which are capable of creating and sustaining controlled fog that can simulate specific fog conditions. Extending optical capability in numerous scattering environments is important for security and situational awareness scenarios.

Polarized Radar for Detection and Automatic Non-Visual Assessment of Unmanned Aerial Systems

200190 | Year 1 of 3

Principal Investigator: M. E. Bratton

Executive Summary:

This project will develop new techniques to automatically detect and classify Unmanned Aerial Systems using polarimetric radar. New hardware configurations and algorithms will be developed to reduce false alarms caused by birds and weather, which can significantly reduce the effectiveness of the radar system. The successful completion of this project could ultimately benefit the NNSA national security missions (nuclear security, energy security), DoD agencies, DHS, and the intelligence community.

Quantifying Uncertainty in Emulations

200191 | Year 1 of 3

Principal Investigator: J. Crussell

Executive Summary:

Emulated testbeds aid in our understanding of large scale cyber systems, yet we have barely begun to understand how well they represent the real world and how much we can rely on them to support our missions. This project aims to discover the usefulness of emulytics for modeling multi-node network phenomena. We will develop a fundamental understanding of the accuracy, and limitations, of these testbeds.

Rapid Automated Pathogen Identification by Enhanced Ribotyping (RAPIER)

191175 | Year 2 of 3

Principal Investigator: M. Bartsch

Executive Summary:

This project seeks to adapt cutting-edge nanopore sequencing technology to rapid broad-spectrum pathogen diagnostics with potential impact to Sandia missions in biodefense and biosurveillance of emerging infectious diseases. In particular, we have developed a novel real-time selective sequencing architecture that we anticipate will dramatically reduce time-to-detection and enhance sensitivity and specificity when identifying and characterizing pathogens in clinical samples.

Sampling-Based Algorithms for Estimating Structure in Big Data

186366 | Year 3 of 3

Principal Investigator: K. M. Matulef

Executive Summary:

This project aims to develop sampling-based algorithms to discover hidden structure in massive datasets. Inferring structure in large datasets is critical for many national security applications. The datasets are so large that traditional techniques are infeasible. We focused on algorithms that use sampling to compute an approximate answer using fewer resources. Cybersecurity benefits greatly from the ability to make better inferences about data based on sampling.

System Theoretic Framework for Mitigating Risk Complexity in the Nuclear Fuel Cycle

191154 | Year 2 of 2

Principal Investigator: A. D. Williams

Executive Summary:

This research aimed to research system theoretic approaches and develop dynamic risk assessment frameworks for understanding risk complexity in the nuclear fuel cycle. Specifically, the project established complex system models and 3S (safety, security, and safeguards) risk mitigation strategies for international spent nuclear fuel (SNF) transportation and demonstrated how to assess, manage, mitigate, and eliminate such complex risks.

Using Data Science to Improve Theorems of Human Performance in National Security Domains

191166 | Year 2 of 2

Principal Investigator: D. J. Stracuzzi

Executive Summary:

This project will update theories of human visual search by analyzing data from mission experts to identify differences between theory and practice. The goal is to provide principles for engineering analyst systems with large visual inspection components. Understanding the nature and boundaries of human performance in national security domains is critical to engineering effective interfaces between users and data. Success will impact homeland security, defense, intelligence analysis, and cybersecurity.

Xenon Atom Trap Trace Analysis Enabled by Optical Isotopic Enrichment

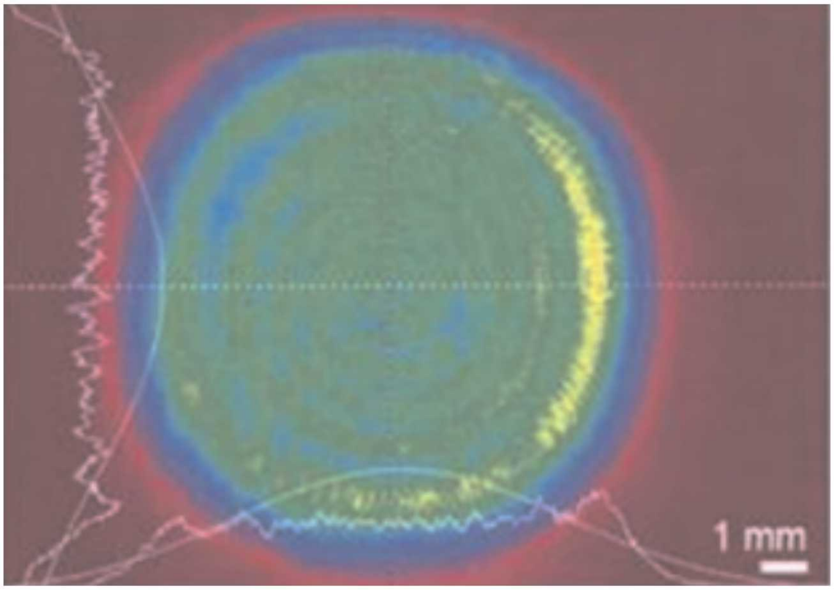
200195 | Year 1 of 3

Principal Investigator: T. J. Kulp

Executive Summary:

This project will develop a new method to allow Atom Trap Trace Analysis to be useful for the quantitative analysis of noble gas isotopes whose abundances are extremely low (< 1 part in 1013). This will be accomplished by generating an isotope-selective method of atomic concentration. The method being pursued is selection via optical deflection. If successful, this project could benefit the NNSA's nuclear nonproliferation mission.

NUCLEAR WEAPONS



The figure above is a Continuum Powerlite output beam spatial profile. [Project 180926, Direct Mechanical Ignition of Reactive Materials for Improved Safety and Performance]

The primary goal of the Nuclear Weapons (NW) Investment Area is to support investments in leading-edge science and the incubation of new technologies and capabilities. These investments are intended to promote innovation in our core products to meet future mission needs and to develop new tools and technologies for design, qualification and surveillance with an overarching goal of improving cost effectiveness, agility, and assurance throughout the life cycle.

PROJECTS

NUCLEAR WEAPONS

A Silicon/III-V Photonics Platform for Optical Data Communications and High Functionality Photonics

200257 | Year 1 of 3

Principal Investigator: A. L. Lentine

Executive Summary:

The goal of this work is to develop a silicon/III-V photonics platform for optical data communications and high functionality photonics. The development of a platform that supports multiple concurrent optical busses with on-board optical processing, reconfigurable routing, and secure communications would have significant impacts to system agility and assurance for numerous national security applications.

Additive Manufacturing of Metallic Components by Laser Powder Forming

181204 | Year 3 of 3

Principal Investigator: C. W. San Marchi

Executive Summary:

The purpose of this project was to develop a quantitative set of benchmarks for materials performance of directed-energy deposited (DED) austenitic stainless steels. These benchmarks include microstructural characteristics and mechanical properties, including strength and fatigue performance. This baseline understanding provides engineers with quantitative information that can be used for materials selection and integration of additive manufacturing into the deployment of advanced technologies.

Additively Manufactured Shock Absorbing Engineered Materials

193407 | Year 2 of 3

Principal Investigator: N. Leathe

Executive Summary:

This project focuses on utilizing additive manufacturing for the development of shock absorbing materials to offer conformal protection in extreme shock events. This capability could facilitate safety enhancements in NNSA systems and in myriad areas ranging from aerospace and defense to the automotive industry. Additionally, the development and calibration of computational models to predict material performance enables iterative design prior to product fabrication.

Advanced Positional Awareness Employing Xtremely Cold Atoms (APEX)

200256 | Year 1 of 3

Principal Investigator: G. Biedermann

Executive Summary:

This project will investigate a new approach to guiding matterwaves for precision inertial measurements with atom interferometers. The guiding of matterwaves holds promise for improved navigation and positional awareness for future nuclear weapon and DoD systems, but the realization has been challenging. By using a combination of theoretical modeling and experimentation, we will explore new techniques for this purpose.

Agile Component Design through Integrated Diagnostics and Computational Optimization

200243 | Year 1 of 3

Principal Investigator: A. Grillet

Executive Summary:

This project will develop agile design tools for vacuum arc sources through model optimization and experimental discovery of the role of surface adsorbates on the initiation of electrical breakdown. Electrical breakdown is key to the operation of several nuclear weapon components but also a critical failure mechanism for others. The new agile design tools developed will enhance future stockpile modernization programs.

Bridging the Gap: Evaluating Compatibility and Reliability of Interfaces between Additively Manufactured and Conventional Gas Transfer System Components

191227 | Year 2 of 3

Principal Investigator: K. Allen

Executive Summary:

This project will characterize the dynamic interfaces formed between machined additively manufactured (AM) surfaces and conventional hardware following explosive valve actuation and resistance forge welding, two gas transfer system processes with severe sliding contact environments. This characterization will aid in understanding the interactions at interfaces between AM and conventional parts and assess AM suitability for nuclear security applications.

Creating Robust and Secure Free-Space Optical Systems for Information and Power Transmission in Confined Environments

191234 | Year 2 of 3

Principal Investigator: P. C. Galambos

Executive Summary:

This project seeks to create free-space optical (FSO) links between electrically isolated subsystem modules, and design/model a novel radiation-hard, high power photodiode. We will demonstrate the link using an FSO transceiver to send/receive foundation bus messages between arming/fuzing/firing modules undergoing vibration. This work benefits national security by providing an enhanced surety optical link (no cables/connectors) enabling agile modular weapon systems.

Defect Characterization for Material Assurance in Metal Additive Manufacturing

180928 | Year 3 of 3

Principal Investigator: B. H. Jared

Executive Summary:

Additive manufacturing offers opportunities to design structures inaccessible through conventional manufacturing. Before adoption in national security applications, questions regarding the reliability and performance of additive metals must be answered. This project coupled material characterization with experimental and computational tool sets to establish a scientific foundation needed to develop a pathway for the qualification and acceptance of additive nonnuclear weapon components.

Direct Mechanical Ignition of Reactive Materials for Improved Safety and Performance

180926 | Year 3 of 3

Principal Investigator: C. Yarrington

Executive Summary:

This project will develop fundamental understanding of direct ignition of reactive nanolaminates through experimental characterization and development of computational shock physics and thermal reaction models. A working knowledge of mechanical ignition will result in simpler weapon component designs that reduce hazardous handling and manufacturing steps, improve performance, and significantly reduced material and manufacturing costs.

Dynamic Strain Aging in Additive Manufactured Alloys and Components

200248 | Year 1 of 3

Principal Investigator: B. R. Antoun

Executive Summary:

This project will expand the environmental and application space for additive manufactured parts by improving our fundamental understanding of microstructurally driven dynamic strain aging that affects material response. The project will develop temporally extreme measurements and advanced microscopy methods focused on nuclear weapon abnormal environments, used to develop dislocation and physics-based modeling capability that bridges length scales from subgrain to continuum level.

Investigation of 10-28 nm Commercial Integrated Circuits for use in Nuclear Weapon Radiation Environments

200260 | Year 1 of 3

Principal Investigator: N. A. Dodds

Executive Summary:

This project will investigate the response of 10-28 nanometer commercial integrated circuits to radiation environments that are of interest for national security applications. These advanced technologies have more processing power than older technology generations, but their reliability in radiation environments is not well understood. Experiments and simulations will characterize their reliability margins and give insight into the radiation-induced failure mechanisms.

Mechanical Communication using Piezoelectric-Magnetoelastic Transducers

201545 | Year 1 of 3

Principal Investigator: I. F. El-Kady

Executive Summary:

The proposed approach is a novel innovative concept for information transmission that has never been demonstrated before. Major fabrication and experimentation risks exist pertaining to mechanical impedance matching the actuated signals to the transmission medium. Successful demonstration will lead to a new paradigm for safety, where a sensor validates the correct configuration of modules or improper assembly/damage.

Microenergetic Logic for Safety Applications

180930 | Year 3 of 3

Principal Investigator: A. S. Tappan

Executive Summary:

This project advanced experimental characterization and modeling capabilities for using vapor-deposited explosives for safety applications. This included developing techniques for studying the geometric effects on small scale explosive behavior and utilizing these results to enhance our modeling capabilities.

Multi-Material Additive Manufacturing for Trusted Ceramic Packages with Embedded Capacitors

191232 | Year 2 of 3

Principal Investigator: S. S. Mani

Executive Summary:

This project is developing and investigating methods to fabricate custom multimaterial electronic packages to include capacitive, conductive, and insulative materials. Direct write additive manufacturing (AM) using multiple materials offers the ability to create novel structures and apply materials in an atypical fashion onto traditional and nontraditional surfaces while providing significant innovation opportunities for microsystems, firesets, and neutron generators for nuclear weapon applications.

Nanocomposite Films with Tunable Physical Properties as Robust Corrosion Barriers

200241 | Year 1 of 3

Principal Investigator: E. J. Schindelholz

Executive Summary:

This project will develop a new class of low-cost conformal corrosion barrier coatings via layer-by-layer (LBL) technology with coating architecture adaptable to chemical/physical function requirements. We will test the hypothesis that LBL nanocomposites impart exceptional corrosion resistance through charge transfer and mass transport inhibition. Success will provide an implementable pathway to increase assurance for stockpile materials and components.

Non-Destructive Evaluation for Encapsulated Component Qualification

200254 | Year 1 of 3

Principal Investigator: A. L. Dagel

Executive Summary:

This project will develop a new nondestructive inspection technique with high sensitivity for low density materials. Foams, fillers, and epoxies serve important roles in preventing critical failure modes in nuclear weapons components due to effects such as thermal fluctuations, shock, or high voltage discharge. This project will enable nondestructive inspection for defects including voids, delamination, and inhomogeneities in these materials.

Rectenna Thermal Power Supply

200245 | Year 1 of 3

Principal Investigator: P. Davids

Executive Summary:

The purpose of our research is to design, fabricate, and demonstrate a new thermal power supply based on direct rectification of infrared radiation from a thermal source. This new form of radiative thermoelectric transduction represents a radical departure from conductive heat transfer and conversion for thermal power supplies and could dramatically reduce cost, improve safety, and provide an alternative source of power for nuclear weapon applications.

Targeting a 100X Reduction from Design to Analysis: An Agile Workflow for Stronglink Design

200242 | Year 1 of 2

Principal Investigator: J. W. Foulk, III

Executive Summary:

The model development and analysis of a stronglink design, dominated by mesh generation, can take up to six months. We are developing new capabilities in higher-order tetrahedral elements, meshing, and contact that could reduce design iteration by over two orders of magnitude. Relieved from the time-intensive burden of discretization, engineers will be able to form and test hypotheses to realize affordability, agility, and assurance for new stronglink designs.

Trust Verification Platform (Trust of Third Party Digital Design Tools using Formal Methods)

180931 | Year 3 of 3

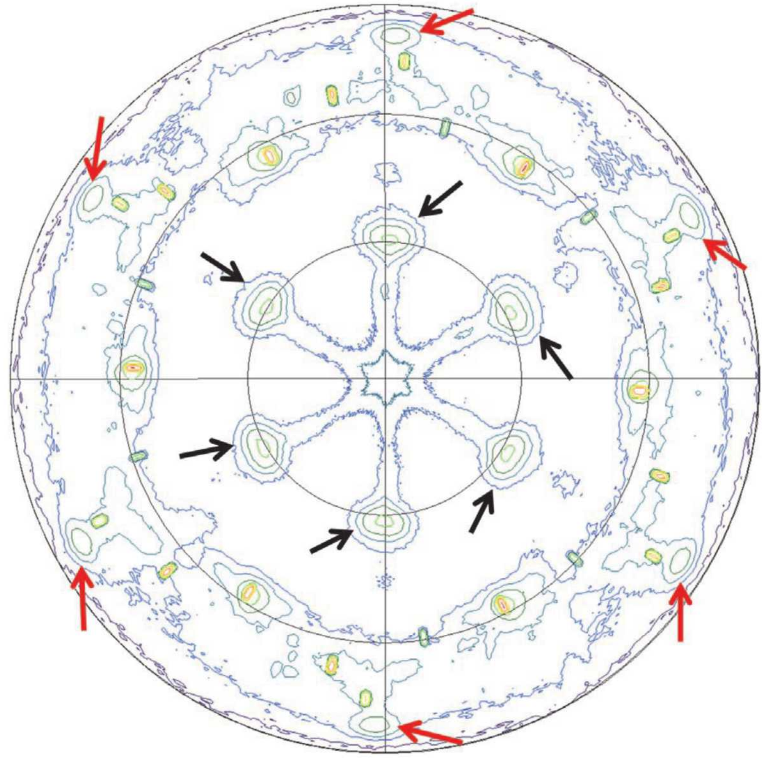
Principal Investigator: T. Mannos

Executive Summary:

Software used to develop critical government microelectronics can be an attractive target for an adversary. We need a way to trust that the circuits designed by these tools are what the designer intended. The Trust Verification Platform (TVP) provides a methodology to perform end-to-end formal equivalence and static timing analysis, closing gaps in the design and verification of integrated circuits.

GRAND CHALLENGES

The figure on the right shows the pole figure for 700 nm thick BGaN film grown on AlN-on-sapphire template. The (3 1 1) and (3 −1 −1) zinc-blende BGaN reflections are clearly present at chi angles of ~30° (black arrows) and ~81° (red arrows), respectively. [Project 180884. Revolutionary Size, Weight, and Power Capability from Ultra-Wide Bandgap Power Electronics]



Grand Challenges are bold, game-changing ideas with the potential for enormous impact to the security of the nation through significant advances in science and engineering. Grand Challenge projects are expected to drive the future of Sandia by providing new directions, capabilities, and solutions and to provide long-term impact to multiple missions and programs. These projects result in a long-term ST&E legacy for Sandia from breakthrough scientific discoveries through development of unique and differentiating technical capabilities. These projects are multimillion dollars in size and utilize multidisciplinary teams, often including external collaborators.

PROJECTS

Changing the Engineering Design and Qualification Paradigm in Component Design and Manufacturing (Born Qualified)

191144 | Year 2 of 3

Principal Investigator: R. A. Roach

Executive Summary:

This project will revolutionize design and manufacturing by combining additive manufacturing techniques with deep materials and process understanding to transform qualification paradigms for materials, designs, and ultimately components for nuclear weapon systems. Margins to requirements, limits of physics, and process uncertainties will be known at birth, and product changes can be swiftly propagated through the design-manufacture-sustainment chain to assess impacts and revolutionize product realization.

Enabling Modular Architectures with Radiation-Hard Bus-Based Power Delivery

200184 | Year 1 of 3

Principal Investigator: J. C. Neely

Executive Summary:

This project will develop a new radiation-hard power conversion and distribution architecture for select space and defense applications. Developing radiation-hard power conversion components and circuits that also support superior efficiency and power density capabilities will greatly enhance the nation's ability to iterate and optimize systems that are constrained by volume, weight, and radiation environment specifications.

Hardware Acceleration of Adaptive Neural Algorithms for Dynamic and Intelligent Threat Detection

180885 | Year 3 of 3

Principal Investigator: C. D. James

Executive Summary:

This project has developed neural algorithms and hardware for national security applications in image processing and cybersecurity. Given that the effectiveness of machine learning algorithms can diminish over time in real-world environments due to noise and drift, our team has generated technologies that support continual adaptation of algorithms. Also, we have built hardware components for accelerating machine learning algorithm training and inference.

NanoCRISPR: A Revolutionary Therapeutic Platform for Rapidly Countering Emerging and Genetically Enhanced Biological Threats

190245 | Year 2 of 3

Principal Investigator: D. Y. Sasaki

Executive Summary:

The goal of this project is to develop a rapid, cost-effective, universal countermeasure for biological pathogens (e.g., Ebola, Zika, Burkholderia) based on the recently discovered Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) gene-editing technology and Sandia-developed technology for efficacious in vivo delivery. This project expands Sandia's national security biodefense applications based on CRISPR technology and further develops our understanding of interfacial interactions between engineered nanomaterials and biology.

Revolutionary Size, Weight, and Power Capability from Ultra-Wide-Bandgap Power Electronics

180884 | Year 3 of 3

Principal Investigator: R. Kaplar

Executive Summary:

This project laid the materials science and device physics foundation for next-generation ultra-wide-bandgap (UWBG) semiconductor devices for revolutionary advancements in power electronics to benefit diverse DOE and NNSA national security applications. It verified that UWBG materials and devices are viable and can enable orders-of-magnitude improvement in size, weight, and power density for power converters, including demonstrating the highest bandgap semiconductor devices ever fabricated.

Smart Sensor Technologies

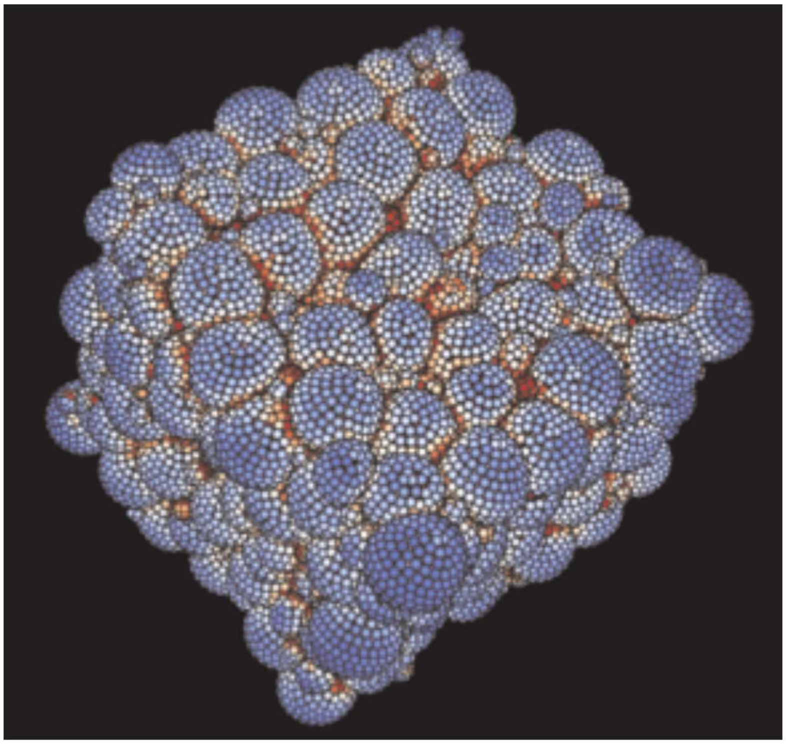
189614 | Year 2 of 3

Principal Investigator: D. W. Peters

Executive Summary:

Sensing is vital for many tactical and strategic applications—alerting warfighters or decision makers to the occurrence of an event. For infrared sensing, a critical tool for national security, the physical sensor is the limiting factor in improving data delivery, as current infrared detectors approach their noise floor. We address this need—offering fast, agile spectral bandwidth control, while simultaneously offering increased signal to noise well beyond the current limit.

The figure to the right shows a peridynamic simulation of compacted and sintered copper powder. The new analysis method combines residual mechanical stress, surface energy, contact, temperature changes, densification, and shape changes of grains. [Project 206533, Peridynamic Theory as a New Paradigm for Multiscale Modeling of Sintering]



The Exploratory Express Investment Area provides a mechanism for maturation and testing of a novel idea that has potential to become very important for one of Sandia's strategic missions. This Investment Area was initiated to provide a vehicle to explore novel ideas that are generated by researchers spontaneously through the year rather than in response to a specific proposal call. Proposals may be submitted throughout the year with the selection of funded projects occurring three times each year. A small amount of funding (≤ $100K) is provided to Exploratory Express projects over a period of no more than a few months to address one critical question as the basis for determining whether the idea is desirable for Sandia to pursue more thoroughly to mature its strategic importance for Sandia's national security missions.

PROJECTS

PROJECTS (continued)

A Hydrogen and He Isotope Nanoprobe

201112 | Year 1 of 1

Principal Investigator: B. L. Doyle

Executive Summary:

This project proved the feasibility that high energy electrons from a transmission electron microscope (TEM) can potentially recoil and subsequently detect Hydrogen (H) and Helium (He) isotopes with nanometer resolution. A TEM-based H/He-isotope nanoprobe would be an important future tool to help ensure the reliability, safety, and upgrading of the US stockpile.

Achieving Optimum Performance in Soft Ferromagnetic Alloys through Additive Manufacturing

206537 | Year 1 of 1

Principal Investigator: A. Kustas

Executive Summary:

This project demonstrated the laser engineered net shaping (LENS) additive manufacturing (AM) process on model soft ferromagnetic alloys and established preliminary process-structure-properties relationships. As a novel processing technology, LENS was shown to overcome the processing issues of conventional thermomechanical methods to enable bulk production of next generation magnetic alloys of high efficiency for use in critical electromagnetic components related to the nuclear security mission.

Alkylammonium Lead-Halide Perovskite for Combined Fast Neutron Detection and Gamma-Ray Spectroscopy

200179 | Year 1 of 1

Principal Investigator: P. L. Feng

Executive Summary:

This project seeks to develop a dual-mode gamma ray and fast neutron detector that functions as a scintillator and/or semiconductor. This represents a presently unmet need for critical nuclear nonproliferation efforts, as relevant to the global nuclear detection architecture and domestic homeland security, respectively.

Artificial Diffusion: Rapid Disease Detection by Driven Magnetic Polybeads

195557 | Year 2 of 3

Principal Investigator: J. E. Martin

Executive Summary:

The goal of this project is to enable rapid disease detection by significantly reducing the incubation time required for immunoassays based on magnetic polybeads. Our approach is to use multiaxial magnetic fields to translocate the polybeads throughout the solution to increase the antigen binding rate. Increasing the assay throughput will enable a faster response to a disease outbreak and is of importance to the biodefense national security mission.

CPHASE Gate with Rydberg Atoms

204390 | Year 1 of 1

Principal Investigator: G. Biedermann

Executive Summary:

We demonstrate a controlled-phase gate approach to entangling neutral atoms using a tunable, Rydberg-dressed interaction. Previous approaches utilize a "dipole blockade", which lacks arbitrary phase control and extensibility to beyond two atoms. We study major error mechanisms that limit the quality of the entangling interaction and chart a definitive path to high-quality entanglement for sensing and other quantum technologies.

Carbon Monofluoride-Based High Voltage Thermal Battery Cathode

204392 | Year 1 of 1

Principal Investigator: B. Perdue

Executive Summary:

This project will develop a thermal battery cathode based on lithium carbon monofluoride (Li-CFx) chemistry that is safer, higher in capacity, and possesses higher voltage than the thermal battery cathodes used presently. By modifying the electrode processing of CFx to make it compatible with molten salt thermal battery technology, we expect to develop a replacement for current thermal battery cathodes. This work is relevant to the nuclear security mission.

Cell Gels - Building Reversible Networks from Boronic Acid and Cell Membrane Chemistry

201319 | Year 1 of 1

Principal Investigator: B. H. Jones

Executive Summary:

This project demonstrates proof of concept of cell-crosslinked networks based on covalent binding of boronic acid polymers to cell membrane saccharides. This approach was tested as an encapsulation strategy for mammalian cells, where it was found to enable preservation of lymphocytes under ambient conditions. These results are expected to have important implications in enabling whole cell biosensors for pathogen and toxin detection.

Detecting Defects in 3D Integrated Devices with Magnetic-Field Probe

201095 | Year 1 of 1

Principal Investigator: P. Tangyunyong

Executive Summary:

The viability of a new approach based on a dynamic magnetic field probe to detect defects in 3D-integrated devices was assessed in this project. Techniques that can effectively detect defects in these 3D devices will give agencies such as DoD and DOE a powerful, new tool to prescreen internally and externally procured microelectronic parts.

Efficient, Predictive Tomography of Multi-Qubit Quantum Processors

201879 | Year 1 of 1

Principal Investigator: R. J. Blume-Kohout

Executive Summary:

This project will prototype a new way to characterize and debug multi-qubit quantum processors. This approach is based on efficient, sparse models for error-producing noise. In addition to conceptual development, this project will apply prototype techniques to characterize an 8-qubit Rigetti Computing processor. (Rigetti Computing is a new cooperative research and development agreement partner). Success will provide the characterization breakthrough needed to support continued rapid development of many-qubit quantum computers.

Engineering Microbial Assassins to Target Bacterial Pathogens

201876 | Year 1 of 2

Principal Investigator: A. Ruffing

Executive Summary:

Bacterial pathogens represent a substantial threat as weapons of bioterrorism and pose unique challenges with regard to large-scale treatment of the infected population and the decontamination of large environmental areas. In this project, we investigated the use of contact-dependent inhibition (CDI) systems to develop engineered 'microbial assassins' for selective killing of a target bacterium.

Evaluating the Capability of High Altitude Infrasound Platforms to Cover Gaps in Existing Networks

206542 | Year 1 of 1

Principal Investigator: D. Bowman

Executive Summary:

This project fielded the world's first low frequency microphone network in the stratosphere. Sound from a ground-based explosion and colliding ocean waves was recorded on four lightweight sensors lofted using solar powered hot air balloons. This is the first step towards persistent geophysical acoustic sensing systems in the atmosphere of Earth and is relevant to understanding the signals generated by chemical and nuclear explosions.

Extending Hypersonic Diagnostics to the Third Dimension

204405 | Year 1 of 1

Principal Investigator: D. R. Guildenbecher

Executive Summary:

A plenoptic camera uses a microlens array to enable 3D imaging from a single snapshot. This work notably extends potential application of plenoptic imaging at Sandia by expanding both the measurement distance and magnification. This is necessary to enable imaging within harsh environments (e.g., flames and energetics) and facilities such as Sandia's hypersonic wind tunnel.

Fingerprinting Microstructural Controls on Larger-Scale Deformation and Fluid Flow in Porous Media

204941 | Year 1 of 1

Principal Investigator: J. E. Heath

Executive Summary:

This project investigated novel applications of topological data analysis to the geosciences. Using persistent homology, we developed accurate digital 3D rock microstructure from noisy x-ray images, and characterized seismic events such as underground explosions and earthquakes. National security, energy security, and resource management will benefit from accurate characterization of seismic events and subsurface rock properties.

Hydrothermal Sintering of Coordination Polymers for High Energy Density Dielectrics

204400 | Year 1 of 1

Principal Investigator: L. Appelhans

Executive Summary:

Coordination polymers (CPs) are hypothesized to be attractive materials for dielectric applications, but processing into forms conducive to dielectric characterization is challenging. In this study, the processing of CPs to form dense samples for dielectric characterization is explored. Enabling preparation of dense CP monoliths will open a new class of materials to evaluation and application as high energy density dielectrics.

In Situ Battery Spectroscopy: A Novel Approach to Investigate Unmodified Working Batteries

206541 | Year 1 of 1

Principal Investigator: E. G. Sorte

Executive Summary:

We investigated lithium (Li) nuclear magnetic resonance on electrochemical systems with the goal of observing electrolyte degradation of Li ion batteries in the stockpile. The research performed under this project aimed to develop new technologies for spectroscopic investigation that would impact Sandia's capability to optimize current energy storage systems and aid in the development of new battery chemistry schemes.

Increasing Yield of Actionable Information from Observational Human Subjects Studies

204404 | Year 1 of 1

Principal Investigator: L. Hund

Executive Summary:

This project applied statistical causal inference methodologies to answer questions about factors impacting susceptibility to email phishing and factors impacting image classification accuracy. This demonstrates the potential impact of a causal inference framework for human subjects research in the homeland security mission space and for predictive assessments in the nuclear weapons mission space.

Peridynamic Theory as a New Paradigm for Multiscale Modeling of Sintering

206533 | Year 1 of 1

Principal Investigator: S. A. Silling

Executive Summary:

We investigated a new way of computationally modeling the sintering process. The model is based on the peridynamic theory of mechanics and uses a high-fidelity, 3D representation with a few hundred nodes per grain. The model successfully reproduces the key features of sintering, including densification, the evolution of microstructure, and the occurrence of random defects in the sintered solid. These accomplishments are relevant to the nuclear weapons security mission.

Quantum Frequency Conversion in Lithium Niobate Microsystems

203538 | Year 1 of 1

Principal Investigator: M. Eichenfield

Executive Summary:

Cryogenically cooled computing concepts are driving the need for efficient transfer of large datasets into/out of cryostats.This project will develop a new architecture for converting the frequency of optical pulses down to the single photon level and with quantum fidelity. This supports development of computers employing superconducting electronics and also eventual linking into a network, over optical fiber, multiple small quantum computation, and communication devices operating at different frequencies.

Renewable Hydrogen Production via Thermochemical/Electrochemical Coupling

204724 | Year 1 of 2

Principal Investigator: A. Ambrosini

Executive Summary:

The goal of this project was a demonstration of a coupled electrochemical/thermochemical reactor, utilizing a proton-conducting membrane to separate hydrogen, to renewably produce hydrogen from steam utilizing solar energy. This would provide a game-changing path towards conducting thermochemistry at lower temperatures, resulting in a high efficiency solar-to-hydrogen process, which will decrease the cost and scale to impactful sizes, enhancing and securing America's energy future.

Scalable Track Detection in Synthetic Aperture Radar Coherent Change Detection Images

200178 | Year 1 of 1

Principal Investigator: J. G. Chow

Executive Summary:

Synthetic aperture radar coherent change detection images exhibit subtle surface changes such as those created by vehicles. These changes are indicators of activity that are valuable to law enforcement and defense/intelligence missions. Current algorithms do not effectively connect tracklets or are computationally expensive. We present a novel, scalable approach using Deep Learning to make track detection practical on large images.

Temporal Cyber Attack Detection

201113 | Year 1 of 1

Principal Investigator: J. B. Ingram

Executive Summary:

This project investigated the use of temporal generative models to learn cyber attack graph representations and automatically generate data for experimentation and evaluation. Training and evaluating cyber systems and machine learning models requires significant, annotated data, which is typically collected and labeled by hand for one-off experiments. Automatically generating such data helps derive/evaluate detection models and ensures reproducibility of results that would be useful for cyber defense analysts.

Testing the Possibility of Magnetic Contrast Imaging Based on Circular and Linear Dichroism using Photoemission Electron Microscopy

206536 | Year 1 of 2

Principal Investigator: T. Ohta

Executive Summary:

The project's goal is to show proof-of-concept of magnetic circular dichroism-photoemission electron microscopy using 213 nanometer wavelength pulsed laser. Our results demonstrate the feasibility of in-plane and out-of-plane magnetic imaging with the limitations in the resolution and measurement time. The knowledge of magnetic domain behaviors is among the fundamental aspects for materials and nano science research, and an important factor for controlling variability of magnetic materials for future computing applications.

Tunable Impedance Spectroscopy Sensors via Selective Nanoporous Materials

204391 | Year 1 of 1

Principal Investigator: T. M. Nenoff

Executive Summary:

This project will develop an electrical read-out sensing device that is highly selective under ambient conditions for particular gas(es) in the environment. The ability to sense and identify individual gases from the complexity of the environment requires highly selective materials. Potential applications are relevant to environmental science, DoD and NNSA nuclear security missions.

Validation of Electron-Photon-Phonon Interaction Model for Laser-Triggered Sprytron

206538 | Year 1 of 1

Principal Investigator: C. H. Moore

Executive Summary:

This project will implement a first-principle treatment of electron-photon-phonon interaction physics and compare the model to existing experimental data. The model will allow systematic engineering design study of optically triggered switches which are expected to have improved performance, reliability, and lifetime over conventional switches. The physics investigated apply to any plasma with significant self-radiation (e.g., streamers near surfaces). Successful completion will reduce risk important in the development of nuclear weapons.

UNPUBLISHED SUMMARIES

For information on the following FY 2017 LDRD Projects, please contact the LDRD Office:
Laboratory Directed Research and Development
Sandia National Laboratories
Albuquerque, NM 87185-0359

Project	Title
180845	Hyperspectral Hypertemporal Database for Predictive End-to-End Remote Sensing Tool and Signature Simulation
180852	An Ultra-low Size, Weight, and Power Multi-Mission Bi-Static Sensor
180929	Additive Manufacturing of Porous Materials
190971	Green Monopropellant System Design and Characterization for Threat Signature Analyses
190974	Optical Technology
190976	Patterns of Life Algorithm Development via Semantic Graphs
190989	Creating Data for Validating Machine Learning Methods
190994	Shot Noise Limited Imaging with Lock-In Based Focal Plane Arrays
190997	Assessment of Non-Traditional Phenomenologies for Proliferation Detection
190998	Microscale Transient Detection
191000	Advanced Materials and Devices for Communications
191005	Development and Demonstration of Alternative Precision Navigation Capabilities in GPS-Denied Environments
191006	Understanding Photon / Free Carrier Interaction in Low Vapor Pressure Signals on Ultra-Thin Silicon Integrated Circuits
191229	Advanced Neutron Generator
191239	Adjoint-Based Methods for Optimization and Uncertainty Quantification in Particle Transport
200013	Exploring Active Metal Spectroscopic Emissions in Explosive Detonations for Improved Weapon Discrimination
200018	Assessment of Post-Quantum Cryptographic Algorithms
200019	Featureless Radio Frequency/Microwave Structures
200058	Landscape Monitoring using High-Resolution Remotely Sensed Imagery
200061	Ionospheric Impacts on Space-Based Radars: Characterization and Mitigation
200062	Assessing Novel Applications of Magneto-Optical Kerr Effect Microscopy (MOKEM)
200064	Automated Analysis of Data Structures for Program Understanding
200068	Understanding the Scientific Basis Behind Assumptions in Aerothermal Modeling
200074	Visible Atmospheric Processing using Optical-Flow Routines
200115	Low Cost, Large Area Neutron Sensor
200227	Additional Processing of Commercial Fin Field Effect Transistor Devices and their Radiation Properties
200253	Novel Materials to Enable Future Weapon Architectures
201234	Can IBM Watson be Taught to be a Nonproliferation Analyst Tool?

AWARD DESCRIPTION	LDRD CONTRIBUTION
R&D 100 Award, *R&D Magazine*: High-Fidelity Adaptive Deception and Emulation System (HADES) Platform: *Vincent Urias*	Project 191165, "Instrumentation Infrastructure for Cyber Emulations"
R&D 100 Award, *R&D Magazine*: Ultra-Wide Bandgap Power Electronic Devices: *Bob Kaplar*	Project 180884, "Revolutionary Size, Weight, and Power Capability from Ultra-Wide-Bandgap Power Electronics," and others
R&D 100 Award, *R&D Magazine*: The SolidSense "Gas Analyzer on a Chip:" *Fernando Garzon*	Project 180835, "Microsensor Arrays for Energy Efficiency, Emission Monitoring and Explosives Detection"
2017 Presidential Early Career Award for Scientists and Engineers (PECASE): *Alan Kruizenga*	Project 157145, "Fluid Flow Measurement of High Temperature Molten Nitrate Salts"
2017 Presidential Early Career Award for Scientists and Engineers (PECASE): *Stephanie Hansen*	Project 173104, "New Capabilities for Hostile Environments," and others
Cyril Stanley Smith Award, Minerals, Metals and Materials Society: *Stephen Foiles*	Project 165825, "The Role of Grain Boundary Energy on Grain Boundary Complexion Transitions"
Emerging Leader Award, Society of Women Engineers: *Kelly Hahn*	Project 173104, "New Capabilities for Hostile Environments," and others
Prism Award, Society of Women Engineers: *Leslie Phinney*	Project 171054, "Revisiting the Applied Mechanics Paradigm: Multiscale Modeling of Transport Processes in Complex Materials," and others
Richard M. Fulrath Award: American Ceramic Society: *Jon Ihlefeld*	Project 180923, "Emergent Phenomena in Oxide Nanostructures"
Life Time Achievement Award: International Sol-Gel Society: *Jeff Brinker and others*	Project 190960, "Modular Abiotic/Biotic Systems (MABS) for Understanding and Directing Biological Function"
Optical Society Fellow: *Hope Michelsen*	Project 173094, "Measurements and Modeling of Black Carbon Aerosols in the Arctic for Climate-Change Mitigation," and others
American Physical Society Fellow: *Andrew Landahl*	Project 152501, "AQUARIUS: Adiabatic Quantum Architectures in Ultracold Systems"
American Physical Society Fellow: *François Léonard*	Project 162907, "Temperature Dependence of the Electronic and Optoelectronic Properties of Carbon Nanotube Devices," and others
American Physical Society Fellow: *Hongyou Fan*	Project 191194, "Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials," and others
American Physical Society Fellow: *Igal Brener*	Project 192786, "A Compact, Spectrally Tunable Source of Entangled Photon Pairs for Quantum Sensing," and others
American Society of Mechanical Engineers Fellow: *Cliff Ho*	Project 173092, "Fractal-Like Materials Design with Optimized Radiative Properties for High-Efficiency Solar Energy Conversion," and others

AWARD DESCRIPTION	LDRD CONTRIBUTION
American Society of Mechanical Engineers Fellow: *Hy Tran*	Project 138635, "Correlation of Dimensional Measurement Uncertainties for Hybrid Measurement Systems," and others
Outstanding Young Engineer Award: 2016 IEEE Albuquerque Chapter: *Jay Johnson*	Project 180867, "Aggregating Distributed Energy Resources as Secure Virtual Power Plants"
Outstanding Young Engineer Award: IEEE Albuquerque Chapter: *Sheng Liu*	Project 191223, "A New All-Dielectric Nanolaser"
Young Scientist Award: International Union of Radio Science (URSI): *Sheng Liu*	Project 191223, "A New All-Dielectric Nanolaser"
DOE NNSA Stewardship Science Graduate Fellowship: *Gabriel Shipley*	Project 200269: "Benchmarking 3D-Magnetohydrodynamic Simulations of Electrothermal Instability Growth by Studying Z-Pinches with Engineered Defects"
First Place Oral Presentation Award: AVS New Mexico Symposium: *Sean Smith*	Project 191197, "Ferroelectric Tunnel Junctions: A Physics-Based Solution to Reliable Resistive Memory"
Second Place Materials Engineering and Sciences Division: 2016 AIChE Annual Meeting: *Maria Kelly*	Project 200168, "Exploring Fundamental Limitations of Manganese Oxide Cathodes for Reversible Zn/MnO2 Batteries"
Challenge Champion: IEEE High Performance Extreme Computing: *Michael M. Wolf, et al.*	Project 199982, "Multi-Level Memory Algorithmics for Large, Sparse Problems"
Best Paper Award: 2016 AIChE Annual Meeting: *Maher Salloum and David B. Robinson*	Project 180929, "Additive Manufacturing of Porous Materials"
Best Paper Award: IEEE International Parallel and Distributed Processing Symposium Workshops: *Mehmet Deveci, et al.*	Project 199982, "Multi-Level Memory Algorithmics for Large, Sparse Problems"
Best Paper Award: *Society of Experimental Mechanics: Melissa Teague*	Project 195883, "Microstructural Modeling of Brittle Materials for Enhanced Performance and Reliability"
Best Poster Award: Rio Grande Symposium on Advanced Materials: *Honyou Fan*	Project 191194, "Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials"
Best Poster Award: Denver X-Ray Conference: *Mark A. Rodriguez, et al.*	Project 180857, "Trusted Materials using Orthogonal Testing"

PUBLICATIONS

The following peer-reviewed publications, published in 2016, are attributed to the LDRD projects noted in the table below. Because publications are tallied over the calendar year, and Sandia operates on a fiscal year, publication metrics for 2017 will be reported in the 2018 Annual Report.

Authors	Article Title	Source	Volume	Issue	Pages	Project
Dunn, Aaron; Dingreville, Remi; Martinez, Enrique; Capolungo, Laurent	Identification of dominant damage accumulation processes at grain boundaries during irradiation in nanocrystalline alpha-Fe: A statistical study	ACTA MATERIALIA	110	n/a	306-323	178184
Booth, Joshua Dennis; Kim, Kyungjoo; Rajamanickam, Sivasankaran	A Comparison of High-Level Programming Choices for Incomplete Sparse Factorization Across Different Architectures	2016 IEEE 30TH INTERNATIONAL PARALLEL AND DISTRIBUTED PROCESSING SYMPOSIUM WORKSHOPS (IPDPSW)	n/a	n/a	397-406	173029
D'Elia, Marta; Perego, Mauro; Bochev, Pavel; Littlewood, David	A coupling strategy for nonlocal and local diffusion models with mixed volume constraints and boundary conditions	COMPUTERS & MATHEMATICS WITH APPLICATIONS	71	11	2218-2230	173025, 165616
Harmon, Brooke; Bird, Sara W.; Schudel, Benjamin R.; Hatch, Anson V.; Rasley, Amy	A Genome-Wide RNA Interference Screen Identifies a Role for Wnt/beta-Catenin Signaling during Rift Valley Fever Virus Infection	JOURNAL OF VIROLOGY	90	16	7084-7097	177858, 190245
Koudelka, Melissa L.; Dorsey, Daniel J.	A Modular NMF Matching Algorithm for Radiation Spectra	PROCEEDINGS OF 29TH IEEE CONFERENCE ON COMPUTER VISION AND PATTERN RECOGNITION WORKSHOPS, (CVPRW 2016)	n/a	n/a	284-289	180846
Wahl, Daniel E.; Yocky, David A.; Jakowatz, Charles V., Jr.; Simonson, Katherine M.	A New Maximum-Likelihood Change Estimator for Two-Pass SAR Coherent Change Detection	IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING	54	4	2460-2469	150122
Haass, Michael J.; Matzen, Laura E.; Butler, Karin M.; Armenta, Mika	A New Method for Categorizing Scanpaths from Eye Tracking Data	2016 ACM SYMPOSIUM ON EYE TRACKING RESEARCH & APPLICATIONS (ETRA 2016)	n/a	n/a	35-38	165535, 190967
Porras, Maria A. Gonzalez; Durfee, Paul N.; Gregory, Ashley M.; Sieck, Gary C.; Brinker, C. Jeffrey	A novel approach for targeted delivery to motoneurons using cholera toxin-B modified protocells	JOURNAL OF NEUROSCIENCE METHODS	273	n/a	160-174	190960
Frank, Michael P.; DeBenedictis, Erik P.	A Novel Operational Paradigm for Thermodynamically Reversible Logic Adibatic Transformation of Chaotic Nonlinear Dynamical Circuits	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180819
DeBenedictis, Erik P.; Frank, Michael P.; Ganesh, Natesh; Anderson, Neal G.	A Path Toward Ultra-Low-Energy Computing	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180819
Lehoucq, R. B.; Rowe, S. T.	A radial basis function Galerkin method for inhomogeneous nonlocal diffusion	COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING	299	n/a	366-380	15-0971
Bent, Zachary W.; Poorey, Kunal; LaBauve, Annette E.; Hamblin, Rachelle; Williams, Kelly P.	A Rapid Spin Column-Based Method to Enrich Pathogen Transcripts from Eukaryotic Host Cells Prior to Sequencing	PLOS ONE	11	12	n/a	173111

Authors	Article Title	Source	Volume	Issue	Pages	Project
Abhyankar, Vinay V.; Wu, Meiye; Koh, Chung-Yan; Hatch, Anson V.	A Reversibly Sealed, Easy Access, Modular (SEAM) Microfluidic Architecture to Establish In Vitro Tissue Interfaces	PLOS ONE	11	5	n/a	151350
Ball, C. S.; Renzi, R. F.; Priye, A.; Meagher, R. J.	A simple check valve for microfluidic point of care diagnostics	LAB ON A CHIP	16	22	4436-4444	173111
Yadav, Vineet; Michalak, Anna M.; Ray, Jaideep; Shiga, Yoichi P.	A statistical approach for isolating fossil fuel emissions in atmospheric inverse problems	JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES	121	20	12490-12504	151293
Parkes, Marie V.; Greathouse, Jeffery A.; Hart, David B.; Sava Gallis, Dorina F.; Nenoff, Tina M.	Ab initio molecular dynamics determination of competitive O-2 vs. N-2 adsorption at open metal sites of M-2(dobdc)	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	18	16	11528-11538	165632
Sarobol, Pylin; Cook, Adam; Clem, Paul G.; Keicher, David; Hirschfeld, Deidre	Additive Manufacturing of Hybrid Circuits	ANNUAL REVIEW OF MATERIALS RESEARCH, VOL 46	46	n/a	41-62	177962
Sarobol, Pylin; Vackel, Andrew; Adamczyk, Jesse; Holmes, Thomas; Rodriguez, Mark	AEROSOL METHOD FOR ROOM TEMPERATURE THICK-FILM DEPOSITION Aerosol deposition offers an alternative to conventional thin film processes when mesoscale coatings are needed	ADVANCED MATERIALS & PROCESSES	174	10	40-43	200184
Allerman, A. A.; Armstrong, A. M.; Fischer, A. J.; Dickerson, J. R.; Crawford, M. H.	Al0.3Ga0.7N PN diode with breakdown voltage > 1600 V	ELECTRONICS LETTERS	52	15	1319-1320	180884
Salinger, Andrew G.; Bartlett, Roscoe A.; Bradley, Andrew M.; Chen, Qiushi; Demeshko, Irina P.	ALBANY: USING COMPONENT-BASED DESIGN TO DEVELOP A FLEXIBLE, GENERIC MULTIPHYSICS ANALYSIS CODE	INTERNATIONAL JOURNAL FOR MULTISCALE COMPUTATIONAL ENGINEERING	14	4	415-438	163747
Awad, Muhammad A.; Rushdi, Ahmad A.; Abbas, Misarah A.; Mitchell, Scott A.; Mahmoud, Ahmed H.	All-Hex Meshing of Multiple-Region Domains without Cleanup	25TH INTERNATIONAL MESHING ROUNDTABLE	163	n/a	251-261	165617
Cai, Hong; Boynton, Nicholas; Lentine, Anthony L.; Pomerene, Andrew; Trotter, Douglas C.	An Adiabatic/Diabatic Polarization Beam Splitter	2016 IEEE OPTICAL INTERCONNECTS CONFERENCE (OI)	n/a	n/a	102-103	173103
Baca, Albert G.; Armstrong, Andrew M.; Allerman, Andrew A.; Douglas, Erica A.; Sanchez, Carlos A.	An AlN/Al0.85Ga0.15N high electron mobility transistor	APPLIED PHYSICS LETTERS	109	3	n/a	180884
Lee, David S.; Swift, Gary; Wirthlin, Michael	An Analysis of High-Current Events Observed on Xilinx 7-Series and UltraScale Field-Programmable Gate Arrays	2016 IEEE RADIATION EFFECTS DATA WORKSHOP (REDW)	n/a	n/a	175-179	165724
Zhou, X. W.; Ward, D. K.; Foster, M. E.	An analytical bond-order potential for the aluminum copper binary system	JOURNAL OF ALLOYS AND COMPOUNDS	680	n/a	752-767	165724

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Authors	Article Title	Source	Volume	Issue	Pages	Project
Keating, Tyler; Baldwin, Charles H.; Jau, Yuan-Yu; Lee, Jongmin; Biedermann, Grant W.	Arbitrary Dicke-State Control of Symmetric Rydberg Ensembles	PHYSICAL REVIEW LETTERS	117	21	n/a	173130
Barlow, Andrew J.; Maire, Pierre-Henri; Rider, William J.; Rieben, Robert N.; Shashkov, Mikhail J.	Arbitrary Lagrangian-Eulerian methods for modeling high-speed compressible multimaterial flows	JOURNAL OF COMPUTATIONAL PHYSICS	322	n/a	603-665	FY14-0945
Mielenz, Manuel; Kalis, Henning; Wittemer, Matthias; Hakelberg, Frederick; Warring, Ulrich	Arrays of individually controlled ions suitable for two-dimensional quantum simulations	NATURE COMMUNICATIONS	7	n/a	n/a	13-0082
Weck, Philippe F.; Kim, Eunja	Assessing Hubbard-corrected AM05+U and PBEsol plus U density functionals for strongly correlated oxides CeO2 and Ce2O3	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	18	38	26816-26826	191056
Xiao, Xiaoyin; Miller, Lance L.; Parchert, Kylea J.; Hayes, Dulce; Hochrein, James M.	Atmospheric solids analysis probe mass spectrometry for the rapid identification of pollens and semi-quantification of flavonoid fingerprints	RAPID COMMUNICATIONS IN MASS SPECTROMETRY	30	13	1639-1646	173069
Emery, J. M.; Grigoriu, M. D.; Field, R. V., Jr.	Bayesian methods for characterizing unknown parameters of material models	APPLIED MATHEMATICAL MODELLING	40	13-14	6395-6411	180878
Arefiev, A. V.; Khudik, V. N.; Robinson, A. P. L.; Shvets, G.; Willingale, L.	Beyond the ponderomotive limit: Direct laser acceleration of relativistic electrons in sub-critical plasmas	PHYSICS OF PLASMAS	23	5	n/a	151367
Campione, Salvatore; Liu, Sheng; Basilio, Lorena I.; Warne, Larry K.; Langston, William L.	Broken Symmetry Dielectric Resonators for High Quality Factor Fano Metasurfaces	ACS PHOTONICS	3	12	2362-2367	189614
Ortega, Jesus D.; Yellowhair, Julius E.; Ho, Clifford K.; Christian, Joshua M.; Andraka, Charles E.	Calorimetric Evaluation of Novel Concentrating Solar Receiver Geometries with Enhanced Effective Solar Absorptance	PROCEEDINGS OF THE ASME 10TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2016, VOL 1	1	n/a	n/a	173092
Geng, Haifeng; Tran-Gyamfi, Mary B.; Lane, Todd W.; Sale, Kenneth L.; Yu, Eizadora T.	Changes in the Structure of the Microbial Community Associated with Nannochloropsis salina following Treatments with Antibiotics and Bioactive Compounds	FRONTIERS IN MICROBIOLOGY	7	n/a	n/a	158835
Miller, Mary A.; Tangyunyong, Paiboon; Cole, Edward I., Jr.	Characterization of electrically-active defects in ultraviolet light-emitting diodes with laser-based failure analysis techniques	JOURNAL OF APPLIED PHYSICS	119	2	n/a	176400
Grest, Gary S.	Communication: Polymer entanglement dynamics: Role of attractive interactions	JOURNAL OF CHEMICAL PHYSICS	145	14	n/a	15-0548

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Appelhans, L. N.; Keicher, D. M.; Lavin, J. M.	Comparison of Dielectric Properties of Additively Manufactured vs. Solvent Cast Polyimide Dielectrics	2016 IEEE CONFERENCE ON ELECTRICAL INSULATION AND DIELECTRIC PHENOMENA (IEEE CEIDP)	n/a	n/a	62-65	191232
Hall, Elise M.; Thurow, Brian S.; Guildenbecher, Daniel R.	Comparison of three-dimensional particle tracking and sizing using plenoptic imaging and digital in-line holography	APPLIED OPTICS	55	23	6410-6420	161867
DeBenedictis, Erik P.	Computational Complexity and New Computing Approaches	COMPUTER	49	12	76-79	180819
Deng, Bobin; Srikanth, Sriseshan; Hein, Eric R.; Rabbat, Paul G.; Conte, Thomas M.	Computationally-Redundant Energy-Efficient Processing for Y'all (CREEPY)	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180819
Rothganger, Fred; James, Conrad D.; Aimone, James B.	Computing with Dynamical Systems	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180885, 180886
Stygar, W. A.; Reisman, D. B.; Stoltzfus, B. S.; Austin, K. N.; Ao, T.	Conceptual design of a 10(13)-W pulsed-power accelerator for megajoule-class dynamic-material-physics experiments	PHYSICAL REVIEW ACCELERATORS AND BEAMS	19	7	n/a	173191, 191238
Lu, Xujie; Chen, Aiping; Luo, Yongkang; Lu, Ping; Dai, Yaomin	Conducting Interface in Oxide Homojunction: Understanding of Superior Properties in Black TiO2	NANO LETTERS	16	9	5751-5755	191196
Grillet, Anne M.; Humplik, Thomas; Stirrup, Emily K.; Roberts, Scott A.; Barringer, David A.	Conductivity Degradation of Polyvinylidene Fluoride Composite Binder during Cycling: Measurements and Simulations for Lithium-Ion Batteries	JOURNAL OF THE ELECTROCHEMICAL SOCIETY	163	9	A1859-A1871	173098
Bishop, Joseph E.; Lim, Hojun	Continuum Approximations	MULTISCALE MATERIALS MODELING FOR NANOMECHANICS	245	n/a	89-129	178667
Schmit, P. F.; Velikovich, A. L.; McBride, R. D.; Robertson, G. K.	Controlling Rayleigh-Taylor Instabilities in Magnetically Driven Solid Metal Shells by Means of a Dynamic Screw Pinch	PHYSICAL REVIEW LETTERS	117	20	n/a	165746
Ortega, Jesus; Khivsara, Sagar; Christian, Joshua; Ho, Clifford; Yellowhair, Julius	Coupled modeling of a directly heated tubular solar receiver for supercritical carbon dioxide Brayton cycle: Optical and thermal-fluid evaluation	APPLIED THERMAL ENGINEERING	109	n/a	970-978	14-0439
Ortega, Jesus; Khivsara, Sagar; Christian, Joshua; Ho, Clifford; Dutta, Pradip	Coupled modeling of a directly heated tubular solar receiver for supercritical carbon dioxide Brayton cycle: Structural and creep-fatigue evaluation	APPLIED THERMAL ENGINEERING	109	n/a	979-987	14-0439
Ortega, Jesus D.; Khivsara, Sagar D.; Christian, Joshua M.; Yellowhair, Julius E.; Ho, Clifford K.	COUPLED OPTICAL-THERMAL-FLUID MODELING OF A DIRECTLY HEATED TUBULAR SOLAR RECEIVER FOR SUPERCRITICAL CO2 BRAYTON CYCLE	PROCEEDINGS OF THE ASME 9TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2015, VOL 1	n/a	n/a	n/a	14-0439

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Rudolph, M.; Harvey-Collard, P.; Jock, R.; Jacobson, T.; Wendt, J.	Coupling MOS Quantum Dot and Phosphorous Donor Qubit Systems	2016 IEEE INTERNATIONAL ELECTRON DEVICES MEETING (IEDM)	n/a	n/a	n/a	200143
Martin, James E.; Solis, Kyle J.	Creating orbiting vorticity vectors in magnetic particle suspensions through field symmetry transitions-a route to multi-axis mixing	SOFT MATTER	12	4	1021-1031	191215
Greene, Adrienne C.; Wheeler, David R.; Spoerke, Erik D.; Bachand, George D.; Jones, Brad H.	Creating Robust and Reversible Cell-Gel Networks using Boronic Acid Chemistry	BIOPHYSICAL JOURNAL	110	3	332A-333A	201319
Meyer, Kelsey E.; Cheaito, Ramez; Paisley, Elizabeth; Shelton, Christopher T.; Braun, Jeffrey L.	Crystalline coherence length effects on the thermal conductivity of MgO thin films	JOURNAL OF MATERIALS SCIENCE	51	23	10408-10417	173117
Ohrhallinger, S.; Mitchell, S. A.; Wimmer, M.	Curve Reconstruction with Many Fewer Samples	COMPUTER GRAPHICS FORUM	35	5	167-176	165617
Jiang, Ruiwei; Guan, Yongpei; Watson, Jean-Paul	Cutting planes for the multistage stochastic unit commitment problem	MATHEMATICAL PROGRAMMING	157	1	121-151	173090
Varman, Arul M.; He, Lian; Follenfant, Rhiannon; Wu, Weihua; Wemmer, Sarah	Decoding how a soil bacterium extracts building blocks and metabolic energy from ligninolysis provides road map for lignin valorization	PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA	113	40	E5802-E5811	16-0758
Baboly, M. Ghasemi; Raza, A.; Brady, J.; Reinke, C. M.; Leseman, Z. C.	Demonstration of acoustic waveguiding and tight bending in phononic crystals	APPLIED PHYSICS LETTERS	109	18	n/a	191080
Ao, T.; Harding, E. C.; Bailey, J. E.; Lemke, R. W.; Desjarlais, M. P.	Demonstration of space-resolved x-ray Thomson scattering capability for warm dense matter experiments on the Z accelerator	HIGH ENERGY DENSITY PHYSICS	18	n/a	26-37	141540
Boubault, Antoine; Yellowhair, Julius; Ho, Clifford K.	DESIGN AND CHARACTERIZATION OF A 7.2 KW SOLAR SIMULATOR	PROCEEDINGS OF THE ASME 9TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2015, VOL 1	1	n/a	n/a	173092
Zhang, Yuewei; Krishnamoorthy, Sriram; Akyol, Fatih; Allerman, Andrew A.; Moseley, Michael W.	Design and demonstration of ultra-wide bandgap AlGaN tunnel junctions	APPLIED PHYSICS LETTERS	109	12	n/a	180884
Sweany, M.; Marleau, P.	Design and expected performance of a fast neutron attenuation probe for light element density measurements	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	833	n/a	134-141	186363

Authors	Article Title	Source	Volume	Issue	Pages	Project
Christian, Joshua M.; Ortega, Jesus D.; Ho, Clifford K.; Yellowhair, Julius	DESIGN AND MODELING OF LIGHT-TRAPPING TUBULAR RECEIVER PANELS	PROCEEDINGS OF THE ASME 10TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2016, VOL 1	n/a	n/a	n/a	173092
Zhang, Yuewei; Krishnamoorthy, Sriram; Akyol, Fatih; Allerman, Andrew A.; Moseley, Michael W.	Design of p-type cladding layers for tunnel-injected UV-A light emitting diodes	APPLIED PHYSICS LETTERS	109	19	n/a	180884
Ortega, Jesus D.; Khivsara, Sagar D.; Christian, Joshua M.; Ho, Clifford K.	DESIGN REQUIREMENTS FOR DIRECT SUPERCRITICAL CARBON DIOXIDE RECEIVER DEVELOPMENT AND TESTING	PROCEEDINGS OF THE ASME 9TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2015, VOL 1	1	n/a	n/a	14-0439
Hibbs, Michael R.; McGrath, Lucas K.; Kang, Seoktae; Adout, Atar; Altman, Susan J.	Designing a biocidal reverse osmosis membrane coating: Synthesis and biofouling properties	DESALINATION	380	n/a	52-59	102737
Li, Jian; Pan, Wei; Bernevig, B. Andrei; Lutchyn, Roman M.	Detection of Majorana Kramers Pairs Using a Quantum Point Contact	PHYSICAL REVIEW LETTERS	117	4	n/a	165717
Burckel, D. Bruce	Device-level and module-level three-dimensional integrated circuits created using oblique processing	JOURNAL OF MICRO-NANOLITHOGRAPHY MEMS AND MOEMS	15	3	n/a	173129
You, Xinli; Chaudhari, Mangesh I.; Rempe, Susan B.; Pratt, Lawrence R.	Dielectric Relaxation of Ethylene Carbonate and Propylene Carbonate from Molecular Dynamics Simulations	JOURNAL OF PHYSICAL CHEMISTRY B	120	8	1849-1853	192678
Bishop, Joseph E.; Emery, John M.; Battaile, Corbett C.; Littlewood, David J.; Baines, Andrew J.	Direct Numerical Simulations in Solid Mechanics for Quantifying the Macroscale Effects of Microstructure and Material Model-Form Error	JOM	68	5	1427-1445	178667
Kaehr, Bryan; Scrymgeour, David A.	Direct-write graded index materials realized in protein hydrogels	APPLIED PHYSICS LETTERS	109	12	n/a	177860
Ebeida, Mohamed S.; Rushdi, Ahmad A.; Awad, Muhammad A.; Mahmoud, Ahmed H.; Yan, Dong-Ming	Disk Density Tuning of a Maximal Random Packing	COMPUTER GRAPHICS FORUM	35	5	259-269	15-0905
O'Brien, Christopher J.; Greathouse, Jeffery A.; Tenney, Craig M.	Dissociation of Sarin on a Cement Analogue Surface: Effects of Humidity and Confined Geometry	JOURNAL OF PHYSICAL CHEMISTRY C	120	49	28100-28109	180896
Du, HuiYun; Deng, Wei; Aimone, James B.; Ge, Minyan; Parylak, Sarah	Dopaminergic inputs in the dentate gyrus direct the choice of memory encoding	PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA	113	37	E5501-E5510	180885
Gan, Shiyuan; Liang, Yufeng; Spataru, Catalin D.; Yang, Li	Dynamical Excitonic Effects in Doped Two-Dimensional Semiconductors	NANO LETTERS	16	9	5568-5573	180836

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Salerno, K. Michael; Agrawal, Anupriya; Peters, Brandon L.; Perahia, Dvora; Grest, Gary S.	Dynamics in entangled polyethylene melts	EUROPEAN PHYSICAL JOURNAL-SPECIAL TOPICS	225	9-Aug	1707-1722	15-0548
van der Laan, John D.; Wright, Jeremy B.; Scrymgeour, David A.; Kemme, Shanalyn A.; Dereniak, Eustace L.	Effects of collection geometry variations on linear and circular polarization persistence in both isotropic-scattering and forward-scattering environments	APPLIED OPTICS	55	32	9042-9048	191184
Moore, Jeremy; Douglas, J. Kenneth; Frank, Ian W.; Friedmann, Thomas A.; Camacho, Ryan M.	Efficient Second Harmonic Generation in Lithium Niobate on Insulator	2016 CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO)	n/a	n/a	n/a	173126
Sava Gallis, Dorina F.; Pratt, Harry D., III; Anderson, Travis M.; Chapman, Karena W.	Electrochemical activity of Fe-MIL-100 as a positive electrode for Na-ion batteries	JOURNAL OF MATERIALS CHEMISTRY A	4	36	13764-13770	177964
Helinski, Ryan L.; Cole, Edward I., Jr.; Robertson, Gideon; Woodbridge, Jonathan; Pierson, Lyndon G.	Electronic Forensic Techniques for Manufacturer Attribution	PROCEEDINGS OF THE 2016 IEEE INTERNATIONAL SYMPOSIUM ON HARDWARE ORIENTED SECURITY AND TRUST (HOST)	n/a	n/a	139-144	159303
Small, Leo J.; Sears, Jeremiah M.; Lambert, Timothy N.; Boyle, Timothy J.; Hess, Ryan F.	Electroreduction of Er3+ in nonaqueous solvents	RSC ADVANCES	6	92	89564-89571	173156
Van Leeuwen, Brian P.; Stout, William M. S.; Urias, Vincent E.	Empirical Assessment of Network-based Moving Target Defense Approaches	MILCOM 2016 - 2016 IEEE MILITARY COMMUNICATIONS CONFERENCE	n/a	n/a	764-769	173071
Whitmore, Mark D.; Grest, Gary S.; Douglas, Jack F.; Kent, Michael S.; Suo, Tongchuan	End-anchored polymers in good solvents from the single chain limit to high anchoring densities	JOURNAL OF CHEMICAL PHYSICS	145	17	n/a	15-0548
Agarwal, Sapan; Cook, Jeanine; DeBenedictis, Erik; Frank, Michael P.; Cauwenberghs, Gert	Energy Efficiency Limits of Logic and Memory	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180819
Agarwal, Sapan; Quach, Tu-Thach; Parekh, Ojas; Hsia, Alexander H.; DeBenedictis, Erik P.	Energy Scaling Advantages of Resistive Memory Crossbar Based Computation and Its Application to Sparse Coding	FRONTIERS IN NEUROSCIENCE	9	n/a	n/a	180885, 171060
Meagher, Robert J.; Negrete, Oscar A.; Van Rompay, Koen K.	Engineering Paper-Based Sensors for Zika Virus	TRENDS IN MOLECULAR MEDICINE	22	7	529-530	173111
Zhang, Yuewei; Allerman, Andrew A.; Krishnamoorthy, Sriram; Akyol, Fatih; Moseley, Michael W.	Enhanced light extraction in tunnel junction-enabled top emitting UV LEDs	APPLIED PHYSICS EXPRESS	9	5	n/a	180884

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Trumbo, Michael C.; Matzen, Laura E.; Coffman, Brian A.; Hunter, Michael A.; Jones, Aaron P.	Enhanced working memory performance via transcranial direct current stimulation: The possibility of near and far transfer	NEUROPSYCHOLOGIA	93	n/a	85-96	165715
Frank, Ian W.; Moore, Jeremy; Douglas, J. K.; Camacho, Ryan; Eichenfield, Matt	Entangled Photon Generation in Lithium Niobate Microdisk Resonators Through Spontaneous Parametric Down Conversion	2016 CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO)	n/a	n/a	n/a	173126
Jau, Y. -Y.; Hankin, A. M.; Keating, T.; Deutsch, I. H.; Biedermann, G. W.	Entangling atomic spins with a Rydberg-dressed spin-flip blockade	NATURE PHYSICS	12	1	71-74	173130
Clarkson, Caitlyn M.; McCoy, John D.; Kropka, Jamie M.	Enthalpy recovery and its relation to shear response in an amine cured DGEBA epoxy	POLYMER	94	n/a	19-30	165649
Cavagnaro, Robert J.; Neely, Jason C.; Fay, Franois-Xavier; Lopez Mendia, Joseba; Rea, Judith A.	Evaluation of Electromechanical Systems Dynamically Emulating a Candidate Hydrokinetic Turbine	IEEE TRANSACTIONS ON SUSTAINABLE ENERGY	7	1	390-399	152503
Thyne, Geoffrey; Brady, Patrick	Evaluation of formation water chemistry and scale prediction: Bakken Shale	APPLIED GEOCHEMISTRY	75	n/a	107-113	171069
Neely, J.; Rashkin, L.; Cook, M.; Wilson, D.; Glover, S.	Evaluation of Power Flow Control for an All-Electric Warship Power System with Pulsed Load Applications	APEC 2016 31ST ANNUAL IEEE APPLIED POWER ELECTRONICS CONFERENCE AND EXPOSITION	n/a	n/a	3537-3544	152503
Schoeniger, Joseph S.; Hudson, Corey M.; Bent, Zachary W.; Sinha, Anupama; Williams, Kelly P.	Experimental single-strain mobilomics reveals events that shape pathogen emergence	NUCLEIC ACIDS RESEARCH	44	14	6830-6839	180816, 180814
Campione, Salvatore; Kim, Iltai; de Ceglia, Domenico; Keeler, Gordon A.; Luk, Ting S.	Experimental verification of epsilon-near-zero plasmon polariton modes in degenerately doped semiconductor nanolayers	OPTICS EXPRESS	24	16	18782-18789	200228
Shan, Tzu-Ray; Wixom, Ryan R.; Thompson, Aidan P.	Extended asymmetric hot region formation due to shockwave interactions following void collapse in shocked high explosive	PHYSICAL REVIEW B	94	5	n/a	151351, 165656
Abraham, J. B. S.; Aguirre, B. A.; Pacheco, J. L.; Vizkelethy, G.; Bielejec, E.	Fabrication and characterization of a co-planar detector in diamond for low energy single ion implantation	APPLIED PHYSICS LETTERS	109	6	n/a	192701
Lu, T. M.; Gamble, J. K.; Muller, R. P.; Nielsen, E.; Bethke, D.	Fabrication of quantum dots in undoped Si/Si0.8Ge0.2 heterostructures using a single metal-gate layer	APPLIED PHYSICS LETTERS	109	9	n/a	173883
Lu, Ping; Yuan, Ren Liang; Ihlefeld, Jon F.; Spoerke, Erik David; Pan, Wei	Fast Atomic-Scale Chemical Imaging of Crystalline Materials and Dynamic Phase Transformations	NANO LETTERS	16	4	2728-2733	180923

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Hai, Bhuiyan Shameem Mahmood Ebna; Bause, Markus; Kuberry, Paul	FINITE ELEMENT APPROXIMATION OF THE EXTENDED FLUID-STRUCTURE INTERACTION (EXFSI) PROBLEM	PROCEEDINGS OF THE ASME FLUIDS ENGINEERING DIVISION SUMMER MEETING, 2016, VOL 1A	1A	n/a	n/a	173025
Fiala, David; Mueller, Frank; Ferreira, Kurt B.	FlipSphere: A Software-based DRAM Error Detection and Correction Library for HPC	2016 IEEE/ACM 20TH INTERNATIONAL SYMPOSIUM ON DISTRIBUTED SIMULATION AND REAL TIME APPLICATIONS (DS-RT)	n/a	n/a	19-28	158802
Colombo, Anthony P.; Carter, Tony R.; Borna, Amir; Jau, Yuan-Yu; Johnson, Cort N.	Four-channel optically pumped atomic magnetometer for magnetoencephalography	OPTICS EXPRESS	24	14	15403-15416	R01EB0 13302
Ruffing, Anne M.; Jensen, Travis J.; Strickland, Lucas M.	Genetic tools for advancement of Synechococcus sp PCC 7002 as a cyanobacterial chassis	MICROBIAL CELL FACTORIES	15	n/a	n/a	170804, 190962
Durniak, Mark T.; Bross, Adam S.; Elsaesser, David; Chaudhuri, Anabil; Smith, Michael L.	Green Emitting Cubic GaInN/GaN Quantum Well Stripes on Micropatterned Si(001) and Their Strain Analysis	ADVANCED ELECTRONIC MATERIALS	2	3	n/a	15-0777
Bauer, Stephen J.; Gardner, W. Payton; Heath, Jason E.	Helium release during shale deformation: Experimental validation	GEOCHEMISTRY GEOPHYSICS GEOSYSTEMS	17	7	2612-2622	165670
DeBenedictis, Erik P.; Williams, R. Stanley	Help Wanted: A Modern-Day Turing	COMPUTER	49	10	76-79	180819
Middleton, L. Robert; Tarver, Jacob D.; Cordaro, Joseph; Tyagi, Madhusudan; Soles, Christopher L.	Heterogeneous Chain Dynamics and Aggregate Lifetimes in Precise Acid-Containing Polyethylenes: Experiments and Simulations	MACROMOLECULES	49	23	9176-9185	141506
McPherson, L. Armon; Ampleford, David J.; Coverdale, Christine A.; Argo, Jeffrey W.; Owen, Albert C.	High energy X-ray pinhole imaging at the Z facility	REVIEW OF SCIENTIFIC INSTRUMENTS	87	6	n/a	165733, 173104
Martinez, Nicholas J. D.; DeRose, Christopher T.; Brock, Reinhard W.; Starbuck, Andrew L.; Pomerene, Andrew T.	High performance waveguide-coupled Ge-on-Si linear mode avalanche photodiodes	OPTICS EXPRESS	24	17	19072-19081	LDRD
Seagle, Christopher T.; Reinhart, William D.; Lopez, Andrew J.; Hickman, Randy J.; Thornhill, Tom F., III	High precision Hugoniot measurements on statically pre-compressed fluid helium	JOURNAL OF APPLIED PHYSICS	120	12	n/a	165739
Armstrong, A. M.; Allerman, A. A.; Fischer, A. J.; King, M. P.; van Heukelom, M. S.	High voltage and high current density vertical GaN power diodes	ELECTRONICS LETTERS	52	13	1170-1171	180884

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Meier, William; Meyer, Kelsey Elizabeth; Sava Gallis, Dorina F.; Blea-Kirby, Mia Angelica; Roth, Joshua	Highly Textured BaTiO3 via Templated Grain Growth and Resulting Polarization Reversal Dynamics	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	99	3	922-929	LDRD
Bouchard, Kristofer E.; Aimone, James B.; Chun, Miyoung; Dean, Thomas; Denker, Michael	High-Performance Computing in Neuroscience for Data-Driven Discovery, Integration, and Dissemination	NEURON	92	3	628-631	180885
Guildenbecher, Daniel R.; Cooper, Marcia A.; Sojka, Paul E.	High-speed (20 kHz) digital in-line holography for transient particle tracking and sizing in multiphase flows	APPLIED OPTICS	55	11	2892-2903	180876
Choi, Byung Joon; Torrezan, Antonio C.; Strachan, John Paul; Kotula, P. G.; Lohn, A. J.	High-Speed and Low-Energy Nitride Memristors	ADVANCED FUNCTIONAL MATERIALS	26	29	5290-5296	180885
Chao, Paul; Karnesky, Richard A.	Hydrogen isotope trapping in Al-Cu binary alloys	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	658	n/a	422-428	165724
O'Brien, Christopher J.; Foiles, Stephen M.	Hydrogen segregation to inclined Sigma 3 < 110 > twin grain boundaries in nickel	PHILOSOPHICAL MAGAZINE	96	26	2808-2828	173116
Jagannathan, Kaushik; Benson, David M.; Robinson, David B.; Stickney, John L.	Hydrogen Sorption Kinetics on Bare and Platinum-Modified Palladium Nanofilms, Grown by Electrochemical Atomic Layer Deposition (E-ALD)	JOURNAL OF THE ELECTROCHEMICAL SOCIETY	163	12	D3047-D3052	180929
King, M. P.; Kaplar, R. J.; Dickerson, J. R.; Lee, S. R.; Allerman, A. A.	Identification of the primary compensating defect level responsible for determining blocking voltage of vertical GaN power diodes	APPLIED PHYSICS LETTERS	109	18	n/a	180884
Wang, George T.; Li, Changyi; Liu, Sheng; Wright, Jeremy B.; Leung, Benjamin	III-Nitride Nanowires Lasers	2016 IEEE PHOTONICS SOCIETY SUMMER TOPICAL MEETING SERIES (SUM)	n/a	n/a	25-26	165704
Wierer, Jonathan J., Jr.; Tansu, Nelson; Fischer, Arthur J.; Tsao, Jeffrey Y.	III-nitride quantum dots for ultra-efficient solid-state lighting	LASER & PHOTONICS REVIEWS	10	4	612-622	186113
Lim, Hojun; Abdeljawad, Fadi; Owen, Steven J.; Hanks, Byron W.; Foulk, James W.	Incorporating physically-based microstructures in materials modeling: Bridging phase field and crystal plasticity frameworks	MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING	24	4	n/a	186053
Nordquist, Christopher D.; Henry, M. David; Nguyen, Janet H.; Clews, Peggy; Lepkowski, Stefan	Inductive Coupling for Increased Bandwidth of Aluminum Nitride Contour-Mode Microresonator Filters	2016 IEEE MTT-S INTERNATIONAL MICROWAVE SYMPOSIUM (IMS)	n/a	n/a	n/a	165708

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McNamara, Laura A.; Bauer, Travis L.; Haass, Michael; Matzen, Laura	Information Theoretic Measures for Visual Analytics: The Silver Ticket?	BEYOND TIME AND ERRORS: NOVEL EVALUATION METHODS FOR VISUALIZATION, BELIV 2016	n/a	n/a	53-61	198367
Leonard, F.; Dickerson, J. R.; King, M. P.; Armstrong, A. M.; Fischer, A. J.	In-Operando Spatial Imaging of Edge Termination Electric Fields in GaN Vertical p-n Junction Diodes	IEEE ELECTRON DEVICE LETTERS	37	6	766-769	180884
Roberts, Scott A.; Mendoza, Hector; Brunini, Victor E.; Trembacki, Bradley L.; Noble, David R.	Insights Into Lithium-Ion Battery Degradation and Safety Mechanisms From Mesoscale Simulations Using Experimentally Reconstructed Mesostructures	JOURNAL OF ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE	13	3	n/a	173098
Abdeljawad, Fadi; Foiles, Stephen M.	Interface-Driven Phenomena in Solids: Thermodynamics, Kinetics and Chemistry	JOM	68	6	1594-1595	15-1052
Li, Changyi; Liu, Sheng; Luk, Ting. S.; Figiel, Jeffrey J.; Brener, Igal	Intrinsic polarization control in rectangular GaN nanowire lasers	NANOSCALE	8	10	5682-5687	165704
Lim, Hojun; Dingreville, Remi; Deibler, Lisa A.; Buchheit, Thomas E.; Battaile, Corbett C.	Investigation of grain-scale microstructural variability in tantalum using crystal plasticity-finite element simulations	COMPUTATIONAL MATERIALS SCIENCE	117	n/a	437-444	173116
Brocato, Terisse A.; Hess, Ryan F.; Moorman, Matthew; Simonson, Robert J.	Investigations into the chemical structure based selectivity of the microfabricated nitrogen-phosphorus detector	SENSORS AND ACTUATORS B-CHEMICAL	224	n/a	618-623	141520
Stevens, Mark J.; Rempe, Susan L. B.	Ion-Specific Effects in Carboxylate Binding Sites	JOURNAL OF PHYSICAL CHEMISTRY B	120	49	12519-12530	200167
Wolf, Michael M.; Edwards, H. Carter; Olivier, Stephen L.	Kokkos/Qthreads Task-Parallel Approach to Linear Algebra Based Graph Analytics	2016 IEEE HIGH PERFORMANCE EXTREME COMPUTING CONFERENCE (HPEC)	n/a	n/a	n/a	173029
Chou, Stanley S.; Swartzentruber, Brian S.; Janish, Matthew T.; Meyer, Kristin C.; Biedermann, Laura B.	Laser Direct Write Synthesis of Lead Halide Perovskites	JOURNAL OF PHYSICAL CHEMISTRY LETTERS	7	19	3736-3741	200179, 164677
Harvey-Thompson, A. J.; Sefkow, A. B.; Wei, M. S.; Nagayama, T.; Campbell, E. M.	Laser propagation measurements in long-scale-length underdense plasmas relevant to magnetized liner inertial fusion	PHYSICAL REVIEW E	94	5	n/a	173190
Yao, Virginia J.; D'Angelo, Sara; Butler, Kimberly S.; Theron, Christophe; Smith, Tracey L.	Ligand-targeted theranostic nanomedicines against cancer	JOURNAL OF CONTROLLED RELEASE	240	n/a	267-286	190960
Henderson, Ian M.; Collins, Aaron M.; Quintana, Hope A.; Montano, Gabriel A.; Martinez, Julio A.	Lights on: Dye dequenching reveals polymersome fusion with polymer, lipid and stealth lipid vesicles	POLYMER	83	n/a	239-245	185269

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Choi, Sukwon; Griffin, Benjamin A.	Local residual stress monitoring of aluminum nitride MEMS using UV micro-Raman spectroscopy	JOURNAL OF MICROMECHANICS AND MICROENGINEERING	26	2	n/a	191198
Geng, Haifeng; Sale, Kenneth L.; Tran-Gyamfi, Mary Bao; Lane, Todd W.; Yu, Eizadora T.	Longitudinal Analysis of Microbiota in Microalga Nannochloropsis salina Cultures	MICROBIAL ECOLOGY	72	1	14-24	158835
Dieni, Cristina V.; Panichi, Roberto; Aimone, James B.; Kuo, Chay T.; Wadiche, Jacques I.	Low excitatory innervation balances high intrinsic excitability of immature dentate neurons	NATURE COMMUNICATIONS	7	n/a	n/a	180885
Muller, Giel; Scheer, Adam; Osborn, David L.; Taatjes, Craig A.; Meloni, Giovanni	Low Temperature Chlorine-Initiated Oxidation of Small-Chain Methyl Esters: Quantification of Chain-Terminating HO2-Elimination Channels	JOURNAL OF PHYSICAL CHEMISTRY A	120	10	1677-1690	151308
Ling, Julia; Jones, Reese; Templeton, Jeremy	Machine learning strategies for systems with invariance properties	JOURNAL OF COMPUTATIONAL PHYSICS	318	n/a	22-35	180823
Harper, Jason C.; Andrews, Jenna M.; Ben, Candice; Hunt, Andrew C.; Murton, Jaclyn K.	Magnetic-adhesive based valves for microfluidic devices used in low-resource settings	LAB ON A CHIP	16	21	4142-4151	158813
Tidwell, Vincent; Moreland, Barbie	Mapping water consumption for energy production around the Pacific Rim	ENVIRONMENTAL RESEARCH LETTERS	11	9	n/a	165630
Schroder, Tim; Trusheim, Matthew E.; Walsh, Michael; Pacheco, Jose; Li, Luozhou	Maskless Creation of Silicon Vacancy Centers in Photonic Crystal Cavities	2016 CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO)	n/a	n/a	n/a	192701
Snyder, Chelsea; Apblett, Christopher; Grillet, Anne; Beechem, Thomas; Duquette, David	Measuring Li+ Inventory Losses in LiCoO2/Graphite Cells Using Raman Microscopy	JOURNAL OF THE ELECTROCHEMICAL SOCIETY	163	6	A1036-A1041	173098
Mendoza, Hector; Roberts, Scott A.; Brunini, Victor E.; Grillet, Anne M.	Mechanical and Electrochemical Response of a LiCoO2 Cathode using Reconstructed Microstructures	ELECTROCHIMICA ACTA	190	n/a	15-Jan	173098
Buchheit, Thomas E.; Susan, Donald F.; Massad, Jordan E.; McElhanon, James R.; Noebe, Ronald D.	Mechanical and Functional Behavior of High-Temperature Ni-Ti-Pt Shape Memory Alloys	METALLURGICAL AND MATERIALS TRANSACTIONS A-PHYSICAL METALLURGY AND MATERIALS SCIENCE	47A	4	1587-1599	151358
Nordquist, Christopher D.; Branch, Darren W.; Pluym, Tammy; Choi, Sukwon; Nguyen, Janet H.	MEMS switching of contour-mode aluminum nitride resonators for switchable and reconfigurable radio frequency filters	JOURNAL OF MICROMECHANICS AND MICROENGINEERING	26	10	n/a	LDRD
Durfee, Paul N.; Lin, Yu-Shen; Dunphy, Darren R.; Muniz, Ane J.; Butler, Kimberly S.	Mesoporous Silica Nanoparticle-Supported Lipid Bilayers (Protocells) for Active Targeting and Delivery to Individual Leukemia Cells	ACS NANO	10	9	8325-8345	190960

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Dinca, Mircea; Leonard, Francois	Metal-organic frameworks for electronics and photonics	MRS BULLETIN	41	11	854-857	180898
Talin, A. Alec; Jones, Reese E.; Hopkins, Patrick E.	Metal-organic frameworks for thermoelectric energy-conversion applications	MRS BULLETIN	41	11	877-882	LDRD
La Bauve, Elisa; Vernon, Briana C.; Ye, Dongmei; Rogers, David M.; Siegrist, Cathryn M.	Method for measuring the unbinding energy of strongly-bound membrane-associated	BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES	1858	11	2753-2762	190961
Miller, Philip R.; Narayan, Roger J.; Polsky, Ronen	Microneedle-based sensors for medical diagnosis	JOURNAL OF MATERIALS CHEMISTRY B	4	8	1379-1383	151337
Wright, A. F.; Modine, N. A.	Migration processes of the As interstitial in GaAs	JOURNAL OF APPLIED PHYSICS	120	21	n/a	180932
Balajewicz, Maciej; Tezaur, Irina; Dowell, Earl	Minimal subspace rotation on the Stiefel manifold for stabilization and enhancement of projection-based reduced order models for the compressible Navier-Stokes equations	JOURNAL OF COMPUTATIONAL PHYSICS	321	n/a	224-241	164678
Ferrie, Christopher; Blume-Kohout, Robin	Minimax Quantum Tomography: Estimators and Relative Entropy Bounds	PHYSICAL REVIEW LETTERS	116	9	n/a	165581
O'Brien, Christopher J.; Medlin, Douglas L.; Foiles, Stephen M.	Misoriented grain boundaries vicinal to the (111) < 1(1)over-bar0 > twin in nickel Part I: thermodynamics & temperature-dependent structure	PHILOSOPHICAL MAGAZINE	96	13	1285-1304	15-1052
O'Brien, Christopher J.; Foiles, Stephen M.	Misoriented grain boundaries vicinal to the (111) < 1(1)over-bar0 > twin in Nickel part II: thermodynamics of hydrogen segregation	PHILOSOPHICAL MAGAZINE	96	14	1463-1484	173116
Flicker, Jack; Brocato, Robert; Delhotal, Jarod; Neely, Jason; Sumner, Bjorn	Module-Level Paralleling of Vertical GaN PiN Diodes	2016 IEEE 4TH WORKSHOP ON WIDE BANDGAP POWER DEVICES AND APPLICATIONS (WIPDA)	n/a	n/a	139-142	180884
Stavila, Vitalie; Parthasarathi, Ramakrishnan; Davi, Ryan W.; El Gabaly, Farid; Sale, Kenneth L.	MOF-Based Catalysts for Selective Hydrogenolysis of Carbon Oxygen Ether Bonds	ACS CATALYSIS	6	1	55-59	180812
Ahmed, Adam S.; Wen, Hua; Ohta, Taisuke; Pinchuk, Igor V.; Zhu, Tiancong	Molecular beam epitaxy growth of SrO buffer layers on graphite and graphene for the integration of complex oxides	JOURNAL OF CRYSTAL GROWTH	447	n/a	12-May	165713
Chaudhari, Mangesh I.; Rempe, Susan B.; Asthagiri, D.; Tan, L.; Pratt, L. R.	Molecular Theory and the Effects of Solute Attractive Forces on Hydrophobic Interactions	JOURNAL OF PHYSICAL CHEMISTRY B	120	8	1864-1870	190365, 190961

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Dunn, Aaron; Dingreville, Remi; Capolungo, Laurent	Multi-scale simulation of radiation damage accumulation and subsequent hardening in neutron-irradiated alpha-Fe	MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING	24	1	n/a	178184
Siegal, Michael P.; Yelton, W. Graham; Perdue, Brian R.; Sava Gallis, Dorina F.; Schwarz, Haiqing L.	Nanoporous-Carbon as a Potential Host Material for Reversible Mg Ion Intercalation	JOURNAL OF THE ELECTROCHEMICAL SOCIETY	163	6	A1030-A1035	176606, 200269
Tuan Anh Ho; Criscenti, Louise J.; Wang, Yifeng	Nanostructural control of methane release in kerogen and its implications to wellbore production decline	SCIENTIFIC REPORTS	6	n/a	n/a	173102
Campione, Salvatore; Wendt, Joel R.; Keeler, Gordon A.; Luk, Ting S.	Near-Infrared Strong Coupling between Metamaterials and Epsilon-near-Zero Modes in Degenerately Doped Semiconductor Nanolayers	ACS PHOTONICS	3	2	293-297	200228
Merkel, Cory; Hasan, Raqibul; Soures, Nicholas; Kudithipudi, Dhireesha; Taha, Tarek	Neuromemristive Systems: Boosting Efficiency through Brain-Inspired Computing	COMPUTER	49	10	56-64	180885
Kent, Michael S.; La Bauve, Elisa; Vernon, Briana C.; Ye, Dongmei; Rogers, David M.	New Method for Measuring the Anchoring Energy of Strongly-Bound Membrane-Associated Proteins	BIOPHYSICAL JOURNAL	110	3	578A-578A	158832
Ting, Christina L.; Sorensen-Unruh, Karen E.; Stevens, Mark J.; Frischknecht, Amalie L.	Nonequilibrium simulations of model ionomers in an oscillating electric field	JOURNAL OF CHEMICAL PHYSICS	145	4	n/a	165824
Christian, Joshua M.; Ortega, Jesus D.; Ho, Clifford K.	NOVEL TUBULAR RECEIVER PANEL CONFIGURATIONS FOR INCREASED EFFICIENCY OF HIGH-TEMPERATURE SOLAR RECEIVERS	PROCEEDINGS OF THE ASME 9TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2015, VOL 1	1	n/a	n/a	173092
Burckel, D. Bruce; Finnegan, Patrick S.; Henry, M. David; Resnick, Paul J.; Jarecki, Robert L., Jr.	Oblique patterned etching of vertical silicon sidewalls	APPLIED PHYSICS LETTERS	108	14	n/a	173129
Wendt, Jeremy D.; Wells, Randy; Field, Richard V., Jr.; Soundarajan, Sucheta	On data collection, graph construction, and sampling in Twitter	PROCEEDINGS OF THE 2016 IEEE/ACM INTERNATIONAL CONFERENCE ON ADVANCES IN SOCIAL NETWORKS ANALYSIS AND MINING ASONAM 2016	n/a	n/a	985-992	180878
Seleson, Pablo; Du, Qiang; Parks, Michael L.	On the consistency between nearest-neighbor peridynamic discretizations and discretized classical elasticity models	COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING	311	n/a	698-722	165616
Dingreville, Remi; Berbenni, Stephane	On the interaction of solutes with grain boundaries	ACTA MATERIALIA	104	n/a	237-249	173116
Martin, James E.	On the origin of vorticity in magnetic particle suspensions subjected to triaxial fields	SOFT MATTER	12	25	5636-5644	LDRD

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Dehollain, Juan P.; Muhonen, Juha T.; Blume-Kohout, Robin; Rudinger, Kenneth M.; Gamble, John King	Optimization of a solid-state electron spin qubit using gate set tomography	NEW JOURNAL OF PHYSICS	18	n/a	n/a	165581
Waisman, E. M.; Reisman, D. B.; Stoltzfus, B. S.; Stygar, W. A.; Cuneo, M. E.	Optimization of current waveform tailoring for magnetically driven isentropic compression experiments	REVIEW OF SCIENTIFIC INSTRUMENTS	87	6	n/a	16-0870
Bochev, Pavel; Ridzal, Denis	Optimization-based additive decomposition of weakly coercive problems with applications	COMPUTERS & MATHEMATICS WITH APPLICATIONS	71	11	2140-2154	173025
Ting, Christina L.; Composto, Russell J.; Frischknecht, Amalie L.	Orientational Control of Polymer Grafted Nanorods	MACROMOLECULES	49	3	1111-1119	165824
Gopal, Chirranjeevi Balaji; El Gabaly, Farid; McDaniel, Anthony H.; Chueh, William C.	Origin and Tunability of Unusually Large Surface Capacitance in Doped Cerium Oxide Studied by Ambient-Pressure X-Ray Photoelectron Spectroscopy	ADVANCED MATERIALS	28	23	4692-4697	158702
Vineyard, Craig M.; Verzi, Stephen J.	Overcoming the Static Learning Bottleneck - the Need for Adaptive Neural Learning	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180885
Sershen, Cheryl L.; Plimpton, Steven J.; May, Elebeoba E.	Oxygen Modulates the Effectiveness of Granuloma Mediated Host Response to Mycobacterium tuberculosis: A Multiscale Computational Biology Approach	FRONTIERS IN CELLULAR AND INFECTION MICROBIOLOGY	6	n/a	n/a	LDRD
DeBenedictis, Erik	PERSPECTIVE: NEXT-GENERATION COMPUTING PARADIGMS AND THE INFORMATION REVOLUTION	COMPUTER	49	9	16-17	180819
Leenheer, Andrew J.; Jungjohann, Katherine L.; Zavadil, Kevin R.; Harris, Charles T.	Phase Boundary Propagation in Li-Alloying Battery Electrodes Revealed by Liquid-Cell Transmission Electron Microscopy	ACS NANO	10	6	5670-5678	158810
Reinke, Charles M.; El-kady, Ihab	Phonon-based scalable platform for chip-scale quantum computing	AIP ADVANCES	6	12	n/a	173029
Kadlec, Emil A.; Jarecki, Robert L.; Starbuck, Andrew; Peters, David W.; Davids, Paul S.	Photon-Phonon-Enhanced Infrared Rectification in a Two-Dimensional Nanoantenna-Coupled Tunnel Diode	PHYSICAL REVIEW APPLIED	6	6	n/a	200245, 189614
Ebeida, Mohamed S.; Mitchell, Scott A.; Swiler, Laura P.; Romero, Vicente J.; Rushdi, Ahmad A.	POF-Darts: Geometric adaptive sampling for probability of failure	RELIABILITY ENGINEERING & SYSTEM SAFETY	155	n/a	64-77	165617
Armstrong, Andrew M.; Allerman, Andrew A.	Polarization-induced electrical conductivity in ultra-wide band gap AlGaN alloys	APPLIED PHYSICS LETTERS	109	22	n/a	180884

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Phaneuf, Christopher R.; VanderNoot, Victoria A.; Koh, Chung-Yan	Portable Centrifugal Microfluidic System for Diagnostics in Resource-Limited Settings	2016 IEEE HEALTHCARE INNOVATION POINT-OF-CARE TECHNOLOGIES CONFERENCE (HI-POCT)	n/a	n/a	89-91	158820
Mickel, Patrick R.; Hughart, David; Lohn, Andrew J.; Gao, Xujiao; Mamaluy, Denis	Power signatures of electric field and thermal switching regimes in memristive SET transitions	JOURNAL OF PHYSICS D-APPLIED PHYSICS	49	24	n/a	173024
Matzen, Laura E.; Trumbo, Michael C.; Haass, Michael J.; Hunter, Michael A.; Silva, Austin	Practice makes imperfect: Working memory training can harm recognition memory performance	MEMORY & COGNITION	44	8	1168-1182	141529
Radvansky, Gabriel A.; D'Mello, Sidney K.; Abbott, Robert G.; Bixler, Robert E.	Predicting Individual Action Switching in Covert and Continuous Interactive Tasks Using the Fluid Events Model	FRONTIERS IN PSYCHOLOGY	7	n/a	n/a	158764
Jones, Reese E.; Templeton, Jeremy; Zimmerman, Jonathan	Principles of Coarse-Graining and Coupling Using the Atom-to-Continuum Method	MULTISCALE MATERIALS MODELING FOR NANOMECHANICS	245	n/a	223-259	151294
Butler, Kimberly S.; Durfee, Paul N.; Theron, Christophe; Ashley, Carlee E.; Carnes, Eric C.	Protocells: Modular Mesoporous Silica Nanoparticle-Supported Lipid Bilayers for Drug Delivery	SMALL	12	16	2173-2185	190960
Mowry, Curtis D.; Pimentel, Adam S.; Sparks, Elizabeth S.; Moorman, Matthew W.; Achyuthan, Komandoor E.	Pulsed Discharge Helium Ionization Detector for Highly Sensitive Aquametry	ANALYTICAL SCIENCES	32	2	177-182	199974, 173131, 151318
Vineyard, Craig M.; Verzi, Stephen J.; James, Conrad D.; Aimone, James B.	Quantifying Neural Information Content: A Case Study of the Impact of Hippocampal Adult Neurogenesis	2016 INTERNATIONAL JOINT CONFERENCE ON NEURAL NETWORKS (IJCNN)	n/a	n/a	5181-5188	180885, 194773
Moussa, Jonathan E.	QUANTUM CIRCUITS FOR QUBIT FUSION	QUANTUM INFORMATION & COMPUTATION	16	13-14	1113-1124	178675
DeBenedictis, Erik P.	Rebooting Computers as Learning Machines	COMPUTER	49	6	84-87	180819
Tencer, John; Carlberg, Kevin; Hogan, Roy; Larsen, Marvin	REDUCED ORDER MODELING APPLIED TO THE DISCRETE ORDINATES METHOD FOR RADIATION HEAT TRANSFER IN PARTICIPATING MEDIA	PROCEEDINGS OF THE ASME SUMMER HEAT TRANSFER CONFERENCE, 2016, VOL 2	2	n/a	n/a	186367
Rallard, Grey; Siefer, Christopher; Hu, Jonathan	REDUCING COMMUNICATION COSTS FOR SPARSE MATRIX MULTIPLICATION WITHIN ALGEBRAIC MULTIGRID	SIAM JOURNAL ON SCIENTIFIC COMPUTING	38	3	C203-C231	16-0790
Bauer, Stephen J.; Gardner, W. Payton; Lee, Hyunwoo	Release of radiogenic noble gases as a new signal of rock deformation	GEOPHYSICAL RESEARCH LETTERS	43	20	10688-10694	191137
Sun, Bingbing; Wang, Xiang; Liao, Yu-Pei; Ji, Zhaoxia; Chang, Chong Hyun	Repetitive Dosing of Fumed Silica Leads to Profibrogenic Effects through Unique Structure-Activity Relationships and Biopersistence in the Lung	ACS NANO	10	8	8054-8066	190960

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Schwarz, Thomas S. J.; Amer, Ahmed; Kroeger, Thomas; Miller, Ethan; Long, Darrell	RESAR: Reliable Storage at Exabyte Scale	2016 IEEE 24TH INTERNATIONAL SYMPOSIUM ON MODELING, ANALYSIS AND SIMULATION OF COMPUTER AND TELECOMMUNICATION SYSTEMS (MASCOTS)	n/a	n/a	211-220	13-1062
Agarwal, Sapan; Plimpton, Steven J.; Hughart, David R.; Hsia, Alexander H.; Richter, Isaac	Resistive Memory Device Requirements for a Neural Algorithm Accelerator	2016 INTERNATIONAL JOINT CONFERENCE ON NEURAL NETWORKS (IJCNN)	n/a	n/a	929-938	180885
Salerno, K. Michael; Agrawal, Anupriya; Perahia, Dvora; Grest, Gary S.	Resolving Dynamic Properties of Polymers through Coarse-Grained Computational Studies	PHYSICAL REVIEW LETTERS	116	5	n/a	15-0548
Dingreville, Remi; Karnesky, Richard A.; Puel, Guillaume; Schmitt, Jean-Hubert	Review of the synergies between computational modeling and experimental characterization of materials across length scales	JOURNAL OF MATERIALS SCIENCE	51	3	1178-1203	173116
Ling, Julia; Kurzawski, Andrew; Templeton, Jeremy	Reynolds averaged turbulence modelling using deep neural networks with embedded invariance	JOURNAL OF FLUID MECHANICS	807	n/a	155-166	180823
Kouri, D. P.; Surowiec, T. M.	RISK-AVERSE PDE-CONSTRAINED OPTIMIZATION USING THE CONDITIONAL VALUE-AT-RISK	SIAM JOURNAL ON OPTIMIZATION	26	1	365-396	180822
Jiang, Ruiwei; Guan, Yongpei; Watson, Jean-Paul	Risk-averse stochastic unit commitment with incomplete information	IIE TRANSACTIONS	48	9	838-854	173090
Rider, William; Witkowski, Walt; Kamm, James R.; Wildey, Tim	Robust verification analysis	JOURNAL OF COMPUTATIONAL PHYSICS	307	n/a	146-163	165612
Bondi, Robert J.; Fox, Brian P.; Marinella, Matthew J.	Role of atomistic structure in the stochastic nature of conductivity in substoichiometric tantalum pentoxide	JOURNAL OF APPLIED PHYSICS	119	12	n/a	180885
Armstrong, Andrew M.; Crawford, Mary H.; Jayawardena, Asanka; Ahyi, Ayayi; Dhar, Sarit	Role of self-trapped holes in the photoconductive gain of beta-gallium oxide Schottky diodes	JOURNAL OF APPLIED PHYSICS	119	10	n/a	180884, 191199
Sarobol, Pylin; Chandross, Michael; Carroll, Jay D.; Mook, William M.; Bufford, Daniel C.	Room Temperature Deformation Mechanisms of Alumina Particles Observed from In Situ Micro-compression and Atomistic Simulations	JOURNAL OF THERMAL SPRAY TECHNOLOGY	25	2-Jan	82-93	177962
Mount, Emily; Gaultney, Daniel; Vrijsen, Geert; Adams, Michael; Baek, So-Young	Scalable digital hardware for a trapped ion quantum computer	QUANTUM INFORMATION PROCESSING	15	12	5281-5298	13-0082

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Chaudhari, Mangesh I.; Nair, Jijeesh R.; Pratt, Lawrence R.; Soto, Fernando A.; Balbuena, Perla B.	Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion	JOURNAL OF CHEMICAL THEORY AND COMPUTATION	12	12	5709-5718	192678
Zeng, Lishan; Zhang, Jun; Sarovar, Mohan	Schedule path optimization for adiabatic quantum computing and optimization	JOURNAL OF PHYSICS A-MATHEMATICAL AND THEORETICAL	49	16	n/a	152501
Sava Gallis, Dorina F.; Chapman, Karena W.; Rodriguez, Mark A.; Greathouse, Jeffery A.; Parkes, Marie V.	Selective O-2 Sorption at Ambient Temperatures via Node Distortions in Sc-MIL-100	CHEMISTRY OF MATERIALS	28	10	3327-3336	165632
Li, Leigang; Sun, Liuyang; Gomez-Diaz, Juan Sebastian; Hogan, Nicki L.; Lu, Ping	Self-Assembled Epitaxial Au-Oxide Vertically Aligned Nanocomposites for Nanoscale Metamaterials	NANO LETTERS	16	6	3936-3943	180923
Su, Qing; Zhang, Wenrui; Lu, Ping; Fang, Shumin; Khatkhatay, Fauzia	Self-Assembled Magnetic Metallic Nanopillars in Ceramic Matrix with Anisotropic Magnetic and Electrical Transport Properties	ACS APPLIED MATERIALS & INTERFACES	8	31	20283-20291	180923
Beechem, Thomas E.; Shaffer, Ryan A.; Nogan, John; Ohta, Taisuke; Hamilton, Allister B.	Self-Heating and Failure in Scalable Graphene Devices	SCIENTIFIC REPORTS	6	n/a	n/a	165713, 173124
Meddens, Marjolein B. M.; Liu, Sheng; Finnegan, Patrick S.; Edwards, Thayne L.; James, Conrad D.	Single objective light-sheet microscopy for high-speed whole-cell 3D super-resolution	BIOMEDICAL OPTICS EXPRESS	7	6	2219-2236	173021
Beechem, Thomas E.; McDonald, Anthony E.; Fuller, Elliot J.; Talin, A. Alec; Rost, Christina M.	Size dictated thermal conductivity of GaN	JOURNAL OF APPLIED PHYSICS	120	9	n/a	180884
Braun, Jeffrey L.; Baker, Christopher H.; Giri, Ashutosh; Elahi, Mirza; Artyushkova, Kateryna	Size effects on the thermal conductivity of amorphous silicon thin films	PHYSICAL REVIEW B	93	14	n/a	LDRD
Wolf, Omri; Campione, Salvatore; Kim, Jin; Brener, Igal	Spectral filtering using active metasurfaces compatible with narrow bandgap III-V infrared detectors	OPTICS EXPRESS	24	19	21512-21520	189614
Severa, William; Parekh, Ojas; Carlson, Kristofor D.; James, Conrad D.; Aimone, James B.	Spiking Network Algorithms for Scientific Computing	2016 IEEE INTERNATIONAL CONFERENCE ON REBOOTING COMPUTING (ICRC)	n/a	n/a	n/a	180885
Pratt, Lawrence R.; Chaudhari, Mangesh I.; Rempe, Susan B.	Statistical Analyses of Hydrophobic Interactions: A Mini-Review	JOURNAL OF PHYSICAL CHEMISTRY B	120	27	6455-6460	190365

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Magyar, R. J.; Shulenburger, L.; Baczewski, A. D.	Stopping of Deuterium in Warm Dense Deuterium from Ehrenfest Time-Dependent Density Functional Theory	CONTRIBUTIONS TO PLASMA PHYSICS	56	5	459-466	165731
Pan, Kai; Guan, Yongpei; Watson, Jean-Paul; Wang, Jianhui	Strengthened MILP Formulation for Certain Gas Turbine Unit Commitment Problems	IEEE TRANSACTIONS ON POWER SYSTEMS	31	2	1440-1448	173090
Argibay, N.; Furnish, T. A.; Boyce, B. L.; Clark, B. G.; Chandross, M.	Stress-dependent grain size evolution of nanocrystalline Ni-W and its impact on friction behavior	SCRIPTA MATERIALIA	123	n/a	26-29	180900
LaFranchi, B. W.; McFarlane, K. J.; Miller, J. B.; Lehman, S. J.; Phillips, C. L., Lui, Z.	Strong regional atmospheric C-14 signature of respired CO2 observed from a tall tower over the midwestern United States	JOURNAL OF GEOPHYSICAL RESEARCH-BIOGEOSCIENCES	121	8	2275-2295	LDRD
Ortega, Jesus D.; Christian, Joshua M.; Ho, Clifford K.	STRUCTURAL ANALYSIS OF A DIRECT HEATED TUBULAR SOLAR RECEIVER FOR SUPERCRITICAL CO2 BRAYTON CYCLE	PROCEEDINGS OF THE ASME 9TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2015, VOL 1	1	n/a	n/a	14-0439
Alam, Todd M.; Kinnan, Mark K.; Wilson, Brendan W.; Wheeler, David R.	Sub-Equimolar Hydrolysis and Condensation of Organophosphates	CHEMISTRYSELECT	1	11	2698-2705	173115
Wheeler, Sarah S.; Ball, Cameron S.; Langevin, Stanley A.; Fang, Ying; Coffey, Lark L.	Surveillance for Western Equine Encephalitis, St. Louis Encephalitis, and West Nile Viruses Using Reverse Transcription Loop-Mediated Isothermal Amplification	PLOS ONE	11	1	n/a	173111
Dunn, Aaron; Dingreville, Remi; Martinez, Enrique; Capolungo, Laurent	Synchronous parallel spatially resolved stochastic cluster dynamics	COMPUTATIONAL MATERIALS SCIENCE	120	n/a	43-52	178184
Dingreville, Remi; Karnesky, Richard A.; Puel, Guillaume; Schmitt, Jean-Hubert	Synergies between computational modeling and experimental characterization of materials across length scales	JOURNAL OF MATERIALS SCIENCE	51	3	1176-1177	173116
Boyle, Timothy J.; Sivonxay, Eric	Synthesis and characterization of 2-hydroxy-pyridine modified Group 4 alkoxides	JOURNAL OF COORDINATION CHEMISTRY	69	9	1419-1438	LDRD
Boyle, Timothy J.; Neville, Michael L.; Parkes, Marie V.	Synthesis and characterization of a series of Group 4 phenoxy-thiol derivatives	POLYHEDRON	110	n/a	13-Jan	LDRD
Yang, Mengna; Jackson, David R.; Chen, JI; Xiong, Zubiao; Williams, Jeffery T.	TDOA Localization Method Based on De-embedding the Propagation Background	PROCEEDINGS OF THE 2016 TEXAS SYMPOSIUM ON WIRELESS AND MICROWAVE CIRCUITS AND SYSTEMS (WMCS)	n/a	n/a	n/a	158773
Cyr, Eric C.; Shadid, John N.; Tuminaro, Raymond S.	TEKO: A BLOCK PRECONDITIONING CAPABILITY WITH CONCRETE EXAMPLE APPLICATIONS IN NAVIER-STOKES AND MHD	SIAM JOURNAL ON SCIENTIFIC COMPUTING	38	5	S307-S331	180821

Authors	Article Title	Source	Volume	Issue	Pages	Project
Kearney, Sean P.; Guildenbecher, Daniel R.	Temperature measurements in metalized propellant combustion using hybrid fs/ps coherent anti-Stokes Raman scattering	APPLIED OPTICS	55	18	4958-4966	180876
DeBenedictis, Erik P.	The Boolean Logic Tax	COMPUTER	49	4	79-82	180819
Hooper, R. J.; Adams, D. P.; Hirschfeld, D.; Manuel, M. V.	The Effect of Substrate Microstructure on the Heat-Affected Zone Size in Sn-Zn Alloys Due to Adjoining Ni-Al Reactive Multilayer Foil Reaction	JOURNAL OF ELECTRONIC MATERIALS	45	1	11-Jan	173653
DeBenedictis, Erik P.	The Search for Computing's Secretariat	COMPUTER	49	8	88-91	180819
Dahms, Rainer N.; Oefelein, Joseph C.	The significance of drop non-sphericity in sprays	INTERNATIONAL JOURNAL OF MULTIPHASE FLOW	86	n/a	67-85	2015-3314
George, Matthew C.; Rodriguez, Mark A.; Kent, Michael S.; Brennecka, Geoff L.; Hopkins, Patrick E.	Thermal Conductivity of Self-Assembling Symmetric Block Copolymer Thin Films of Polystyrene-Block-Poly(methyl methacrylate)	JOURNAL OF HEAT TRANSFER-TRANSACTIONS OF THE ASME	138	2	n/a	10-0018
Xiao, Xiaoyin; Miller, Lance L.; Bernstein, Robert; Hochrein, James M.	Thermal degradation of -carotene studied by ion mobility atmospheric solid analysis probe mass spectrometry: full product pattern and selective ionization enhancement	JOURNAL OF MASS SPECTROMETRY	51	4	309-314	14-0193
van Swol, Frank; Zhou, Xiaowang W.; Challa, Sivakumar R.; Martin, James E.	Thermodynamic properties of model CdTe/CdSe mixtures	MOLECULAR SIMULATION	42	1	14-24	165697
Miller, Philip; Moorman, Matthew; Manginell, Ron; Ashlee, Carlee; Brener, Igal	Towards an Integrated Microneedle Total Analysis Chip for Protein Detection	ELECTROANALYSIS	28	6	1305-1310	151337
Barrows, Wesley; Dingreville, Remi; Spearot, Douglas	Traction-separation relationships for hydrogen induced grain boundary embrittlement in nickel via molecular dynamics simulations	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	650	n/a	354-364	173116
Ullman, Andrew M.; Brown, Jonathan W.; Foster, Michael E.; Leonard, Francois; Leong, Kirsty	Transforming MOFs for Energy Applications Using the Guest@MOF Concept	INORGANIC CHEMISTRY	55	15	7233-7249	180898
Moussa, Jonathan E.	Transversal Clifford gates on folded surface codes	PHYSICAL REVIEW A	94	4	n/a	178675
Wang, Jian-jun; Wang, YI; Ihlefeld, Jon F.; Hopkins, Patrick E.; Chen, Long-Qing	Tunable thermal conductivity via domain structure engineering in ferroelectric thin films: A phase-field simulation	ACTA MATERIALIA	111	n/a	220-231	LDRD
Suwardi, Ady; Prasad, Bhagwati; Lee, Shinbuhm; Choi, Eun-Mi; Lu, Ping	Turning antiferromagnetic Sm0.34Sr0.66MnO3 into a 140 K ferromagnet using a nanocomposite strain tuning approach	NANOSCALE	8	15	8083-8090	180923

Authors	Article Title	Source	Volume	Issue	Pages	Project
Boubanga-Tombet, Stephane; Wright, Jeremy B.; Lu, Ping; Williams, Michael R. C.; Li, Changyi	Ultrafast Carrier Capture and Auger Recombination in Single GaN/InGaN Multiple Quantum Well Nanowires	ACS PHOTONICS	3	12	2237-2242	191196, 165704
Baboly, M. Ghasemi; Alaie, S.; Reinke, C. M.; El-Kady, I.; Leseman, Z. C.	Ultra-high frequency, high Q/volume micromechanical resonators in a planar AlN phononic crystal	JOURNAL OF APPLIED PHYSICS	120	3	n/a	173029, 191080
Ling, Julia; Ruiz, Anthony; Lacaze, Guilhem; Oefelein, Joseph	UNCERTAINTY ANALYSIS AND DATA-DRIVEN MODEL ADVANCES FOR A JET-IN-CROSSFLOW	PROCEEDINGS OF THE ASME TURBO EXPO: TURBINE TECHNICAL CONFERENCE AND EXPOSITION, 2016, VOL 5C	5C	n/a	n/a	LDRD
Coltrin, Michael E.; Kee, Robert J.	Unified Nusselt- and Sherwood-number correlations in axisymmetric finite-gap stagnation and rotating-disk flows	INTERNATIONAL JOURNAL OF HEAT AND MASS TRANSFER	102	n/a	122-132	LDRD
Zarzar, Lauren D.; Swartzentruber, B. S.; Donovan, Brian F.; Hopkins, Patrick E.; Kaehr, Bryan	Using Laser-Induced Thermal Voxels to Pattern Diverse Materials at the Solid-Liquid Interface	ACS APPLIED MATERIALS & INTERFACES	8	33	21134-21139	164677
Gamble, John King; Harvey-Collard, Patrick; Jacobson, N. Tobias; Baczewski, Andrew D.; Nielsen, Erik	Valley splitting of single-electron Si MOS quantum dots	APPLIED PHYSICS LETTERS	109	25	n/a	173883
Weck, Philippe F.; Kim, Eunja; Wang, Yifeng	van der Waals forces and confinement in carbon nanopores: Interaction between CH4, COOH, NH3, OH, SH and single-walled carbon nanotubes	CHEMICAL PHYSICS LETTERS	652	n/a	22-26	173102
Dickerson, Jeramy R.; Allerman, Andrew A.; Bryant, Benjamin N.; Fischer, Arthur J.; King, Michael P.	Vertical GaN Power Diodes With a Bilayer Edge Termination	IEEE TRANSACTIONS ON ELECTRON DEVICES	63	1	419-425	180884
Cooper, Candice F.; Taylor, Paul A.	VIRTUAL SIMULATION OF BLAST, BEHIND-ARMOR BLUNT TRAUMA, AND PROJECTILE PENETRATION LEADING TO INJURY OF LIFE-CRITICAL ORGANS IN THE HUMAN TORSO	PROCEEDINGS OF THE ASME INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION, 2015, VOL 3	3	n/a	n/a	165554
Haniff, Shivonne; Taylor, Paul; Brundage, Aaron; Burnett, Damon; Cooper, Candice	VIRTUAL SIMULATION OF THE EFFECTS OF INTRACRANIAL FLUID CAVITATION IN BLAST-INDUCED TRAUMATIC BRAIN INJURY	PROCEEDINGS OF THE ASME INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION, 2015, VOL 3	n/a	n/a	n/a	165554
Pruski, Marek; Sadow, Aaron D.; Slowing, Igor I.; Marshall, Christopher L.; Stair, Peter	Virtual Special Issue on Catalysis at the US Department of Energy's National Laboratories	ACS CATALYSIS	6	5	3227-3235	180812

Authors	Article Title	Source	Volume	Issue	Pages	Project
Ho, Clifford K.; Mills, Brantley; Christian, Joshua M.	VOLUMETRIC PARTICLE RECEIVERS FOR INCREASED LIGHT TRAPPING AND HEATING	PROCEEDINGS OF THE ASME 10TH INTERNATIONAL CONFERENCE ON ENERGY SUSTAINABILITY, 2016, VOL 1	n/a	n/a	n/a	14-0439
Baczewski, A. D.; Shulenburger, L.; Desjarlais, M. P.; Hansen, S. B.; Magyar, R. J.	X-ray Thomson Scattering in Warm Dense Matter without the Chihara Decomposition	PHYSICAL REVIEW LETTERS	116	11	n/a	165731

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ABSTRACT

This report summarizes progress from the Laboratory Directed Research and Development (LDRD) program during fiscal year 2017. In addition to the programmatic overview, the report includes progress reports from 344 individual R&D projects in 14 categories.

LDRD ANNUAL REPORT STAFF

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