



Los Alamos National Laboratory

Laboratory Directed Research and Development

FY18 Annual Progress Report



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Structure of this Report

In accordance with U.S. Department of Energy Order (DOE) 413.2C, the Laboratory Directed Research and Development (LDRD) annual report for fiscal year 2018 (FY18) provides summaries of each LDRD-funded project for the fiscal year, as well as technical outcomes for completed projects. The report is organized as follows:

Overview: An introduction to the LDRD program at Los Alamos National Laboratory (LANL), the program's structure and strategic values, the LDRD portfolio management process, and highlights of outstanding accomplishments by LDRD researchers.

Project Summaries: The project summaries are organized by Focus Areas – Complex Natural and Engineered Systems, Information Science and Technology, Materials for the Future, Nuclear and Particle Futures, and Science of Signatures. Project descriptions are included for continuing projects and project descriptions and technical outcomes are included for projects that ended in FY18.

Los Alamos LDRD project identification numbers consists of three parts. The first is the fiscal year in which the project was initially funded, the second is a unique numerical identifier, and the third identifies the project component.

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Leadership Perspectives

“LDRD is central to science, technology, and engineering strategy at Los Alamos as articulated in our Laboratory Agenda, and I cannot imagine being successful without it. Our LDRD objectives of advancing mission agility, capability, and people align with and derive from this strategy. Because of LDRD's importance we must also ensure that we execute our LDRD program with the highest standards of transparency and objectivity and an unwavering commitment to robust peer review.”

– **John Sarrao**, Deputy Director for Science, Technology, & Engineering

Retrospective from LDRD Program Director Bill Priedhorsky

“LDRD has remarkable power in convening the Laboratory’s staggering talent to consider the problems that lie between ourselves and our future.”

– **Bill Priedhorsky**, LDRD Program Director



Even 12 years into my service as Laboratory Directed Research and Development (LDRD) Program Director, I am impressed every day by what LDRD delivers to this great Laboratory. With a proposal success rate that hovers around 15% obtaining LDRD funding is a rigorous challenge, and we demand the same rigor in project execution. What LDRD delivers, dollar for dollar, is worth all of the effort. We see the future of the Laboratory being built project by project on the path to new mission solutions – accelerators for the future, the nexus of climate change and infrastructure, new sensors and materials for nuclear deterrence – to touch just a few examples. Mission capabilities ranging across fundamental materials science, biochemical fundamentals of life, and the nature of atoms, nuclei, and quarks enable us to achieve solutions once thought impossible.

As we committed to ourselves in the 2016 LDRD charter, LDRD will always insist on the highest standards of creativity and innovation, equaling or exceeding our national and international peers. This has not changed under the new Triad leadership at Los Alamos (which began shortly after the start of fiscal year 2019). In fact, the LDRD Program Office has been streamlined and elevated in the new organization, reporting directly to the Deputy Director for Science, Technology, & Engineering. LDRD’s success is due to an extraordinary Program Office that encompasses technical leadership, administration, budget, and IT tools; each vacancy on our team attracts extraordinary applicants, testifying to the drawing power of the program.

LDRD has remarkable power in convening the Laboratory’s staggering talent to consider the problems that lie between ourselves and our future. Proposal writing, though it might feel like a chore at times, is the place where ideas and teams come together and where the charter of future LDRD projects is built. That LDRD demands interdisciplinary collaboration is deeply ingrained in Laboratory culture, and participation in LDRD is seen by management as an essential step in career development. LDRD panels are a place for staff to come together to discuss evolving science and engineering across the breadth of the Laboratory. We insist that LDRD project leaders contribute to workforce development whether through

recruiting new talent, growing mid-career leadership, or expanding the reputation of our senior staff. One of our contributions to staff development is the Assistant Chair program for Directed Research review panels, which brings in promising early career staff in a non-voting role, giving them a window into strategy that was formerly reserved for more senior staff.

LDRD is not unique to Los Alamos. LDRD leaders from Los Alamos, Livermore, Sandia, Nevada, and Headquarters convene quarterly to learn each other's best practices and share the great successes of LDRD with all who will listen. We are particularly interested in learning from each other about how we can best understand the many long-term impacts of LDRD. Furthermore, LDRD is not unique to NNSA. During my tenure as LDRD lead for Los Alamos, I have seen LDRD increase in its scale and rigor across the DOE Complex, becoming central to the strategy of our sister Labs. Notably, LDRD rates at the major non-NNSA labs are now within a fraction of a percent of the NNSA standard. Every Lab agrees on the goals of LDRD: mission agility, ST&E excellence (capability), and workforce development (people). We at LDRD remain firmly committed to our investment in the future of the Laboratory and the Nation.

Future prospects from LDRD Program Deputy Director Laura Stonehill

“I am struck by the remarkable talent at this Laboratory and the creativity and innovation displayed in LDRD projects and proposals. The commitment of our technical staff to cutting-edge ST&E in support of Lab missions is inspiring.”
– **Laura Stonehill**, LDRD Program Deputy Director



I am pleased to have joined the Los Alamos LDRD program as the new Deputy Program Director early in fiscal year 2019. As Deputy Program Director, I will share in the formulation, implementation, and strategic direction of LDRD and will work closely with Laboratory and external leadership at all levels.

Even just a few months into my time in the LDRD program, I am struck by the remarkable talent at this Laboratory and the creativity and innovation displayed in LDRD projects and proposals. The commitment of our technical staff to cutting-edge ST&E in support of Lab missions is inspiring. I am also thrilled to be working with the talented and dedicated professionals who make up the LDRD Program Office staff – working with this team every day is such a pleasure.

One of my first activities as LDRD Deputy Director has been to engage in a series of meetings with Division-level leadership across the Laboratory. These conversations have given me a clearer perspective on the breadth and diversity of the Laboratory and have sparked thinking and discussion within the LDRD program about evolving the Los Alamos LDRD program to make it even more inclusive and impactful. As we look to the future, we recommit ourselves to the ongoing effectiveness and excellence of LDRD, while working to better document its long-term impacts, to ensure that LDRD includes the highest-impact transformative work, and to communicate LDRD outcomes across the Lab and beyond.

“We at LDRD remain firmly committed to our investment in the future of the Laboratory and the Nation.” – **Bill Priedhorsky**, LDRD Program Director

Overview

The heart of the LDRD program is high-risk, high-reward research that creates innovative technical solutions for some of our nation's most difficult challenges. The program follows strategic guidance derived from the missions of the U.S. Department of Energy, the National Nuclear Security Administration, and the Laboratory. To execute that strategy, the LDRD program creates a free market for ideas that draws upon the bottom-up creativity of the Laboratory's best and brightest researchers. The combination of strategic guidance and free-market competition provides a stream of capabilities that position the Laboratory for mission agility.

The LDRD program provides the Laboratory Director with the opportunity to strategically invest in potentially transformative research that strengthens the Laboratory's capabilities to address national security challenges. Funded in FY18 with approximately 5.5% of the Laboratory's overall budget, the LDRD program helps Los Alamos anticipate, innovate, and deliver world-class science and engineering.

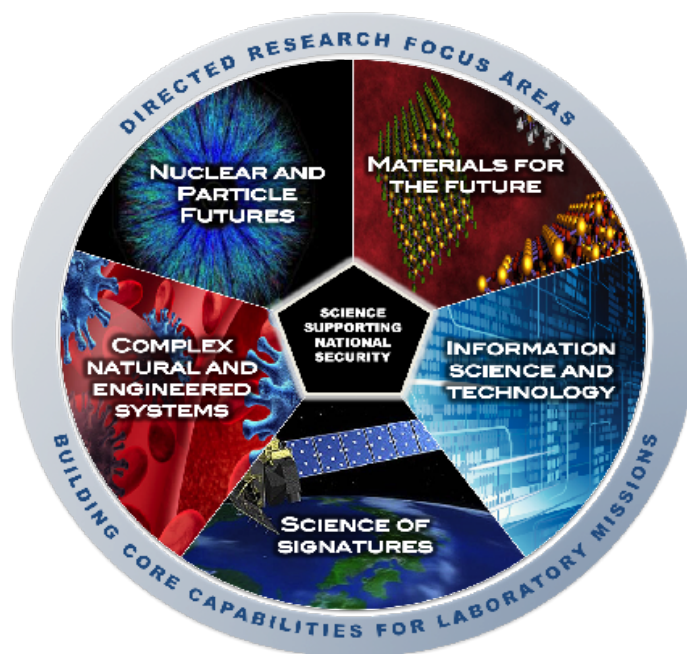
Program Structure

The Los Alamos LDRD program is organized into five program components with distinct institutional objectives: Directed Research (DR), flagship investments in mission solutions; Exploratory Research (ER), smaller projects that invest in people and skills that underpin key Laboratory capabilities; Early Career Research (ECR), supporting the development of early-career researchers; Mission Foundations Research (MFR), translating discovery into innovative solutions; and Postdoctoral Research and Development (PRD), recruiting bright, qualified, early-career scientists and engineers. In FY18, the LDRD program funded 342 projects with total costs of \$124.5 million. These projects were selected through a rigorous and highly competitive peer review process and are reviewed formally and informally throughout the fiscal year. The LDRD program holds a reserve each year to make modest investments that address new opportunities. In FY18, the reserve budget grew mid-year to approximately \$7M due to Lab growth and a rebate from the absence of weather-related closures.

Directed Research

The DR component makes long-range investments in multidisciplinary scientific projects in key competency or technology-development areas. In FY18, LDRD funded 50 DR projects, which represents approximately 51% of the program's

research funds. Directed Research projects are typically funded up to a maximum of \$1.7M per year for three years. Directed Research is organized around Focus Areas that define key areas of science, technology, and engineering in support of Los Alamos missions. The Focus Areas map to the Los Alamos science pillars, plus an additional multi-disciplinary Focus Area that is not captured by the pillars. Between them, they capture the capabilities that are essential to our Laboratory missions in the long term (3-15 years). For each Focus Area, coordinators led a process to engage broadly with the Lab to set investment priorities for the FY18 Strategic Investment Plan, published Lab-wide.



Exploratory Research

The ER component is focused on developing and maintaining technical staff competencies in key strategic disciplines that form the foundation of the Lab's readiness for future national missions. Largely focused on a single discipline, ER projects explore highly innovative ideas that underpin Lab programs. In FY18, LDRD funded 173 ER projects, which represents approximately 36% of the program's research funds. Exploratory Research projects are funded up to an average maximum of \$350K per year for three years.

Unlike DR proposals, division endorsements are not required for ER proposals; instead, this component of the LDRD program is operated as an open and competitive path for every staff member to pursue funding for his/her great idea. The ER component is a critical channel for bottom-up creativity. Nonetheless, it is strongly driven by mission needs via the definition of the ER research categories and investment between them.

Directed Research Focus Areas	Mission Impact
Information Science and Technology	Advance theory, algorithms, and high-performance computing to address national security challenges.
Materials for the Future	Enable controlled functionality and performance prediction through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano to microscopic scales, to bulk material.
Science of Signatures	Develop and deploy new measurement systems whereby understanding the unique elements of threats or events allows us to identify and assess them within complex environments.
Nuclear and Particle Futures	Ensure the safety, security, and surety of the Nation's nuclear stockpile, address emerging global threats, enable and safeguard future nuclear energy systems, and increase our understanding of the universe.
Complex Natural and Engineered Systems	Understand, predict, integrate, design, engineer, and/or control complex systems that significantly impact national security.

Exploratory Research Technical Categories	Capability Development
Atomic, Molecular, Quantum, and Optical Sciences	Quantum atomic, molecular and optical systems
Biological Sciences	Biosciences
Chemical Sciences	Chemistry
Computational and Numerical Methods	Information and knowledge sciences, computer and computational sciences
Computer Science, Mathematics, and Data Science	High-performance computing, data analysis, and data-driven science
Defects and Interfaces in Materials	Theoretical, computation and modeling, and experimental methods to understand defects and interfaces in materials
Earth, Planetary, and Space Sciences	Earth and space sciences
Emergent Phenomena in Materials Functionality	Theory, computation and modelling, and experimental methods to understand behavior of materials
Engineering Applications	Weapons science and engineering, advanced manufacturing, sensors, and remote sensing
High-Energy Density, Plasma, and Fluid Physics	High-energy density plasmas and fluids and beams
Measurement Science, Instrumentation, and Diagnostics	Measurement methods that enable new scientific discovery
Nuclear and Particle Physics, Astrophysics, and Cosmology	Nuclear physics, astrophysics, and cosmology

Early Career Research

The ECR component of the LDRD program is designed to strengthen the Laboratory's scientific workforce by providing support to exceptional staff members during their crucial early career years. In FY18, the LDRD program funded 34 ECR projects, which represents approximately 4% of the program's research funds. This included 18 new starts, which is a significant increase from previous fiscal years (i.e. 9 new starts in FY17; 8 in FY16). The increased support for early career staff reflects a response to the steady demand for early career support across the Laboratory, as well as an intent to aid in the sometimes challenging transition from postdoc to full-time staff member and to stimulate research in disciplines supported by the LDRD program. ECR projects are funded up to \$225K per year for two years.

Postdoc Research and Development

The PRD component ensures the vitality of the Laboratory by recruiting outstanding researchers. Through this investment, the LDRD program funds postdoctoral fellows to work under the mentorship of PIs. The primary criterion for selection of LDRD-supported postdocs is the raw scientific and technical talent of the candidate, with his or her specialty a secondary factor. In FY18, LDRD funded 73 PRD projects, which represents approximately 6% of the program's research funds.

PRD projects are funded under two appointment types intended to represent the most promising among the Laboratory postdoc population—Director's Postdoctoral Fellows and Distinguished Postdoctoral Fellows. Distinguished fellows are supported at a higher salary and typically show evidence of providing a new approach or insight to a major problem that will likely have a major impact in their research field. To recognize their role as future science and technology leaders, Distinguished postdoc fellows are named after some of the greatest leaders of the Laboratory's past, such as Los Alamos Medal laureate Darleane Christian Hoffman. In FY18, LDRD supported 52 Director's and 14 Distinguished fellows, with 3 Director's fellows selected as Distinguished during the fiscal year. Throughout a Director's postdoc fellow appointment (2 years, extendable to 3) or Distinguished (3 years), the LDRD program encourages conversion to staff. In FY18, the LDRD program continued support for 4 former Director's postdoc fellows who converted to staff prior to FY18.

LDRD also encourages collaboration between postdocs and Laboratory staff. More postdocs are hired through DR and ER projects than directly through PRD appointments. Counting both avenues, in FY18 the LDRD program supported 51% of the 556 postdocs who spent at least part of the year at the Laboratory. The average population throughout the year was 281.

LDRD Postdocs Receive 2018 Postdoctoral Distinguished Performance Awards

The Laboratory established the Postdoctoral Distinguished Performance Awards to honor outstanding postdoc achievements that significantly impact the Laboratory's scientific efforts and status in the scientific community.



Lukasz Cincio's research interests lie at the interface between Condensed Matter Physics and Quantum Information Theory. The main goal of his project is to create a scalable, numerical tool that will enable insights into two-dimensional quantum systems.



Osman El-Atwani is developing a fundamental understanding of radiation effects and plasma material interactions in tungsten-based materials. Osman converted to a scientist in the Materials Science and Technology Division in early FY19.

Mission Foundations Research (MFR)

Initiated in FY17, the underlying objective of Mission Foundations Research (MFR) is to translate discovery into innovative solutions. The MFR component funds applied science and engineering in the technology readiness level (TRL) 3-5 range, targeting mission problems defined in advance by mission champions across the Laboratory. Technical readiness levels are used by many federal agencies, such as the U.S. Department of Homeland Security, to estimate the maturity of a technology. Proposed MFR projects must be at TRL 2 and have a solid scientific foundation. They are funded for up to 2 years. In FY18, the LDRD program funded 12 MFR projects, which represents a \$4.2M total investment.

FY18 MFR Projects		
FY Start	Title	Problem Statement
FY17	Pellet Cracking During Fabrication of Pu-238 Oxide Fuel	Manufacturing Process Agility and Innovation
FY17	Direct Electrolytic Reduction of Plutonium Oxide Surrogates	Manufacturing Process Agility and Innovation
F17	Coherent Radio Frequency Collection Through Computation for CubeSat Constellations	Dominance of the Electromagnetic Spectrum
FY17	Insensitive High Explosives using 3-picrylamino-triazole (PATO)	Alternative Insensitive High Explosive
FY18	Additive Re-Manufacturing Guided by Process and Hydrodynamic Modeling	Advanced manufacturing for non-SNM Nuclear Explosive Package components and materials
FY18	Engineered Functionality and Structural Hierarchy in Additively Manufactured Materials	Advanced manufacturing for non-SNM Nuclear Explosive Package components and materials
FY18	New Methods for Producing Stockpile Equivalent High Explosive Components	Advanced manufacturing for non-SNM Nuclear Explosive Package components and materials
FY18	Long-Range In-Situ Acoustic Diagnosis and Monitoring of Molten-Salt Systems	Electro-Chemistry of Molten-Salt Systems under Extreme Radiation Environments
FY18	Noninvasive Thermal Mass Flow Meter for Safeguards	Analytics for WMD Monitoring
FY18	Nonlinear Elastic Wave Measurements for Diagnosing Aging in Pentaerythritol Tetranitrate	Analytics for WMD Monitoring
FY18	Multiscale Relational Analytics for Weapons of Mass Destruction (WMD) and Proliferation Activity Monitoring	Analytics for WMD Monitoring
FY18	Disrupting Actinide Aqueous Processing: Additively Manufacturing High-Speed Counter-Current Chromatography Devices	Manufacturing Process Agility and Innovation

■ Project selected for Phase II funding in FY19

Selecting and Managing LDRD Projects

The LDRD program is the vehicle by which the Laboratory harvests the ideas of some of our best and brightest scientists and engineers to execute DOE and NNSA missions. This bottom-up approach is balanced by a program management strategy in which Senior Laboratory leadership sets science and technology priorities, then opens an LDRD competition for ideas across the breadth of the Laboratory. Panels formed from the Laboratory's intellectual leaders rigorously review proposals. Conflict of interest is mitigated, and carefully formulated evaluation criteria support the commitment to fair assessment practices. In FY18, DR proposal assessment criteria was refactored to emphasize the LDRD goals—capability, mission agility, and people. The selection processes are modeled on best practices established by the National Science Foundation (NSF) and National Institutes of Health (NIH).

To guarantee fairness and transparency and to ensure that the strongest proposals are funded, the selection panels include managers and technical staff drawn from the full range of technical divisions. Serving on an LDRD selection panel is often a starting point on the path to leadership roles in the scientific community. Past LDRD panelists have gone on to be Laboratory Fellows, division leaders, program directors, association Fellows, and chief scientists, while others have become leaders in academia.

Benefits of Serving on LDRD Panels

The mission of the Laboratory is to solve the nation's most difficult national security problems. By their nature, these problems lack a well-defined path to solution. In fact, the path is often completely unknown. It is rare that such creative work is done alone; the ideas and results from many colleagues are needed, often drawn out in conferences, hallway conversations, journals, and seminars. LDRD is an internal arena in which Laboratory staff serve as peer reviewers and play a key role of interaction in the scientific process. Proposal selection panelists are chosen for their subject-matter expertise, and the discussions in which they engage are not only critical to the LDRD process, but they also provide an opportunity for panelists to educate themselves on the latest results and practices and expose themselves to opportunities for collaboration. As noted in an evaluation of peer review conducted by the UK House of Commons, "Peer review is regarded as an integral part of a researcher's professional activity; it helps them become part of the research community."

Annual Project Appraisals

In FY18, the LDRD program reviewed every multi-year project funded in the previous year (not including PRDs, which are reviewed by the Postdoc Program Office). This occurred in various formats, from formal appraisals with external reviewers, to assessments organized by line managers, to informal visits with PIs, to written appraisals of ended projects. The primary objective of the reviews is to assess progress and provide peer input to help PIs maintain the highest quality of work. They also help the LDRD Program Office manage the program portfolio.

Continuing DR projects are appraised every year with a half-day project appraisal at the beginning of year 2, a shorter progress appraisal at the beginning of year 3, and a final project appraisal after the project ends, based on the written final project report. External reviewers playing an important role in the second year. The internal-external review is open to all Laboratory staff. Four project appraisers – two internal and two external – are nominated by the PI and approved by the LDRD Program Director. When appropriate, the appraisal is held as part of a broader workshop hosted by the Laboratory. The Chair of the project appraisal panel is responsible for writing a formal report of the review that details how well a project is addressing and meeting its goals and documenting any weaknesses the panel may have observed. The PI is then required to respond to the concerns documented in the report with a revised project plan. The average score for second-year DR projects appraised in FY18 was 4.0, or "excellent." The average score rose to the "excellent/outstanding" range for third-year (4.5) and final appraisals (4.3), pointing to the efficacy of the appraisal process to help PIs maintain the highest quality of work.

Written reviews, held in the LDRD archives, address: (1) accomplishments; (2) quality of science and technology, relevance to Laboratory and national missions, progress toward goals and milestones, project leadership, and the degree to which the project may establish or sustain a position of scientific leadership for the Laboratory; and (3) recommendations by the committee for changes in the scope or approach of the project.

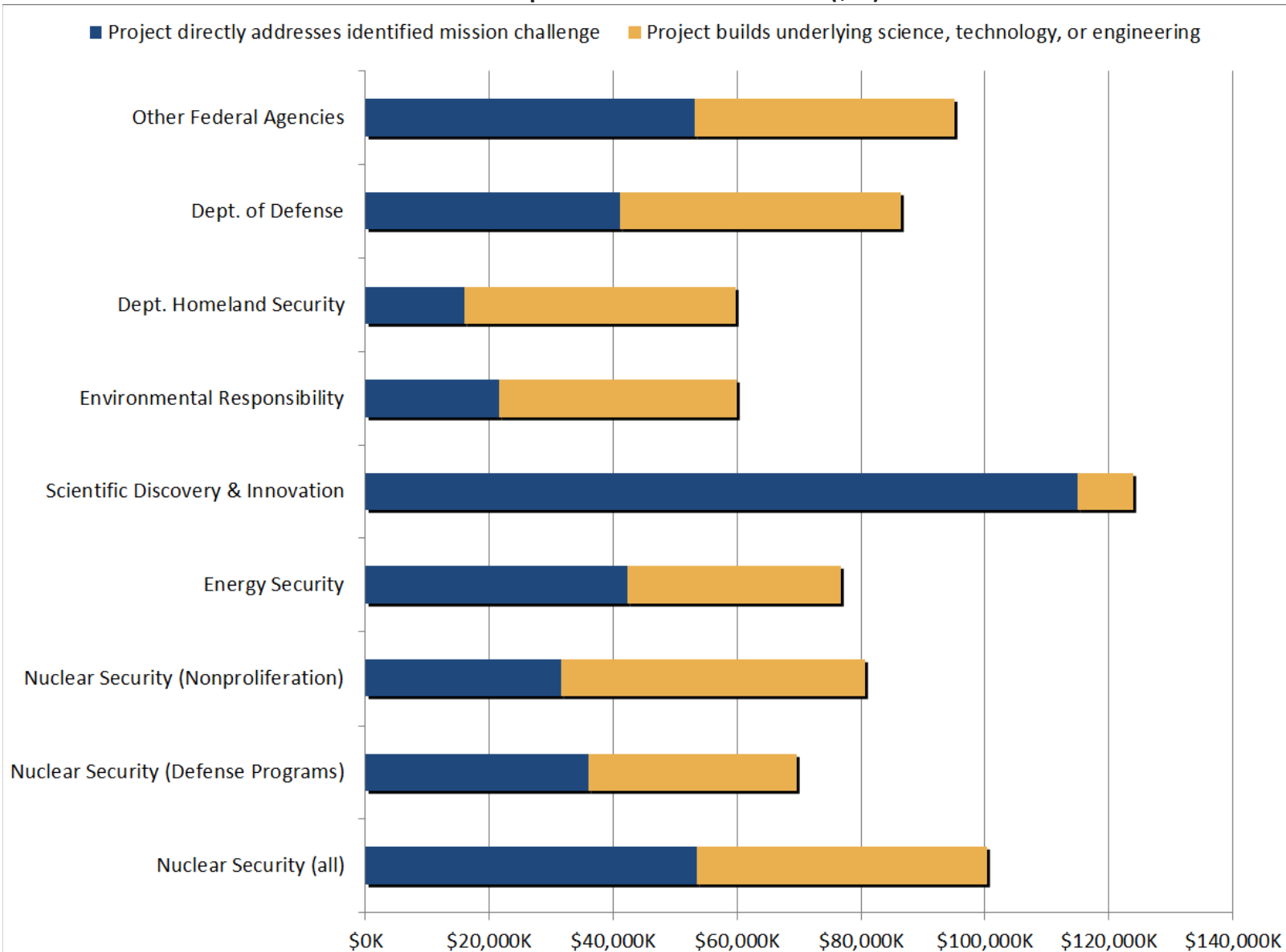
In addition to formal project appraisals, which are conducted annually, the LDRD program leaders meet informally with PIs in their labs. The purpose of these one-on-one meetings is to give PIs individualized assistance and to determine what the LDRD Program Office can do to positively impact success of the project.

Continuing ER and ECR projects are appraised in their first and second years. The LDRD Deputy Program Director collaborates with the technical divisions to conduct project appraisals.

Mission Relevance

Mission relevance is one of the most important criteria in the evaluation of a potential LDRD project; it is carefully considered in project selection and tracked annually through the data sheet process. Many of the technologies that put Los Alamos on the map have deep roots in LDRD and are valuable to DOE and NNSA mission areas of nuclear security, energy security, environmental remediation, and scientific discovery and innovation. LDRD work also benefits the national security missions of the Department of Homeland Security, the Department of Defense, and other Federal agencies. As a result, the scientific advances and technology innovations from LDRD provide multiple benefits to all Los Alamos stakeholders, consistent with Congressional intent and the Laboratory's scientific strategy.

Mission Impact of FY18 LDRD Portfolio (\$M)



First and foremost, Los Alamos LDRD projects are required to address one or more of the DOE or NNSA mission areas. Due to the nature of basic R&D, the work may also benefit the mission challenges of other Federal agencies. The sum of the total LDRD investment in relevant missions is far greater than the annual LDRD budget; investment in one project often contributes to and impacts multiple missions.

Mission Success Highlights

Cold Cathodes for Next Generation Electron Accelerators: Methodologies for Radically Improving Performance and Robustness (20150394DR)

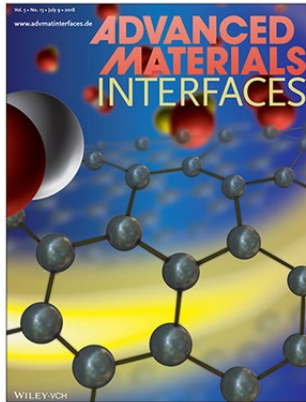


Figure. *Advanced Materials Interfaces* back cover featured LDRD research in July 2018.

DOE-commissioned studies point to electron sources as one of the highest accelerator R&D priorities for the next decade, requiring a transformational advance in cold cathode performance. LDRD researchers and their collaborators have developed a unique approach, decoupling two competing physical mechanisms that have prevented scientists from improving cold cathode efficiency and lifetime. Rational design of cathode materials is a new frontier which can scale to address evolving needs of existing and future accelerators.

Mission Foundations Research Dedicated to Advanced Manufacturing

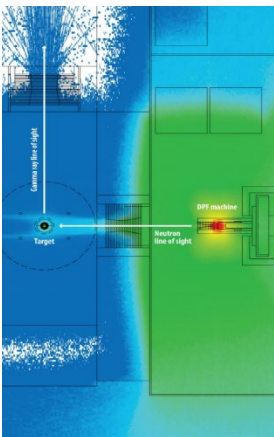
Two FY18 LDRD projects dedicated to advanced manufacturing for non-SNM Nuclear Explosive Package components and materials were selected for Phase II funding extending into FY19.

New Methods for Producing Stockpile Equivalent High Explosive Components (20180605ER)

This innovation aims to provide the basis for rapid, agile production of non-nuclear high energy (HE) weapon components. At present, the United States produces HE components through a time- and labor-intensive process. A new process for HEs allows for significant time and labor savings and provides a capability to prepare hundreds to thousands of parts with quick turnaround.

Additive Re-Manufacturing Guided by Process and Hydrodynamic Modeling (20180551ER)

This research is focused on understanding the applicability of additive techniques for the remanufacture of non-nuclear material components within nuclear weapons. The application directly addresses current challenges in the safety, security, and reliability of nuclear weapons.



A new subcritical measurement tool will help scientists protect and preserve the nation's stockpile.

A central mission of the Stockpile Stewardship Program is to predict, detect, and evaluate potential problems of the Nation's aging and changing stockpile. An LDRD research team proved a single-shot accuracy of better than 0.3% for the Neutron Diagnosed Subcritical Experiments (NDSE) technique using static nuclear targets at the Nevada Site. Through this work, the Laboratory and the Nation have the opportunity of a new test facility for alpha reaction history, similar to traditional reaction diagnostics employed during full-scale testing. (20150044DR) [READ MORE](#)

Science News

Here's a look at just a few of the Laboratory's top science stories from 2018, with links to articles about the work. All of the discoveries, advancements, or technologies mentioned here have roots in LDRD. LDRD investments in new capabilities enable the Laboratory's agile response to emerging national security challenges.



How satellite imagery could combat infectious diseases worldwide

For LANL, forecasting infectious diseases like influenza, HIV, dengue, and others, is a matter of national security. LANL LDRD researchers and collaborators have recognized a need to add more data to the mix and have turned to satellite imagery. Through a partnership with Descartes Labs, LANL has unique access to a data repository that enables consolidated exploitation of all open source global-coverage imagery, in turn enabling the ability to develop, test, and implement such algorithms on broad spatial, sensor, and temporal scales. A LDRD project that started in FY18, "Geospatial Change Surveillance with Heterogeneous Data" (20180529ECR), is leveraging access to this data repository. The project aims to develop cutting-edge signal processing tools for multi-temporal change detection, or change surveillance, across heterogeneous satellite sensors.

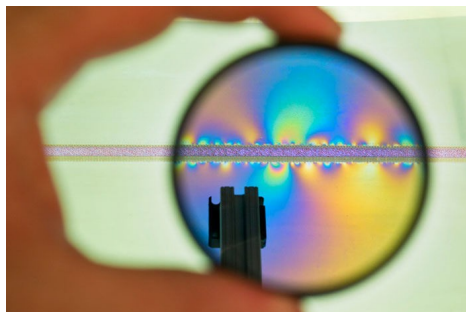
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The race to build Megafire prediction tools

LDRD Researcher Rod Linn has spent almost three decades collaborating with the U.S. Forest Service on a 3D modeling program to predict fires' paths, based on everything from wind and temperature data to the slope of a particular hillside and the situation of adjacent buildings and power lines. California's rising temperatures and worsening droughts are accelerating the need for advanced modeling technology. In Linn's current LDRD project, "Innovating Wildfire Representation in Earth System Models (ESMs)" (20190310ER), Linn aims to revolutionize how wildfire is represented in ESMs, vastly improve simulation of disturbance under climate change, and significantly advance our ability to project wildfire emissions. Read this news story to learn more about this LDRD researcher and progress in this area.

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Machine learning-detected signal predicts time to earthquake

LDRD researchers and collaborators have applied machine-learning expertise to earthquakes along Cascadia, a 700-mile-long fault from northern California to southern British Columbia that flanks cities such as Seattle. Two papers published in Nature Geosciences report the detection of seismic signals accurately predicting slow slippage in laboratory studies, as well as the Cascadia fault's slow slippage—a type of failure observed to precede large earthquakes in other subduction zones.

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Since 1978 Los Alamos has won more than 153 of the prestigious R&D 100 Awards, and in 2018 it took eight. Four of the awards have roots in LDRD and represent the program's investments in science, engineering, and technology impacting the broader scientific community. Notably, the "Universal Bacterial Sensor" invention also received a Gold Award for Corporate Social Responsibility. This award, a first for LANL, honors organizational efforts to be a greater corporate member of society, from a local to global level.

Long-Range Wireless Sensor Network

Informational Video: [Long-Range Wireless Sensor Network](#)

Using decades of experience developing satellite components for the harsh space environment, Los Alamos National Laboratory researchers invented the Long-range Wireless Sensor Network (LRWSN), a low-power sensor network that is self-forming and self-healing and can affordably collect, process, and transmit data over long distances in rugged and remote outdoor environments.

Universal Bacterial Sensor

Informational Video: [Universal Bacterial Sensor](#)

Scientists at Los Alamos National Laboratory have looked to the human immune system to develop the Universal Bacterial Sensor (UBS)—a unique technology that mimics biological recognition of bacterial pathogens, requiring only a small volume of sample to detect all pathogens quickly, simply, and efficiently without prior knowledge of what they might be.

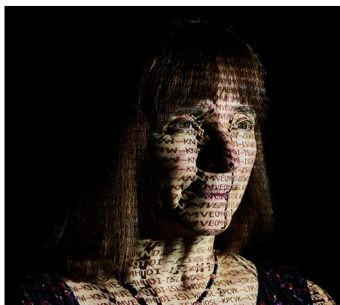
Silicon Strip Cosmic Muon Detectors for Homeland Security

Nevada National Security Site Mission Support and Test Services LLC submitted the joint entry with Fermi National Accelerator Laboratory and Los Alamos National Laboratory researchers. The team developed slim silicon strip muon detectors that provide versatility and enable stealthy deployment into walls, ceilings and portable devices. Muon trackers use the scattering trajectory signature to detect shielded nuclear materials, explosives, and other items of interest.

Video-Based Dynamic Measurement & Analysis

Informational Video: [ViDeoMAGic](#)

Engineers at Los Alamos National Laboratory have developed ViDeoMAGic (Video-based Dynamic Measurement & Analysis), a revolutionary new technology that uses video of a vibrating structure and extracts high-spatial-resolution structural vibration and dynamics information to measure the dynamic response and analyze the health of civil, mechanical, and aerospace structures.



Los Alamos National Laboratory theoretical biologist Bette Korber, PhD

R&D magazine chose Laboratory theoretical biologist **Bette Korber** as its **2018 Scientist of the Year**. Korber has received significant LDRD support throughout her accomplished career. She is responsible for managing and building LANL's HIV Database, which today has over 800,000 sequences of the HIV virus from around the world. Korber was recognized, "not only for her groundbreaking contribution to the mosaic vaccine and the fight against HIV, but also for her continued commitment to trying new and innovative scientific approaches," said Bea Riemschneider, Editorial Director, *R&D Magazine*.

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Performance Metrics

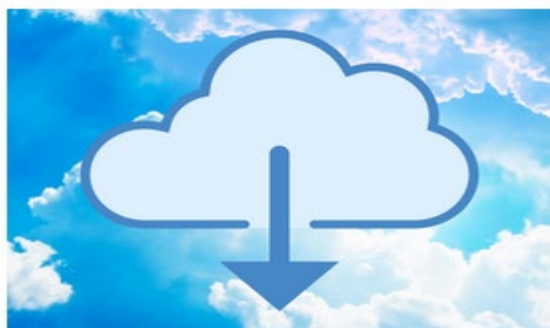
The LDRD program is a key resource for addressing the long-term science and technology goals of the Laboratory, as well as enhancing the scientific capabilities of Laboratory staff. Through careful investment of LDRD funds, the Laboratory builds its reputation, recruits and retains excellent scientists and engineers, and prepares to meet evolving national needs. The impacts of the LDRD program are particularly evident in the number of publications and citations resulting from LDRD funded research, the number of postdoctoral candidates supported and converted by the program, and the breadth of awards LDRD researchers received. The following performance metrics are updated annually.

Intellectual Property

An indication of the cutting-edge nature of research funded by LDRD is the contribution the program makes to the Laboratory's intellectual property.

U.S. Patents Issued				
	FY15	FY16	FY17	FY18
LANL Patents	50	88	43	51
LDRD Supported	10	19	9	10
% due to LDRD	20%	22%	21%	20%

Invention Disclosures				
	FY15	FY16	FY17	FY18
LANL Disclosures	71	133	117	109
LDRD Supported	16	69	24	40
% due to LDRD	23%	52%	21%	37%



In FY18, LDRD-funded research resulted in **19 software copyrights**, which was **17% of the LANL total**. This compares to 7% of the Laboratory total in FY17.

Science and Engineering Talent Pipeline

In an increasingly competitive job market, LDRD remains an important vehicle for recruiting the brightest researchers to Los Alamos National Laboratory, where they become innovators and scientific leaders. LDRD is also instrumental in retaining new talent from the postdoc pool at the Laboratory.

Postdoc Support				
	FY15	FY16	FY17	FY18
LANL Postdocs	488	501	497	556
LDRD Supported >10%	266	272	263	281
% due to LDRD	55%	54%	53%	51%

Postdoc Conversions				
	FY15	FY16	FY17	FY18
LANL Conversions	55	80	69	81
LDRD Supported >10%	24	47	37	37
% due to LDRD	44%	59%	54%	46%



LDRD Postdoc Success Story

Los Alamos celebrates an ever-stronger technical workforce as demonstrated by external recognition. A LDRD-supported Hoffman Distinguished Postdoctoral Fellow, **Stacy Copp**, was recently named one of five recipients of the 2018 [L'Oreal USA For Women in Science Fellowship](#). The fellowships are granted to female postdoctoral scientists annually, awarding grants of \$60,000 each for their contributions in science, technology, engineering and math (STEM) fields and commitment to serving as role models.

[Copp](#) is a soft-matter physicist at the Lab, who researches the creation of materials that emit or interact with light by using soft molecules as building blocks (See LDRD project 20180701PRD1, "Soft Matter-Directed Photonic Materials by Data-Driven Design.") Her work has potential applications in biomedical diagnostics, solar energy and energy-efficient lighting.

Peer-reviewed Publications and Citations

The LDRD program produces a large volume of high-quality scientific contributions relative to its portion of the Laboratory's budget. The numerous publications made possible with LDRD funding help the Laboratory maintain a strong presence and scientific reputation in the broader scientific community. The quality of these publications is evidenced by the number of times they were cited. The most highly cited LDRD paper published in FY18, *Multi-messenger Observations of a Binary Neutron Star Merger*, discusses the first observed gravitational-wave of a binary neutron star merger.

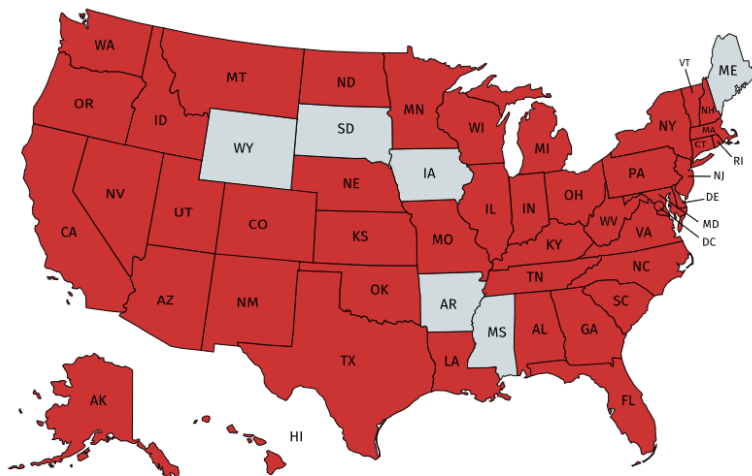
Publications				
	FY15	FY16	FY17	FY18
LANL Pubs	1872	1968	2235	2100
LDRD Supported	392	426	586	613
% due to LDRD	21%	22%	26%	29%

Citations				
	FY15	FY16	FY17	FY18
LANL Citations	31540	24100	15360	6357
LDRD Supported	11314	8117	4991	2386
% due to LDRD	36%	34%	32%	38%

External Collaborations

External collaborations are essential to the conduct of research and development in LDRD. By working with other national laboratories, academia, and industry, LDRD investigators access leading facilities and knowledge in the U.S. and abroad. A collaborator is defined as a likely co-author on a proposal, patent, or publication (including formal internal reports) as a result of the project and someone with whom the reporting PI is in direct contact with. LDRD collaborations from FY18 indicate broad intellectual engagement. Principal investigators from the 342 active LDRD projects in FY18 reported 984 collaborations with approximately 438 institutions.

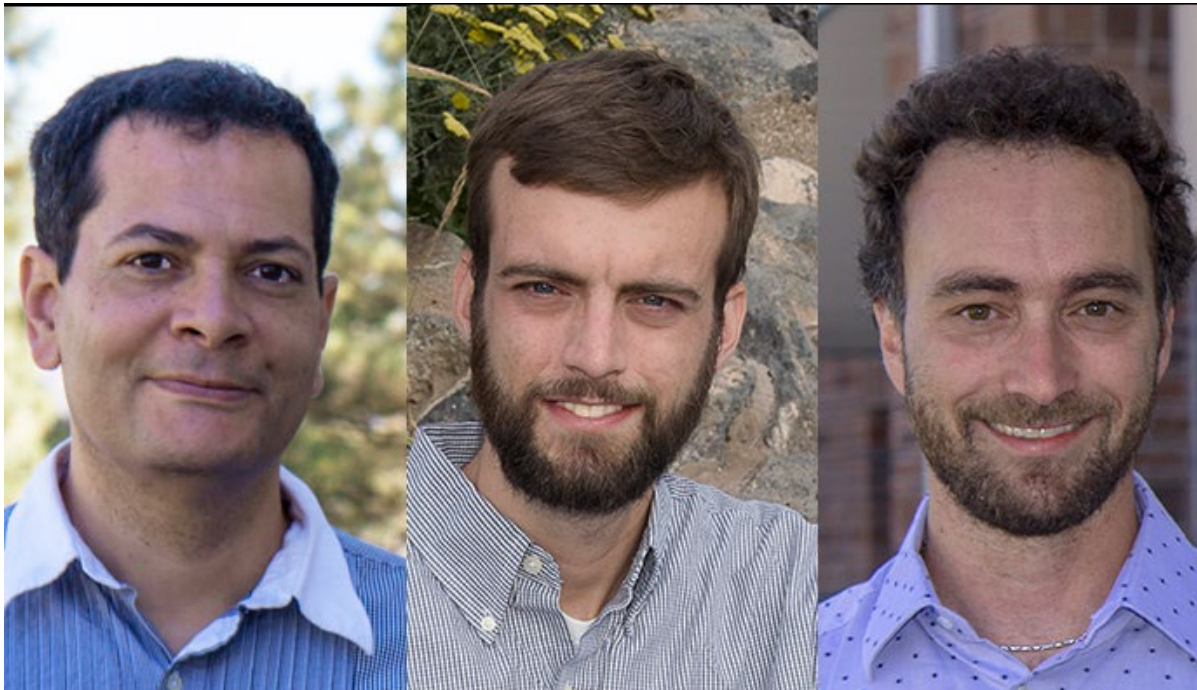
In FY18, LDRD external collaborators within the United States come from 44 states and Washington DC.



Professional Awards & Recognitions

The LDRD program helps Los Alamos National Laboratory anticipate, innovate, and deliver solutions to some of the nation's toughest challenges. The driving force behind each impact has been the focused initiative of many talented scientists and engineers who choose to apply their knowledge and expertise in service to the Nation. The LDRD program is proud to support the work of some of the Laboratory's most accomplished researchers, who in FY18 received many prestigious awards, honors, and recognitions.

Top young Los Alamos researchers honored with DOE Early Career Awards



From left to right: Cesar Luis Da Silva, Alex Zylstra, and Stefano Gandolfi.

Three talented young researchers at Los Alamos National Laboratory are among the recipients of the highly valued Early Career Research Program Funding awards from the U.S. Department of Energy's Office of Science. All three were active with LDRD in FY18. This is the ninth year DOE has provided the awards, designed to bolster the nation's scientific workforce with support to exceptional researchers during their early careers.

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"The strength of Los Alamos National Laboratory is our staff," said former **Director Terry C. Wallace, Jr.** "These early career researchers are being recognized for not only their accomplishments, but also for their potential as future leaders and pushing the frontiers of science and technology. They continue the Laboratory's proud tradition of excellence that has defined us for the last 75 years."

Fellow of the American Physical Society



“I congratulate Brian, Jennifer, Brian, and Brian on their selection as American Physical Society Fellows,” said **John Sarrao**, Deputy Director for Science, Technology & Engineering at Los Alamos. “These individuals highlight the breadth of scientific innovation and expertise that support the Lab’s national security mission.”

From left to right: Brian Albright of XTD Primary Physics (XTD-PRI), Jennifer Hollingsworth of the Center for Integrated Nanotechnologies (MPA-CINT), Brian J. Jensen of Shock and Detonation Physics (M-9) and Brian Kendrick of Physics and Chemistry of Materials (T-1).

Of the four Los Alamos scientists honored, three were active in LDRD in FY18.

Brian Albright was cited for outstanding contributions to the theory and modeling of kinetic plasmas, including pioneering work in laser-driven ion acceleration, laser plasma instabilities, high energy density physics and particle-in-cell simulations.”

Jennifer Hollingsworth was cited for the discovery and development of non-blinking giant quantum dots (gQDs), spanning pioneering contributions to materials chemistry, the photophysics of excited-state processes in nanomaterials and applications in optoelectronics.”

Brian Kendrick was cited for “the development and application of new computational methods to include the geometric (Berry) phase in molecular collisions and spectra using the gauge potential approach.

“Recognition of their accomplishments by the American Physical Society demonstrates the vibrant engagement that the Laboratory’s physicists have with the external scientific community and their contributions to physics research.” – John Sarrao, Deputy Director for Science, Technology & Engineering



Complex Natural and Engineered Systems

Countering Pathogen Interference with Human Defenses

Geoffrey Waldo
20160054DR

Project Description

We will develop a detailed understanding of the way in which pathogens such as influenza virus interfere with human defenses designed to destroy them. This will provide a foundation for new therapeutics and diagnostics for influenza and other pathogens. Human cells can detect when they are infected by a virus or other pathogen and respond by activating machinery that destroys the infecting pathogen. To counter this, many pathogens such as influenza virus have evolved sophisticated methods to manipulate the control networks for these internal defense systems and evade destruction. In this project we will develop a detailed molecular understanding of how influenza virus interferes with "autophagy", a cellular defense system that can engulf and digest pathogens. Our project will create a foundation for the development of a broad range of next-generation therapeutics that block pathogen interference with human defenses and restore the natural ability of infected cells to destroy infecting pathogens. Our work will also provide a framework that can be extended to understand interference with host defenses by intracellular bacterial pathogens, such as Burkholderia, that are pertinent to defense threat reduction.

Technical Outcomes

We developed new types of computer models of flu infections, providing a foundation for developing new therapeutics. Our project generated images of how key flu and human proteins move and interact with each other during actual infections.

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Critical Stress in Earth Crust

Paul Johnson
20170004DR

Project Description

A large earthquake in Cascadia or California would devastate the regional and potentially national economies. The primary national security challenge the project will address is attempting to characterize when a large earthquake may occur and how large it may be so that preparatory action may be taken. Our secondary security challenge is applying this same technology to anthropogenically induced seismicity, particularly in the mid west. Can we tell when a large human-induced earthquake will take place and how large it will be so that we can take action to prevent it? That is the secondary goal. The novelty of our work is the use of machine learning to discover and understand new physics of failure, through examination of the full continuous time signal. The future of earthquake physics will rely heavily on machine learning to process massive amounts of raw seismic data. Our work represents an important step in this direction. Expected outcomes: The work is of broad technical application. Not only does it have import to earthquake forecasting, but also the approach is far-reaching, applicable to potentially all failure scenarios including nondestructive testing, brittle failure of all kinds, avalanche, etc.

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Flow Cells for Scalable Energy Conversion and Storage

Rangachary Mukundan
20170046DR

Project Description

This project aims to develop low-cost, high-energy, high-power-density flow cell systems that have the potential to dramatically increase the amount of energy storage available in the US electrical grid. This increased availability of energy storage is expected to play a key role in increasing the penetration of renewable energies like wind and solar power. Specifically, this project utilizes a multi-pronged approach to develop novel chemistries and materials required to build high energy/power density non-aqueous flow battery systems. The development of such systems is in direct support of the DOE Office of Electricity Energy Storage program and is expected to have a positive impact on the national energy security mission.

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Impacts of Extreme Space Weather Events on Power Grid Infrastructure: Physics-Based Modelling of Geomagnetically-Induced Currents (GICs) During Carrington-Class Geomagnetic Storms

Michael Henderson
20170047DR

Project Description

The project focuses on understanding the impacts that extreme space weather events may have on North-American power grid infrastructure. This will be accomplished by improving physics-based space weather models so that they can realistically simulate extreme events. The output of these improved codes will be used in power grid analysis tools to assess impacts on the ground. Aspects of the work can also be transitioned to the study of impacts on power grids of associated with nuclear weapons effects.

Publications

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Multiscale Modeling of Biological Systems

Angel Garcia
20170509DR

Project Description

This project aims at modeling biological systems using computational and mathematical methods. Biological systems are modeled at different scales: atomistic (proteins, nuclei acids in various environments), systems of proteins described as members of an interacting (biochemical network), and dynamical non-linear systems that can show interesting behaviors in response to small perturbations. These models are used to model diseases and, potentially, to design new drugs that target specific proteins. The research is done in interdisciplinary teams that include biologists, physicists, and mathematicians. Postdoctoral fellows conduct the research under the supervision of Laboratory staff scientists. The modeling of signaling pathways related to cancer align with DOE's interest in developing high-performance computing and modeling approaches to help diagnose cancer patients. The development of new computational and modeling capability to study biomembranes will be relevant to health and biotechnology applications.

Publications

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Establishing a Radiotherapeutic Capability to Counter Biothreats

Stosh Kozimor
20180005DR

Project Description

Our proposed work directly supports our national security by developing and validating a novel, countermeasure pipeline against antimicrobial and multi-drug resistant bacterial pathogens. To protect our nation's health, we are offering a therapeutic alternative to the declining effectiveness of antibiotics. To maintain our national security and protect our nation's warfighters, we are demonstrating a rapid radiotherapies capability to combat bacterial pathogens developed as multi-drug resistant bioweapons.

Publications

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Understanding Actinide-Water Interactions in High Pressure-Temperature (P-T) Environments

Hongwu Xu
20180007DR

Project Description

The overarching goal of this project is to transform our understanding on the speciation, solubility and stability of actinide-bearing phases in high-pressure high-temperature aqueous environments using an integrated experimental and modeling approach. This new field of actinide science has important relevance to a range of nuclear applications and is tied to DOE/NNSA missions in energy and national security. More specifically, successful execution of this project will contribute greatly to addressing the needs to develop accident-tolerant nuclear fuels, build the safety basis for permanent disposal of the tens of thousands of metric tons of spent nuclear fuel accumulated at power plants, and understand actinide environmental signatures from underground nuclear testing in support of Global Security applications. In addition, this project will afford a new unique capability of wide-ranging utility to the DOE complex in the fields of actinide science and technology, as well as materials and chemical systems beyond actinides.

Publications

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Xu, H., X. L\xc3\xbc, P. J. Heaney, and Y. Ren. Structural behavior of a stuffed derivative of alpha-quartz, Mg_{0.5}AlSiO₄, at high temperature: an in situ synchrotron XRD study. Submitted to *Physics and Chemistry of Minerals*. (LA-UR-19-21198)

Adaptation Science for Complex Natural-Engineered Systems

Donatella Pasqualini
20180033DR

Project Description

Half of U.S. population and gross domestic product (GDP) is located in coastal counties. Electrical, water, and other critical infrastructure necessary to support population centers and the nation's economic and national security is disproportionately concentrated on the coast. Coastal regions are at risk of extreme flooding due to major storms, such as Hurricanes Katrina and Sandy, combined with the erosion of shorelines and stress on wetlands which protect the coast, and these risks may increase. This project will address two challenges: (1) predicting how coastlines will change over the next few decades due to the combined action of storms, waves, erosion, groundwater pumping, and other factors; and (2) designing electrical-water infrastructure networks in coastal regions that are more resilient to the flood and saltwater damage anticipated to occur in a changed coastal zone. We will develop a new coastal model that simulates and predicts the complex evolution of the coastline due to ocean, vegetation, and land surface interactions; and an optimization model that redesigns large infrastructure networks for resilience to natural hazards. The result will improve U.S. energy and national security and economic prosperity, by protecting the nation's electrical grid and other infrastructure assets upon which communities and industry depend.

Publications

Samsel, F., P. J. J. Wolfram, A. Barres, T. Turton, and R. B. Bujack. Colormapping Resources and Strategies for Organized Intuitive Environmental Visualization. Submitted to *Environmental Earth Sciences*. (LA-UR-19-20148)

Wang, S., D. Pasqualini, N. M. Urban, C. J. Coffrin, R. W. Bent, and S. Mason. An Optimization-Based Adaptation Framework for Coastal Electrical Infrastructure Resilience To Climate Change. Submitted to *Climatic Change*. (LA-UR-19-22145)

Systems Out of Equilibrium

Angel Garcia
20160588DR

Project Description

This project addresses fluid systems out of equilibrium, such as porous media flows, thermal convection and stably-stratified shear flows, for applications in carbon sequestration, enhanced gas/oil recovery, and ocean dynamics. At the most fundamental level, we will investigate experimentally and numerically a range of fluid instabilities including low-Reynolds number porous media flows, thermal convection, and stably stratified shear flows. Hydrodynamic instability, turbulence, and mixing have application in ocean and atmospheric modeling and the characterization of astrophysical explosions and nuclear weapons physics.

Technical Outcomes

We have developed new methods and algorithms to model many out of equilibrium processes. In particular we developed machine learning approaches to characterize microstructures in materials, the prediction of earthquakes, and the description of fracture flow in layered materials. We developed the Shear-Transformation Zone (STZ) theory of granular flow to perform multiscale modeling of earthquake ruptures. The same STZ model was also applied to study deformation in amorphous crystalline nanolaminates.

Publications

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Desalination Co-mingled: The Path to Affordability

Robert Currier
20180094DR

Project Description

Water will be increasingly important as the century evolves. Reliable fresh water supplies are necessary for human consumption, thermo-electric power generation, core industrial activities, and irrigation. The availability and quality of fresh water are critical to global health, economic growth, and ultimately, political stability. Desalination is the only means to a long term supply of fresh water. However, desalination practices are expensive. The path forward for desalination is to couple it to low cost energy sources, such as raw heat, and the production of valuable co-products. We propose a desalination technique that accomplishes this using raw thermal energy (from solar thermal or natural gas) to push compressed brines into conditions under which the solvent properties of water degrade, thus facilitating salt removal. The approach enables selective precipitation of valuable mineral co-products from deep aquifer brines that can offset costs (e.g. lithium and rare earth elements). The approach also promises liquid discharge-free desalination, thus avoiding costs and environmental concerns associated with concentrated brine disposal. In addition to producing fresh water and strategic metals, applications include treating water produced with oil and gas, limiting seismic activity during carbon sequestration, water mediated sub-surface transport of fission products, and solute recovery from liquid wastes.

Technical Outcomes

Valuable metals can be recovered from brine by manipulating temperature and density to control precipitation. Specifically, selective precipitation of metal co-products appears feasible during a supercritical desalination process. Electrochemical techniques can be used to monitor changes in key physical properties and solubility. Corrosion should also be manageable in a supercritical salt precipitation process (although special alloys may be required). Initial techno-economic analysis suggests the value of recovered metals could exceed the value of desalinated water.

Investigations of the Magnetic Characteristics of Iron-Only Clusters

John Gordon
20160255ER

Project Description

This project will develop new iron clusters as these molecules have the potential to behave as single-molecule magnets. The expected high magnetic spins of these clusters may lend themselves to applications such as quantum computing and high-density information storage using spintronics. The use of spintronics technologies could potentially revolutionize the electronics and computing industries by making it possible to store vastly more data in devices than is currently possible. Efficient spintronics technologies could mean huge energy savings due to the fact that reversing the electronic spins in such systems would require less power than the normal electronic charge. This work will build capabilities in theory, computation and modeling, and experimental chemistry that form the foundation for understating new synthetic materials.

Technical Outcomes

The magnochemistry of an Fe₉ cluster has suggested that the triangular units that comprise the cluster framework may exhibit spin frustration behavior. This is of significant interest to us going forward and we hope to interrogate a series of Fe₃ systems in the future, both experimentally and computationally, as these could yield insight into the behavior of other condensed matter systems (e.g. spin glasses) of relevance to Los Alamos' national security and energy mission.

Molecular Actinide Nitrides

Marisa Monreal
20160261ER

Project Description

This project seeks to prepare new bimetallic complexes that will provide valuable information about how actinide nitrides interact with other metals found in cladding material. Few molecular examples of actinide nitrides are available for study, owing to the difficulties in synthesis. Recent advances have provided routes to actinide azide and nitride complexes that expands the options for developing actinide nitride chemistry. The development of new molecular azide and nitride systems remains a major challenge in the field of actinide chemistry. Several questions now present themselves. What stoichiometric and catalytic reactivity might be achieved with terminal nitride linkages? Could molecular systems, such as the ones we propose to synthesize, constitute useful low-temperature precursors to actinide nitride materials? To answer these questions and more, an understanding of the electronic structure and chemical behavior of actinide nitride functional groups is needed. This proposal will do just that. This effort directly addresses the Los Alamos plutonium science research strategy to address our national security mission.

Technical Outcomes

The project's overall goal was to synthesize actinide (Th, U, Np, Pu) azides and nitrides. After surveying a variety of supporting ligand systems, we identified one that allowed the isolation of the first neptunium azide complex. We completed the full characterization of a series of uranium, thorium, and neptunium halide and azide compounds, using spectroscopy, X-ray crystallography, and electrochemistry. Finally, we have established a new Laboratory capability: an electrochemical system in the Actinide Research Facility.

Black Carbon Interactions with Radiation, Water and Ice: Laboratory Studies to Calibrate Arctic Climate Models

Manvendra Dubey
20160331ER

Project Description

Light-absorbing particles such as soot from forest fires or fossil fuel combustion and wind-generated mineral dust emitted in the atmosphere can be transported over long distances into the Arctic. There they can deposit onto snow and ice packs, darkening their surfaces and promoting melting by enhanced heating via light absorption. Current models treating these processes and effects are uncertain because they are idealized and not validated. In this project, we isolate and interrogate key processes and properties of these particles, including their light-absorbing power, scavenging by clouds and snowfall, and effects on the ice reflectivity in controlled laboratory experiments to test and refine the parameterizations used in models. Our results will increase confidence in quantifying the contributions of natural and anthropogenic light absorbing particles to the observed retreat of the Arctic sea ice and Greenland ice sheets.

Publications

- Bixler, S. L., C. Carrico, C. Allen, J. T. Lam, S. Dabli, A. P. Sullivan, A. C. Aiken, T. A. Rahn, D. Romonosky, P. Chylek, S. A. Sevanto, and M. K. Dubey. Southwestern U.S. biomass burning smoke hygroscopicity: The role of plant phenology, chemical composition chemistry and combustion properties. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-18-20787)
- Romonosky, D., S. L. Gomez, J. T. Lam, C. Carrico, A. C. Aiken, P. Chylek, and M. K. Dubey. Optical Properties of Laboratory and Ambient Biomass Burning Aerosols: Elucidating the Black, Brown, and Organic Carbon Components and Mixing Regimes. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-18-30035)

Using Therapeutic Bacteria to Treat Human Diseases

Jason Gans
20160340ER

Project Description

We aim to develop a technology that can be used to effectively treat gastrointestinal diseases using natural gut bacteria. We will demonstrate its utility by treating one of the deadliest diseases in the nation: *Clostridium difficile*. *Clostridium difficile* (C. diff.), is a major cause of gastrointestinal infections and is responsible for ~30,000 deaths every year in the U.S. alone. By the end of the project, we will demonstrate that a defined mixture of a few specific gut bacterial species can be used to effectively prevent and/or treat C. diff. infections in lab animals. The information gathered in this project will also help others better understand how equilibrium of species in a complex microbiome is established, and how it changes in response to various disturbances. This project will enable us to study the connection between the gut flora and several common inflammatory and auto-immune disorders, such as Crohn's disease, ulcerative colitis, cardiovascular disease, rheumatoid arthritis, etc.

Dwelling Ribotype 078 Strains in Canada Identical to That of the Historic Human Clinical Strain M120 in the United Kingdom. To appear in *Microbiology Resource Announcements*. (12) . (LA-UR-18-22191 DOI: 10.1128/MRA.00853-18)

Technical Outcomes

Major technical outcomes were: (1) Established new capability to perform gut microbiome research, (2) Developed protocol to maintain and cultivate complex gut microbiome in lab conditions (publication in preparation), and (3) Developed novel screening platform to identify microbes that are of therapeutic values in medicine field (patent application).

Publications

Alhmoud, T., A. Kumar, C. C. Lo, R. Al-Sadi, S. Clegg, I. Alomari, T. Zmeili, C. D. Gleasner, K. K. McMurry, A. E. K. Dichosa, M. Vuyisich, P. S. G. Chain, S. Mishra, and T. Ma. Intestinal Permeability and Microbial Dysbiosis in Acute Coronary Syndrome (MIACS study). Submitted to *Microbiome*. (LA-UR-18-26913)

Kumar, A. LDRD ER Final Report. Unpublished report. (LA-UR-18-30028)

Rodriguez-P, A., A. E. K. Dichosa, P. S. G. Chain, S. L. Johnson, Y. A. Kunde, G. Vuyisich, K. W. Davenport, and A. Kumar. Complete Genome Sequences of Historic Food-

Tracking Microbial Effects on Water-Uptake and Productivity of Plants

Sanna Sevanto
20160373ER

Project Description

We use a combination of methods for non-invasive imaging and genomics to understand, for the first time, the complex interactions between the roots of plants and their microbial associates in the soil and how these influence plant survival. A successful project will deliver 1) world-class methods for studying plant-soil interactions, 2) in-vivo observations of the effects of mycorrhizal fungi on plant water uptake and drought responses, and 3) plant activity on root associates. We will combine unique capabilities to lead an emerging scientific field integrating fungal associates with plant functional responses. We will also develop non-invasive, high-resolution methods needed for understanding soil-plant interactions. Our results could revolutionize theories on plant stress responses and tolerance addressing significant gaps in our ability to predict plant productivity, vegetation changes and ecosystem-scale carbon cycling under changing climate.

Technical Outcomes

In this project we developed methods to identify influence of root and soil microbial communities on plant water uptake and productivity. We successfully imaged in situ water transport in the soil and roots with neutron radiography, and identified bacterial and fungal communities affecting water retention and transport rates, and plant drought tolerance.

Publications

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Malone, M., J. Yoder, J. F. Hunter, M. A. Espy, L. T. Dickman, R. O. Nelson, S. C. Vogel, J. H. Sandin, and S. A. Sevanto. In vivo Observation of Tree Drought Response with Low-Field NMR and Neutron Imaging. 2016. *Frontiers in Plant Science*. 564. (LA-UR-16-20572 DOI: 10.3389/fpls.2016.00564)

Raivonen, M., S. A. Sevanto, S. Smolander, L. Backman, J. Susiluoto, T. Aalto, T. Markkanen, J. Makela, J. Rinne, O. Peltola, M. Aurela, M. Tomasic, X. Li, T. Larmola, S. Juutinen, E. S. Tuittila, M. Heimann, T. Klainen, V. Brovkin, and T. Vesala. HIMMELI v1.0: Helsinki Model of MEthane build-up and emission for peatlands. To appear in *Geoscientific Model Development*. (12) 4665-4691. (LA-UR-17-22271 DOI: 10.5194/gmd-10-4665-2017)

Ryan, M. G., S. A. Sevanto, L. T. Dickman, A. D. Collins, and H. D. Adams. Stomatal Control Area as a simple hydraulic trait for evaluating drought response. Submitted to *Tree Physiology*. (LA-UR-19-21916)

Ryan, M. G., S. A. Sevanto, L. T. Dickman, D. E. Ulrich, A. D. Collins, and H. Adams. An alternative to (an)isohydry: stomatal closure point as a simply hydraulic trait. Submitted to *Plant, Cell and Environment*. (LA-UR-18-25773)

Sevanto, S. A. The influence of leaf size and shape on leaf thermal dynamics: does theory hold up under natural conditions?. 2017. *Plant, Cell & Environment*. (2) 237-248. (LA-UR-17-27765 DOI: 10.1111/pce.12857)

Sevanto, S. A. An empirical method that separates irreversible stem radial growth from bark water content changes in trees: theory and case studies. 2017. *Plant, Cell & Environment*. (2) 290-303. (LA-UR-17-27764 DOI: 10.1111/pce.12863)

Sevanto, S. A. Drought impacts on phloem transport. 2018. *Current Opinion in Plant Biology*. 76-81. (LA-UR-17-28969 DOI: 10.1016/j.pbi.2018.01.002)

Sevanto, S. A. Is desiccation tolerance and avoidance reflected in xylem and phloem anatomy of two co-existing arid-zone coniferous trees?. 2018. *Plant, Cell & Environment*. (LA-UR-17-23770 DOI: 10.1111/pce.13198)

Vesala, T., S. A. Sevanto, Y. Salmon, T. Gronholm, L. Lindfors, E. Juurola, E. Nikinmaa, I. Riipinen, P. Hari, M. Mencuccini, and T. Holttä. Effect of Leaf Water Potential on Internal Humidity and CO₂ Dissolution: Reverse Transpiration and Improved Water Use Efficiency under Negative Pressure. 2017. *Frontiers in Plant Science*. (LA-UR-17-22009 DOI: 10.3389/fpls.2017.00054)

Expediting the Genetic Engineering of Microalgae for Industrial Production

Scott Hennelly
20160393ER

Project Description

This work in algal research will drive its development as an industrially viable systemic technology. Using genetic tools we will elucidate the algal genome and make algal genetic engineering more routine. Extensive genetic manipulations are required to realize algae's inherent potential as a systemic technology. To date, progress has been slow, due to poorly characterized algal genetics and a lack of genetic tools such as plasmids, reliable transformation methods and viral vectors. Our goal is to make algal genetic engineering routine. We will deliver a set of tools and methods to deliver genes to algae, stably integrate them into the genome, and express them. Beyond simple feedstock for energy production, harnessing the complex biosynthetic power algae would open new avenues for the production of a wide array of complex chemicals and materials of interest for national security applications.

Technical Outcomes

This project created editing strains that stably express CRISPR/Cas genes. These will be the starting point for the development of engineered algae with enhanced capacities in growth and productivity. These strains are in use by collaborators at Los Alamos National Laboratory and the New Mexico Consortium, and will undoubtedly improve the efficiency of strain development going forward. We also made progress on the development of exciting new tools for the delivery of exogenous homologous recombination systems.

Mapping Cotranscriptional Assembly of the 30S Ribosomal Subunit to Illuminate Mechanisms of Antibiotic Interference

Peter Goodwin
20170156ER

Project Description

The ribosome, the primary machinery for protein synthesis in all living organisms, is an exquisitely complex, self-assembled multi-component structure, and as such, has become "the" model system for the study of self-assembly. Moreover, it is also the target for about 50 percent of clinical antibiotics. Our goal is a molecular-level understanding of the assembly of the 30S ribosomal subunit during transcription of its Ribonucleic Acid (RNA) scaffold. This new level of understanding will give unprecedented insight into mechanisms of antibiotic interference with ribosome assembly and identify new targets and assays for drug design. As such, this research supports Los Alamos missions to combat threats to U.S. health security, such as tuberculosis and methicillin-resistant staphylococcus aureus (MRSA), and provide defense against bio-threats such as anthrax and plague.

Breaking the "Curse of Dimensionality" for Boltzmann-like Systems

Gianmarco Manzini
20170207ER

Project Description

The goal of this project is to develop a new Information, Science and Technology capability for computer simulations of high-dimensional problems based on kinetic equations. A wide range of topics from computational science can benefit from its successful outcome, with potential mission-critical applications such as atmospheric and climate modeling and space weather simulation (global security/threat reduction) and magnetic fusion energy (energy security). This project will extend world-class numerical algorithms to high performance architectures, thus providing the DOE with unique computational capabilities useful for large proposals in computational co-design and extreme-scale solvers categories.

Manzini, G., and G. L. Delzanno. The Legendre-discontinuous Galerkin discretization of the 1D-1V Vlasov-Poisson system. Unpublished report. (LA-UR-17-28540)

Manzini, G., and G. L. Delzanno. A discontinuous Galerkin-Hermite discretization of the Vlasov-Poisson system. Unpublished report. (LA-UR-17-28541)

Roytershteyn, V., S. Boldyrev, G. L. Delzanno, C. Chen, D. Groselj, and N. Loureiro. Numerical Study of Inertial Kinetic-Alfven Turbulence. Submitted to *Astrophysical Journal*. (LA-UR-18-28710)

Roytershteyn, V., and G. L. Delzanno. Spectral Approach to Plasma Kinetic Simulations Based on Hermite Decomposition in the Velocity Space. To appear in *Frontiers in Astronomy and Space Sciences*. (LA-UR-18-23813 DOI: 10.3389/fspas.2018.00027)

Publications

Fatone, L., D. Funaro, and G. Manzini. Arbitrary-Order Time-Accurate Semi-Lagrangian Spectral Approximations of the Vlasov-Poisson System. Submitted to *Journal of Computational Physics*. (LA-UR-18-22660)

Manzini, G., D. Funaro, and G. L. Delzanno. Convergence of Spectral Discretizations of the Vlasov-Poisson System. 2017. *SIAM Journal on Numerical Analysis*. (5) 2312-2335. (LA-UR-16-22601 DOI: 10.1137/16M1076848)

Manzini, G., G. L. Delzanno, and L. J. Vernon. Breaking the 'curse of dimensionality' for Boltzmann-like system. Unpublished report. (LA-UR-17-24420)

Manzini, G., L. Fatone, and D. Funaro. A Semi-Lagrangian Spectral Method for the Vlasov-Poisson System based on Fourier, Legendre and Hermite Polynomials. Submitted to *Communication on Applied Mathematics and Computation*. (LA-UR-18-25332)

Manzini, G., L. Fatone, and D. Funaro. On the Use of Hermite Functions for the Vlasov-Poisson System. Presented at *ICOSAHOM*. (London, United Kingdom, 2018-07-09 - 2018-07-13). (LA-UR-18-30323)

Exploiting Quantum Interference to Control Ultracold Molecular Collisions

Brian Kendrick
20170221ER

Project Description

The proposed research will develop new fundamental capabilities in modeling and simulation for exploiting a newly discovered quantum interference mechanism to control the outcome of ultracold molecular collisions. The unprecedented dynamic range of this new mechanism provides the realization of a quantum switch capable of turning the collision outcome on or off. Thus, it opens up an entirely new domain of quantum control. The proposed work will lay the foundation for several transformative technological applications based on cold molecules, which is important to the DOE/NNSA missions in information science and technology and global security. These include: a new framework for realizing quantum computing, the development of sensors with unprecedented sensitivity, enable new tests of fundamental symmetries, improved astrophysics models of the interstellar medium/molecular clouds, and the synthesis of specific molecular species. The control of cold molecular collisions will also enable the formation of dense ensembles of cold molecules relevant for studying new exotic states of condensed matter and quantum phases.

Publications

- Balakrishnan, N., and B. K. Kendrick. Geometric Phase and Interference Effects in Ultracold Chemical Reactions. Submitted to *Proceedings of the QSCP-XXI in Progress in Theoretical Chemistry and Physics*. (LA-UR-17-21188)
- E. Croft, J. F., C. Makrides, M. Li, A. Petrov, B. K. Kendrick, N. Balakrishnan, and S. Kotochigova. Universality and chaoticity in ultracold K+KRb chemical reactions. 2017. *Nature Communications*. 15897. (LA-UR-17-20822 DOI: 10.1038/ncomms15897)
- Croft, J. F., N. Balakrishnan, and B. K. Kendrick. Long-lived complexes and quantum chaos in ultracold elastic K₂+Rb collisions. Submitted to *Physical Review A*. (LA-UR-17-29347)

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- Kendrick, B. K. Non-adiabatic quantum reactive scattering calculations for the ultracold hydrogen exchange reaction: H + H₂(ν) → H + H₂(ν'). 2018. *Chemical Physics*. (LA-UR-18-23192 DOI: 10.1016/j.chemphys.2018.07.001)
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- Teplukhin, A., B. K. Kendrick, and D. Babikov. Calculation of molecular vibrational spectra on a quantum annealer. Submitted to *Nature Communications*. (LA-UR-18-29586)
- Xie, C., B. K. Kendrick, D. R. Yarkony, and H. Guo. Constructive and Destructive Interference in Nonadiabatic Tunneling via Conical Intersections. 2017. *Journal of Chemical Theory and Computation*. (5) 1902-1910. (LA-UR-17-20533 DOI: 10.1021/acs.jctc.7b00124)

Sensitive Optical Super-resolution Neuroimaging

Anatoly Efimov
20170249ER

Project Description

This project will produce advances in neural measurement and analysis technology, and enhance our ability to investigate, understand, and ultimately to emulate the function of the brain. Obvious applications include biomedical applications for diagnostics, therapeutics and prosthetic devices. Ultimately, such work will enable neural emulation: image understanding, natural language comprehension; closed loop control of motor function; and navigation in complex, dynamic environments. Similar processing techniques will generalize to problems outside of biological experience: analysis of hyperspectral imagery, detecting ultrasonic or electromagnetic signatures over wide frequency ranges; solution of ill-posed inverse problems; reasoning by inference or analogy based on very dense and complex data. Such applications have clear implications for national security responsibilities of the DoD and DoE.

Measuring Messenger Ribonucleic Acid (mRNA) and Protein Content from Single Cells: Single Molecule Fluorescence In-Situ Hybridization on a Chip

James Werner
20170256ER

Project Description

This work is building the foundational tools to understand and detect the initial stages of bacterial versus viral infections. A biological attack is possible in both warfighter and civilian (e.g. terrorist) scenarios. The proper course of treatment of such attacks requires an understanding of the agent deployed (e.g. is it a toxin, or bacterial or viral in nature). This work is building the tools to understand how immune cells respond differently to bacterial versus viral infections at the single cell level. It will advance the state of the art in bioanalysis, measuring a suite of biomarkers (both proteins and nucleic acids) at the single cell level. We hypothesize that early events in disease diagnosis and progression will be clearer at the level of single cells, the level where infection starts and grows. This work will impact DOE/NNSA missions in warfighter and civilian protection from biological attacks, as well as helping with national needs in preventing the spread of infectious disease.

Publications

Kalb, D. M., S. H. Adikari, E. Hong-Geller, and J. H. Werner.
Single-Cell Correlations of mRNA and Protein Content
in Human Monocytic Cell Line after LPS Stimulation.
Submitted to *PLOS One*. (LA-UR-19-20143)

Probing Ionosphere and Magnetosphere Connections with an Electron Gun

Gian Delzanno
20170423ER

Project Description

This project aims to remove the major obstacle (i.e. catastrophic spacecraft charging) to using high-power, relativistic electron beams for space applications relevant to science as well as to national security. In one potential application, known as radiation belt remediation, relativistic electron beams can be used to trigger plasma waves in the space environment. Waves can interact with the energetic particles of the environment and precipitate them at the poles, thus returning hazardous fluxes of energetic particles to more benign levels. Energetic particles in the near-Earth environment, the so-called 'killer electrons,' can cause catastrophic failure of our space infrastructure and pose a significant threat to national security. In another application, relativistic electron beams emitted from a magnetospheric spacecraft are used to probe ionosphere/magnetosphere connections with unprecedented accuracy. If successful, the long-term goals of the project are to (1) open up a new field of experimental space plasma physics based on electron beams, (2) enable the development of radiation belt remediation schemes to protect our space-based infrastructure, and (3) enable for the first time the resolution of several long-standing questions in ionospheric/magnetospheric physics.

beams. Submitted to *Physical Review Letters*. (LA-UR-17-30198)

Marchand, R., and G. L. Delzanno. Tethered capacitor charge mitigation in electron beam experiments. Submitted to *Frontiers in Space Physics and Astronomy*. (LA-UR-18-30554)

Miars, G. C., G. L. Delzanno, F. Lucco Castello, O. Leon, and B. E. Gilchrist. Enabling Electron Beam Use in Tenuous Space Plasmas using Plasma Contactors: the Ion Emission Model. Presented at *Spacecraft charging and technology conference*. (kobe, Japan, 2018-06-25 - 2018-06-25). (LA-UR-18-30588)

Miars, G., O. Leon, B. Gilchrist, G. L. Delzanno, F. Lucco Castello, and J. Borovsky. Ion Emission from a Positively Biased Hollow Cathode Plasma. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-18-28711)

Publications

Borovsky, J. E., and G. L. Delzanno. Active Experiments in Space: The Future. Submitted to *Frontiers in Astronomy and Space Physics*. (LA-UR-18-31542)

Lucco Castello, F., G. L. Delzanno, O. Leon, B. Gilchrist, J. Borovsky, and G. Miars. Spacecraft-Charging Mitigation of a High-Power Electron Beam Emitted by a Magnetospheric Spacecraft: Simple Theoretical Model for the Transient of the Spacecraft Potential. To appear in *Journal of Geophysical Research: Space Physics*. (8) 6424-6442. (LA-UR-17-27668 DOI: 10.1029/2017JA024926)

Delzanno, G. L., and V. Roytershteyn. High-frequency plasma waves and pitch-angle scattering induced by electron

Aromatic Actinide Metallacycles

Jaqueline Kiplinger
20170529ER

Project Description

The proposed research directly addresses the Los Alamos Plutonium Science and Research Strategy and Laboratory missions in Energy Security and Materials for the Future. A better understanding and control of covalency in the actinides will likely lead to new chemistries and reactivity trends that can be exploited to meet the needs of next-generation actinide science. This includes critical national priorities such as design of next-generation nuclear fuels, efficient separations in nuclear materials processing, a greater scientific basis for waste management, and materials stabilization issues relevant to weapons aging and corrosion processes. In essence, the insight we gain through this project could have widespread impact on designing stable aromatic and antiaromatic actinide complexes and to "turn-on" unique 5f-element electronic and optical phenomenon and reaction chemistry; thereby, directly addressing the BES grand challenge to Control Matter at the Most Basic Level of the Electron.

Publications

- Cope, S., K. Erickson, J. Xie, J. K. Pagano, R. Waterman, P. Yang, R. Wu, B. L. Scott, J. L. Kiplinger, L. Gagliardi, and D. E. Morris. Synthesis and characterization of actinide metallabiphenylene complexes. Submitted to *Science*. (LA-UR-18-23690)
- Erickson, K., A. G. Lichtscheidl, M. J. Monreal, A. T. Nelson, B. L. Scott, D. E. Morris, and J. L. Kiplinger. Exploiting the reactivity of actinide fluoride bonds for the synthesis and characterization of a new class of monometallic bis(azide) uranium complexes. 2018. *Journal of Organometallic Chemistry*. 180-186. (LA-UR-17-28097 DOI: 10.1016/j.jorganchem.2017.10.044)
- Erickson, K., J. K. Pagano, A. G. Lichtscheidl, D. E. Morris, B. L. Scott, and J. L. Kiplinger. A sustainable methodology for the synthesis of uranium(III) and uranium(IV) chlorides: Replacing hexachloropropene with trimethylsilyl chloride. Submitted to *Chemical Communications*. (LA-UR-17-25715)
- Erickson, K., J. L. Kiplinger, D. E. Morris, B. D. Kagan, and B. L. Scott. Revisiting the bis(dimethylamido) metallocene complexes of thorium and uranium: improved syntheses, structure, spectroscopy, and redox energetics of $(C_5Me_5)_2An(NMe_2)_2$ ($An = Th, U$). *Dalton Trans.* (34) 11208-11213. (LA-UR-17-23836 DOI: 10.1039/C7DT02373A)
- Erickson, K., N. Dandu, S. Cope, P. Dub, B. L. Scott, D. E. Morris, S. Odoh, and J. L. Kiplinger. Metal-Dependent σ -H Agostic Bonding to Actinides: Synthesis, Characterization, and Electronic Structure of Bis(amidoborane) Complexes, $(C_5Me_5)_2An(NH_2)_2(BH_3)_2$ ($An = Th, U$). Submitted to *Journal of the American Chemical Society*. (LA-UR-18-29510)
- Michalczyk, R., J. L. Kiplinger, L. A. I. Silks, K. Erickson, D. O. Baumann, and B. L. Scott. A Sterically Biased Unsymmetrical Azobenzene Derivative: Synthesis, Molecular Structure, and ^{15}N NMR Spectroscopic Analysis of (E)-1-(2,6-Diisopropylphenyl)-2-phenyldiazine. 2017. *Journal of Chemical Crystallography*. (6) 245-248. (LA-UR-17-25868 DOI: 10.1007/s10870-017-0700-4)
- Pagano, J. K., B. L. Scott, and J. L. Kiplinger. Synthesis, characterization, and reactivity of the first uranium metallocene 1,2-bis(diphenylphosphino)acetylene complexes. 2018. *Inorganica Chimica Acta*. 347-352. (LA-UR-17-31363 DOI: 10.1016/j.ica.2018.06.010)
- Pagano, J. K., D. S. J. Arney, B. L. Scott, D. E. Morris, J. L. Kiplinger, and C. J. Burns. A sulphur and uranium fiesta! Synthesis, structure, and characterization of neutral terminal uranium(VI) monosulphide, uranium(VI) σ -disulphide, and uranium(IV) phosphine sulphide complexes. *Dalton Transactions*. (LA-UR-18-26567 DOI: 10.1039/C8DT02932F)
- I. Silks, L. A., R. Wu, E. Nicholas, K. Erickson, D. E. Morris, B. L. Scott, J. L. Kiplinger, and T. Cantat. Trapping a Uranium Schrock-Type Alkylidene Species Affords the Uranacyclobutene Complex, $(C_5Me_5)_2U[1,3-C(SiMe_3)C(SiMe_3)C_2H_2CPh_2]$. Submitted to *Journal of the American Chemical Society*. (LA-UR-18-24002)

Powering the Resolution Revolution with Multi-Resolution Algorithms: Merging Image Analysis, Molecular Simulation and Model Building

Karissa Sanbonmatsu
20180139ER

Project Description

Fundamental biology science and health security have important applications in national security. Molecules in living systems and biomedicine have highly intricate, complex structures and shapes. Their shape often determines how they work and the role they play in our own bodies and in harmful bacteria. If we can understand how these molecules work in atomic detail, we may be able to control them, laying the foundation for new drugs to treat disease and the defend against harmful bacteria. This field is called structural biology. To date, structural biology has played an instrumental role in almost every aspect of life science and biomedicine. This project focuses on cryogenic electron microscopy, a technique revolutionizing the field of structural biology. By satisfying the large demand for computational tools in cryogenic electron microscopy, our project stands to position Los Alamos National Laboratory at the forefront of a revolution in structural biology.

Publications

Jung, J., W. Nishima, M. G. Daniels, G. Bascom, C. Kobayashi, A. A. Adedoyin, M. E. Wall, A. Lappala, W. M. Fischer, C. S. Tung, T. Schlick, Y. Sugita, and K. Y. Sanbonmatsu. Scaling Molecular Dynamics Past 500000 Processor Cores for Large-Scale Biophysical Simulations. Submitted to *Journal of Computational Chemistry*. (LA-UR-18-31413)

Visualizing and Understanding Complex Fluid Transport in 3-Dimensional Microstructure

Hari Viswanathan
20180151ER

Project Description

Flow through fractures is critical for national security applications such as nuclear nonproliferation. Fractures act as the superhighways of flow in the subsurface and characterizing fracture flow is critical for predicting gas seepage from underground nuclear tests from other nation states.

Publications

Nguyen, T. P. Effectiveness of supercritical-CO₂ and N₂ huff-and-puff methods of enhanced oil recovery in shale fracture networks using microfluidic experiments. Submitted to *Applied Energy*. (LA-UR-18-30569)

Geophysical Signatures of Changing Water Resources

Ellen Syracuse
20180158ER

Project Description

Water is necessary for all facets of life, and energy production and water resources are inextricably intertwined. Increasing strains on water resources due to groundwater withdrawals and frequent drought conditions, particularly in the US West, has the potential to threaten US energy production. By combining a set of non-traditional geophysical measurements, we will be able to quantify the distribution of groundwater resources and changes in them over time in response to changing meteorological conditions in a way that has not been possible previously, thereby improving understanding of energy security threats. Our results will have direct impact to the DOE cross-cutting initiative Water-Energy Nexus, as well as the DOE EPSA and BER programs.

In Situ Characterization of Uranium Hydriding Corrosion

Terry Holesinger
20180295ER

Project Description

Hydride formation / corrosion is a materials problem that affects a broad range of diverse industries that includes manufacturing, transportation, energy and national security. This work focuses on uranium hydride (UH₃), which has direct relevance to and is an active research area for laboratory mission for stockpile stewardship. Each step in the hydride formation process contains a number of fundamental unanswered questions – basic gaps in the knowledge that make it currently impossible to predict timing and locations of uranium hydride corrosion on any given surface. Our overall goal is to change this and produce a predictive (theory) and verification (experiment) framework for understanding and directly observing the hydrogen(H) corrosion process in uranium. The pioneering research we propose is to predict and directly observe across all length scales the first early-stage nucleation and growth processes of UH₃. This includes identifying the pathways and structural conditions that facilitate hydride formation, no easy task given that the hydride process starts as a subsurface phenomena in technologically applied materials. The results of our work will have an immediate impact on DOE/NNSA missions for stockpile stewardship. Understanding and controlling hydride formation is an important aspect of ensuring material reliability in an aging weapons stockpile.

ERIS: Electrolysis Rocket Ignition System

Nicholas Dallmann
20180382ER

Project Description

Low cost-to-orbit can now be achieved by launching small satellites as secondary payloads alongside larger missions. However, there is a barrier to these 'rideshare' opportunities. Hazardous and cumbersome propellants can pose a risk to the primary mission. This is generally not tolerated, effectively eliminating the most common high thrust propulsion options from such missions. Electrolysis Rocket Ignition System (ERIS) will provide unique solutions to this problem. The enabling capability development of ERIS is a simple, compact, water electrolyzer for space. The electrolyzer will be based on the Laboratory's innovative fuel cell programs. A satellite carrying ERIS would launch with benign liquid water. Only after reaching orbit -well away from the primary satellite(s)- would ERIS disassociate that water into pressurized oxygen (O₂) and hydrogen (H₂) for (cold-gas or reactive) propulsion or for the truly novel Laboratory interest of ignition/throttling another propellant like the Laboratory's solid-fuel-solid-oxidizer propulsion system (SFOS). The high-impulse segregated SFOS is a combination of novel materials unique in its safety and high energy density. The system has been successfully ground tested in small satellite formats and in rockets. SFOS has unique potential to be stopped-and-restarted, providing a safe, multi-pulse ignition system. ERIS will add these revolutionary capabilities to SFOS.

Removing and Swapping Photoreceptors in Algae to Improve Biomass Yield

Shawn Starkenburg
20180393ER

Project Description

This project directly supports the energy security mission of DOE and NNSA. The major hurdle impeding renewable fuel sourcing from algae is cost. Therefore, research efforts focused on increasing algal yields will directly reduce the price of algal derived gasoline and other transportation fuels. The goal of this project is to improve the yield and lower the cost of algal biofuel production 2 fold to improve the state of technology to meet the DOE targets for renewable energy use.

Publications

Deodato, C., S. Barlow, B. Hovde, and R. A. Cattolico.

Chrysochromulina (Haptophyceae) isolates from lake and river ecosystems: An electron microscopic comparison and discussion of type species diagnosis. Submitted to *Algal Research*. (LA-UR-19-20025)

Sanchez, M., C. Payen, F. Cheong, B. Hovde, S. Bissonnette, A. Arkin, J. Skerker, R. Brem, A. Caudy, and M. Dunham.

Transposon insertional mutagenesis in *Saccharomyces uvarum* reveals trans-acting effects influencing species-dependent essential genes. Submitted to *Genome Research*. (LA-UR-19-20026)

Next Generation Models for Radial Diffusion of Energetic Electrons in the Earth's Radiation Belts

Michael Henderson
20180449ER

Project Description

This project supports development of capabilities for Space Situational Awareness (SSA) both in a predictive realm and in post-facto analyses of spacecraft anomalies (forensics). Accurate specification/prediction of the relativistic electron populations in the radiation belt is critical for understanding and mitigating threats to space-based assets. The enhancement of Los Alamos National Laboratory datasets used in this project also maintains and supports broader national security needs including space-based treaty verification activities on-going at the Laboratory and the ability to plan for future missions. The new models for the radial diffusion transport parameters that will result from this work will constitute a transformational advancement over what is currently available and will place the Laboratory at the forefront of this research area.

Optimization Aware Uncertainty Quantification in Non-Linear Networked Systems

Sidhant Misra
20180468ER

Project Description

In systems of national importance, such as critical infrastructures, where optimization is leveraged to achieve optimal technical performance or economic efficiency, uncertainty creates significant risks. If uncertainty is not accounted for properly during the design and optimization process, the system might be vulnerable even to relatively minor disturbances. Addressing this problem requires Uncertainty Quantification (UQ) to characterize the impact of uncertainty in a mathematical form, as well as integration of the uncertainty characterization in UQ-Aware Optimization. Using nonlinear networked systems as the primary example, we will (i) develop new methods for UQ using non-traditional approaches based on powerful new ideas in modern optimization theory and the theory of Graphical Models and (ii) develop techniques that incorporate both existing and our advanced UQ methods into a larger optimization framework. Our work will make significant contributions to the general fields of UQ and optimization. In addition, these concepts are directly applicable to security assessment and optimization under uncertainty in non-linear infrastructure networks—an integral part of the Laboratory's work on critical infrastructure and energy security. The project is also aligned with other mission relevant non-linear networks, including epidemic spreading, analysis of social or communication networks, and interdiction of networks transporting contraband.

- Ng, Y., S. Misra, L. A. Roald, and S. N. Backhaus. Statistical Learning for DC Optimal Power Flow. Presented at *Power Systems Computation Conference*. (Dublin, Ireland, 2018-06-11 - 2018-06-11). (LA-UR-17-29722)
- Vuffray, M. D., S. Misra, and A. Lokhov. Efficient Learning of Discrete Graphical Models. Presented at *COLT 2019 : Computational Learning Theory*. (Phoenix, Arizona, United States, 2019-06-25 - 2019-06-29). (LA-UR-19-20925)
- Wiesser, T., S. Misra, and L. A. Roald. Chance-Constrained Optimization for Non-Linear Network Flow Problems. Presented at *Semi-Algebraic techniques for the Optimal Power Flow Problem and Stability Assessment of Power Systems*. (Paris, France, 2018-01-16 - 2018-01-16). (LA-UR-17-31414)

Publications

- Lasserre, J. B., S. Marx, T. Weisser, and D. Henrion. A MOMENT APPROACH FOR ENTROPY SOLUTIONS TO NONLINEAR HYPERBOLIC PDES. Submitted to *Mathematical Control and Related Fields*. (LA-UR-19-21398)
- Misra, S., D. Molzahn, and K. Dvijotham. Optimal adaptive linearizations of the AC power flow equations. Presented at *Power Systems Control Conference*. (Dublin, Ireland, 2018-06-11 - 2018-06-11). (LA-UR-17-29721)

Advanced Technology Laser Triggering of High Power Linear Induction Accelerator Pulsed Power Switches

Roger Shurter
20170625ER

Project Description

This project will lead to the development of high energy, multi-kilojoule pulsed power switches with highly precise temporal resolution. With the application of these new switch designs using pressured air rather than the asphyxiants currently in use such as sulfur hexafluoride, the Science Based Stockpile Stewardship program may be significantly impacted. A potential example of this technology application is the new down-hole radiographic research accelerator under development for sub-critical weapons testing at the Nevada Test Site.

Technical Outcomes

This project resulted in the establishment of a tunable laser based experimental system for advanced study of new phenomena relating to high energy pulsed power switching. This work is potentially applicable for existing Laboratory radiography facilities and the new radiographic accelerator system to be commissioned at the Nevada Test Site Underground facility in the mid 2020's.

Long-Range In-Situ Acoustic Diagnosis and Monitoring of Molten-Salt Systems

Alp Findikoglu
20180568ER

Project Description

The proposed work will be a valuable contribution to the technical field because there is currently no commercial technique for long-range in situ acoustic inspection of pipes in conventional nuclear and fuel power plants; availability of such a technique could lead to a better understanding of corrosion effects, enable a non-destructive technique for rapidly testing new reactor materials, and provide a new diagnostic technique for other high temperature applications such as conventional light-water reactors, fusion reactors, or solar-thermal/geothermal energy recovery processes. This work supports Los Alamos National Laboratory's national security missions in Energy Security by providing a system to enable a new type of molten-salt reactor (MSR). The DOE Office of Nuclear Energy and the Office of Science Basic Energy Systems are actively exploring ways to promote the establishment of MSRs in the US. Additionally, the results of this study could lead to Strategic Partnerships and CRADAs with companies to help develop commercial products.

Technical Outcomes

The present work demonstrated in situ detection of corrosion at elevated temperatures of up to 600 °C in a small (1"-diameter, 5"-length) model molten-salt vessel using custom piezoelectric single-crystal sensors. With the current setup, we demonstrated detection limit of approximately 0.1% wall loss, which is considerably better than the target minimum detection limit of 0.5% for nuclear industry.

Cas9 Gene Editing Efficacy

Scott Twary
20180653ER

Project Description

The application of genome editing to modify targeted genes has been simplified by the CRISPR/Cas9 technology. This application has accelerated and broadened the capability to specifically modify targeted genes for both functional discovery, genome corrections (genetic diseases) and engineering new production systems. In addition, this technology can be applied across many diverse organisms broadening the potential for both beneficial and nefarious use. CRISPR/Cas9 systems are continually being improved to optimize the primary editing and minimize any secondary off-target effects. This work will investigate how both modifications in the Cas9 enzyme and altered designs of the gene target guide Ribonucleic Acid (RNA) are reflected in specific and non-specific genome changes. Specificity in the mode of action of the Cas9 enzyme relies on both rapid recognition of target sites and restricted Deoxyribonucleic Acid (DNA) cutting activity. Recent developments have recognized the contribution of these factors into minimizing off-target genome editing. These results will allow us to differentiate natural random mutations changing an organism's characteristics versus directed engineering approaches. This will be important as new emerging threats are recognized and for monitoring specific engineered populations released into natural ecosystems.

Technical Outcomes

Multiple gene target guide sets were tested for CRISPR/Cas editing efficacy on human cell lines. An essential gene was targeted under toxic culture conditions if functional. Multiple gene knock-outs were confirmed. Complete genome analysis was completed to explore the potential for targeted and off-target genome editing and mutation. Kmer analysis of potential mutations identified the targeted gene confirming analysis functionality. Over 900 genome sites with target sequence similarity did not have any editing mutations.

Fast-running Fire Propagation Model for Complex Terrain Environments

Rodman Linn
20180723ER

Project Description

We aim to develop a first-of-its-kind fast-running self-determining wildland fire spread model that works in complex terrain and accounts for the fire/atmosphere feedbacks that are essential to correctly predict fire behavior and fire smoke transport. Development of the fire-modeling tool for complex terrain environments will result in a tool that will support the nuclear weapons effects, emergency response, wildfire protection, and prescribed fire decision-making communities. In addition to directly benefitting future Laboratory site fire preparedness, several outside agencies are also seeking enhanced QUIC-Fire capabilities for use in prediction of fire spread after a nuclear detonation, as this is a major concern for military planners in the nuclear weapons effect community. The USDA Forest Service and other land agencies are showing interest in QUIC-Fire to support fuels management decision-making in the western United States, but they need the ability to handle complex topography. Laboratory emergency response and other government and DoD facilities are similarly expressing interest in these enhanced capabilities to help assess and mitigate the impact of unintentional fires, as well as prescribed fires. This work will also improve source inversion at high-resolution local scales and will assist appropriate NNSA and Air Force nuclear weapons testing monitoring communities.

Technical Outcomes

This project developed two new formulations to capture the influences of topography on the wind fields and worked through a method to account for terrain-induced thermodynamic-related influences on flow fields. We have modified the reduced-order fire spread and energy balance models to allow the model to account for the influences of terrain. This project made significant progress towards enabling QUIC-Fire use on complex topography and increasing its utility for a variety of applications and government agencies.

Control of Turbulence by Design

Heidi Morris
20180728ER

Project Description

The national security challenge that this work will address is to ultimately mitigate turbulence in Omega and National Ignition Facility implosions and help improve the viscosity physics in our codes. Turbulent mix has been invoked to explain many results in Inertial Confinement Fusion and High Energy Density physics, such as reduced yield in capsule implosions. Many simulations use fluid turbulent mix models to help match simulation results to data, but this is not appropriate if fully developed turbulence is not present. Mix, turbulent or not, can turn a plasma of a single material into a multi-component plasma, causing the viscosity to change by orders of magnitude depending on the fraction of high-atomic number (high-Z) material mixed in. Unlike fluids, mixed plasmas can have a change in viscosity that is high enough to ward off further turbulent growth. The project will employ self-consistent simulations to examine the plasma states and viscosities that can be established with the OMEGA laser.

Technical Outcomes

The importance of viscosity in reducing instability growth for possible future shock-tube or MShock experiments was examined. To achieve this, self-consistent Lasnex and xRAGE simulation studies have been performed, which have advanced our understanding beyond what was considered previously using equations alone. It is difficult to achieve high values of ionization and viscosity for the types of experiments considered here. Studies at more energetic conditions might be of interest for future work.

A New Method for Computer-Guided Design and Optimization of Noncovalent Molecular Recognition Motifs

Christopher Neale
20180739ER

Project Description

New drugs require enormous capital investment. Our long-term goal is to dramatically reduce the total cost associated with bringing a drug to market. To do this, we plan to replace collections of disjoint initial leads with swarms of chemically related leads that each define a broad region of chemical space. We reason that these swarms will add flexibility to the process of lead refinement and thereby reduce the likelihood that drug candidates will succumb to late-stage failures. To this end, we are developing an automated computer simulation capability in which the exploration of chemical space is guided by a probabilistic search that rewards conceptually funnel-shaped regions comprising many high-scoring chemicals. This simulation platform is, by design, also applicable to guide macromolecular modifications such that it can empower protein engineering for greater thermal stability (e.g., clean energy innovation via industrial carbon dioxide sequestration) and protein repurposing for binding to exogenous compounds, enabling signature detection and providing possible avenues for forward deployment via transgenic plants.

Technical Outcomes

Many biological processes are regulated by molecular recognition. Examples include signal transduction, viral attachment, and protein/nucleic acid folding and complex formation. To study these processes, and to develop drugs that rectify harmful interactions, we developed a generalized computational framework for the autonomous design and optimization of molecular interfaces in liquid environments. Beyond drugs, this framework will be of interest for the rational design of biosensors, detoxification platforms, and surfaces that resist biofouling.

Climate-driven Disease Models

Carrie Manore
20180740ER

Project Description

As part of the Laboratory's global security mission, this project is an important piece of setting the stage for a system that could truly forecast mosquito-borne disease risk at a small scale across large regions. With increased situational awareness, national and international public health agencies and our national security agencies will have more lead time for resource allocation and mitigation and will be better able to issue appropriate warnings for the public to use personal protection or implement mosquito control.

Technical Outcomes

We developed a mathematical model that links temperature and flooding in waterways in cities to the abundance of the Culex mosquitoes that spread West Nile virus. Our models predict mosquito fluctuations work well for regions of municipal regions where waterways are minimally managed but need to be adapted where waterways are managed intensively. This model is foundational to our future efforts in predicting mosquito populations and disease risk under future climate scenarios.

Magnetic Coupling to the Ionospheric Alfvén Resonator

William Junor
20180749ER

Project Description

We will evaluate this sensing methodology as a tool for detection of clandestine, underground, nuclear tests, and for nuclear treaty monitoring. We anticipate that the technique may provide another diagnostic tool to complement and augment other sensing methods; taken together, these sensing methods would be able to more accurately assess the likelihood that a clandestine test occurred. The impact on DOE/NNSA missions would be to provide another sensing methodology, but one which is not defeated by seismic decoupling.

Technical Outcomes

No excitation of the Ionospheric Alfvén Resonator was seen during our tests for the range of frequencies we used and for the size of the magnetic pulses we generated. Natural ionospheric noise may have masked the signals. TEC measurements using next-gen (L1, L5 equipped) cell phones appears to be possible and very useful.

Modeling Glycan Dynamics and Occupancy using Molecular Dynamics Simulations and Machine Learning

Kshitij Wagh
20180750ER

Project Description

Our long-term goal is to better understand the important role of protein-attached sugars (“glycans”) in infectious disease, immunology, cancer, and several other biological disciplines, and to apply this knowledge for discovery/design of novel vaccines and therapeutics, and biothreat detection and mitigation. The research proposed here encompasses the development of two computational strategies that are key building blocks required for realizing our long-term research program. If successful, our computational strategies will provide basic biological data on glycans that are either inaccessible to experiments or accessible only through resource-intensive experiments, and thus, facilitate high-throughput studies of biological roles of glycans. This research directly supports the basic science efforts of the DOE Office of Science Biological and Environmental Research to understand structure and function of complex, biological systems using computational approaches. Our general modeling framework can also be applied to understand other biological phenomena of interest to the DOE/NNSA such as plant sugars, algal biofuels, etc.

Technical Outcomes

This project achieved: a) initial simulations of glycan subunits that will facilitate coarse-grained approaches for long-time simulations of glycoprotein dynamics, b) helped identify potential problems with published data that will be used for machine learning prediction of site-wise glycan occupancy, and c) organized a workshop on HIV glycan biology that will allow future collaborations and program development.

Integrating Mechanistic Models with Machine Learning and Statistical Approaches to Predict Individual Disease Risks Using Electronic Health Records

Ruian Ke
20180752ER

Project Description

Cardiovascular disease is a leading cause of debility and death in the US. This project combines machine learning (ML) and mechanistic cardiovascular disease modelling to elucidate cause-effect relationships, correct for selection bias, and appropriately formulate the higher order interaction terms. Future efforts could ultimately lead to a powerful tool to make precise predictions of individual disease outcome and thus rational decisions of treatments tailored to individual characteristics. This research is aligned with the recent DOE initiatives in quantitative approaches to precision medicine.

Technical Outcomes

This project developed a novel framework that integrates mechanistic modeling with statistical modeling to describe the changes in key biomarkers of cardiovascular diseases (CVDs) and how changes in the longitudinal measurements of these biomarkers relates to the risk of major subtypes of CVDs. This framework easily integrates into statistical approaches as well as machine learning approaches to analyze a large amount of EHR data to guide precise individualized decisions.

Boosting Algae Biomass for Biofuels with Plant Substrate Utilization

Amanda Barry
20170533ECR

Project Description

A Los Alamos priority is to secure energy solutions for clean energy and to mitigate the impacts of global energy demand growth. Optimizing algal growth through a mixotrophic (using light and carbon for growth) strategy utilizing cellulosic substrates and identifying potential high-value enzymes in biofuel production strains aligns with this focus and with DOE Bioenergy Technologies Office goals for improving algal biomass productivity. The proposed research will enable economical algal biofuel production by increasing algal biomass productivity and contribute to a stable domestic energy future.

Publications

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for Biofuels with Plant Substrate Utilization. Unpublished report. (LA-UR-18-28460)

Rollin, J., S. Pattathil, S. R. Starckenburg, N. M. Sudasinghe Appuhamilage, B. W. Vogler, and A. N. Barry.

Characterization of plant carbon substrate utilization by *Auxenochlorella protothecoides*. 2018. *Algal Research*. 37-48. (LA-UR-18-21621 DOI: 10.1016/j.algal.2018.07.001)

Advanced Understanding of Ocean Heat Storage by Coupling Large Eddy Simulation to a Global Ocean Model

Luke Van Roekel
20180549ECR

Project Description

Modeling the Earth System is a challenging, yet exciting, endeavor. There are physical processes essential to Earth System Models (ESMs) that span a wide range of sizes (meter to hundreds of kilometers). Present ESMs are unable to simulate this broad range of processes as many of these processes are smaller than the model grid cells. Newer ESMs that claim to be able to simulate a wider range of physical processes are unable to do so with high fidelity. This work will yield an unprecedented improvement in ESM ability to accurately simulate the rich tapestry of processes important to the ocean. This research will serve the energy security mission of DOE by helping to revolutionize our understanding and predictive capability of the migration and fate of carbon in the climate system. The resulting improved ESM fidelity will yield more confidence in any planning and policy that results from model predictions.

Modeling Heterogeneous Surveillance Data for Adaptive Real-time Response to Epidemics

Ethan Romero-Severson
20180612ECR

Project Description

Infectious disease outbreaks threaten local, national, and global security not only in their direct destabilizing effects, but also in their secondary effects by perceptions to governmental responses to those outbreaks. We propose that much of the data that is collected as part of routine surveillance can be used to move from a 'surveillance and reporting' paradigm to an active decision support framework where local outbreaks can be directly modeled and the potential efficacy and costs of alternative intervention programs can be tested in an evolving epidemic.

Publications

- Bulla, I., E. Romero-Severson, and D. Gromov. Systematic evaluation of the population-level effects of alternative treatment strategies on the basic reproduction number. 2019. *Journal of Theoretical Biology*. 381-390. (LA-UR-18-31251 DOI: 10.1016/j.jtbi.2018.11.029)
- Leitner, T. K., and E. Romero-Severson. Phylogenetic patterns recover known HIV epidemiological relationships and reveal common transmission of multiple variants. 2018. *Nature Microbiology*. (9) 983-988. (LA-UR-18-28043 DOI: 10.1038/s41564-018-0204-9)
- Romero-Severson, E., I. Spicknal, D. Gromov, and I. Bulla. Sensitivity of joint contagiousness and susceptibility-based dynamic optimal control strategies for HIV prevention. To appear in *PLOS ONE*. (10) . (LA-UR-18-30123 DOI: 10.1371/journal.pone.0204741)
- Romero-Severson, E., and A. Goyal. Screening for hepatitis D and PEG-Interferon over Tenofovir enhance general hepatitis control efforts in Brazil. To appear in *PLOS ONE*. (9) . (LA-UR-18-28686 DOI: 10.1371/journal.pone.0203831)

Joint Critical Thresholds and Extremes for Vulnerability Assessment of Regional Stability

Katrina Bennett
20180621ECR

Project Description

This project will address "what, where, how" of joint thresholds and extreme events (e.g. flooding+high temperatures) to provide a critical, climate-appropriate assessment of vulnerability to regional stability and security in US watersheds. The novel, science-based approach to vulnerability assessment in a no-analog future can be used to support decision-making for national security applications. The project also directly supports wider Department of Energy (DOE) challenges, including DOE Office of Science's focus on energy-water nexus and DOE's mission to provide actionable science to other federal agencies including the Department of Homeland Security and the Department of Defense.

Publications

Bennett, K. E., J. Cherry, B. Balk, and S. Lindsey. Using MODIS estimates of fractional snow cover extent to improve streamflow forecasts in Interior Alaska. Submitted to *Hydrology and Earth System Sciences*. (LA-UR-18-21603)

Bennett, K. E., V. Tidwell, D. Llewellyn, S. Behery, L. Barrett, M. Stansbury, and R. S. Middleton. Threats to a Colorado River Provisioning Basin from Coupled Future Climate and Societal Changes. Submitted to *Environmental Research Letters*. (LA-UR-18-30685)

Next-Generation Sea Level Predictions with Novel Ice Sheet Physics

Matthew Hoffman
20160608ECR

Project Description

This project will generate a robust capability of realistic basal physics for ice-sheet models developed and used by Los Alamos for improved sea level change predictions. Ice sheet basal sliding is the primary control on the flux of ice to the oceans; however, current predictions of sea level change from ice sheet models assume basal sliding will not change in the future, an assumption at odds with decades of research. Incorporating this crucial missing process will generate superior sea level predictions and a novel Earth System Modeling capability at Los Alamos. The impact of this work could be profound as sea-level change could potentially disrupt and displace coastal infrastructure and communities. Close to 150 million people live within 1 meter (m) of current sea level.

Technical Outcomes

The project developed a model for subglacial drainage that includes distributed and channelized drainage, runs in parallel, and is coupled to ice dynamics. Comparing model output to water pressure measurements in Greenland revealed the importance of weakly-connected regions of the bed to basal traction. Further work identified the importance of draining supraglacial lakes in Greenland to the formation of moulins. Model simulations showed that inclusion of subglacial drainage makes simulations more sensitive to external forcing.

Publications

Andrews, L. C., M. J. Hoffman, T. A. Neumann, G. A. Catania, M. P. Luethi, R. L. Hawley, K. M. Schild, C. Ryser, and B. F. Morriss. Seasonal Evolution of the Subglacial Hydrologic System Modified by Supraglacial Lake Drainage in Western Greenland. To appear in *Journal of Geophysical Research: Earth Surface*. (6) 1479-1496. (LA-UR-18-27505 DOI: 10.1029/2017JF004585)

Andrews, L. C., M. J. Hoffman, T. A. Neumann, G. A. Catania, M. P. Luethi, R. L. Hawley, K. M. Schild, C. Ryser, and B. F. Morriss. Seasonal evolution of the subglacial hydrologic system modified by supraglacial lake drainage in western Greenland. Submitted to *Journal of Geophysical Research: Earth Surface*. (LA-UR-18-26150)

de Fleurian, B., M. A. Werder, S. Beyer, D. J. Brinkerhoff, I. Delaney, C. F. Dow, J. Downs, O. Gagliardini, M. J. Hoffman, R. L. Hooke, J. Seguinot, and A. N. Sommers. SHMIP The subglacial hydrology model intercomparison Project. Submitted to *Journal of Glaciology*. (LA-UR-18-30871)

Hoffman, M. J. Next-generation sea level predictions with novel ice sheet physics. Unpublished report. (LA-UR-18-20089)

Hoffman, M. J., L. C. Andrews, S. F. D. Price, G. A. Catania, T. A. Neumann, M. P. Luethi, J. Gulley, C. Ryser, R. L. Hawley, and B. Morriss. Greenland subglacial drainage evolution regulated by weakly connected regions of the bed. 2016. *Nature Communications*. 13903. (LA-UR-16-24080 DOI: 10.1038/ncomms13903)

Hoffman, M. J., M. Perego, L. A. Andrews, S. F. D. Price, T. A. Neumann, J. Johnson, and G. Catania. Widespread Moulin Formation During Supraglacial Lake Drainages in Greenland. 2018. *Geophysical Research Letters*. (2) 778-788. (LA-UR-17-28283 DOI: 10.1002/2017GL075659)

Coupling Kinetic to Fluid Scales in Space and Laboratory Plasmas

Ari Le

20160647PRD2

Project Description

This project will perform advanced computer simulations to more accurately model two types of problems: (1) the interaction between the solar wind and the Earth's magnetosphere, and (2) the implosion of inertial fusion capsules. The fluid equations currently used to model plasmas are not always well justified. This is particularly true in critical regions such as shocks and thin boundary layers. In this project, we will demonstrate the feasibility of simulations that more accurately describe the entire complex system. We anticipate this project may improve our ability to more accurately model a variety of applications, including the space weather environment surrounding the Earth, and also the plasma dynamics within the fuel region of inertial fusion capsules.

Publications

Chen, L. J., A. Y. Le, S. Wang, L. I. Wilson, S. Schwartz, N. Bessho, T. Moore, D. Gershman, B. Giles, D. Malaspina, F. Wilder, R. Ergun, M. Hesse, H. Lai, C. Russell, R. Strangeway, R. Torbert, A. Vinas, J. Burch, S. Lee, C. Pollock, J. Dorelli, W. Paterson, N. Ahmadi, K. Goodrich, B. Lavraud, O. Le Contel, Y. Khotyaintsev, P. Lindqvist, L. Avanov, and H. Wei. Electron Bulk Acceleration and Thermalization at Earth's Quasiperpendicular Bow Shock. 2018. *Physical Review Letters*. (22) 225101. (LA-UR-18-26991 DOI: 10.1103/PhysRevLett.120.225101)

Chen, L. J., D. Gershman, E. Yarger, S. Wang, J. Jara-Almonte, J. Yoo, E. H. Kim, M. Yamada, H. Ji, A. Y. Le, and W. Fox. Whistler Wave Generation by Anisotropic Tail Electrons During Asymmetric Magnetic Reconnection in Space and Laboratory. To appear in

Geophysical Research Letters. (16) 8054-8061. (LA-UR-18-20161 DOI: 10.1029/2018GL079278)

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Le, A. Y. Global Hybrid (Kinetic Ion/Fluid Electron) Simulation of Magnetosphere of Jupiter's Moon Ganymede with Code H3D Performed on Mustang. Unpublished report. (LA-UR-16-29561)

Le, A. Y., T. J. T. Kwan, M. J. Schmitt, H. W. Herrmann, and S. H. Batha. Simulation and assessment of ion kinetic effects in a direct-drive capsule implosion experiment. 2016. *Physics of Plasmas*. (10) 102705. (LA-UR-16-24469 DOI: 10.1063/1.4965913)

Le, A. Y., W. S. Daughton, J. Yoo, S. Wang, H. Ji, J. L. Burch, W. Fox, J. Jara-Almonte, T. Moore, R. B. Torbert, B. Giles, M. Hesse, L. J. Chen, and M. Yamada. The two-fluid dynamics and energetics of the asymmetric magnetic reconnection in laboratory and space plasmas. To appear in *Nature Communications*. (1) 5223. (LA-UR-18-31065 DOI: 10.1038/s41467-018-07680-2)

Le, A. Y., W. S. Daughton, L. J. Chen, and J. Egedal. Enhanced electron mixing and heating in 3-D asymmetric reconnection at the Earth's magnetopause. *Geophysical Research Letters*. (LA-UR-17-27740 DOI: 10.1002/2017GL072522)

Le, A. Y., W. S. Daughton, O. Ohia, L. J. Chen, Y. H. Liu, and S. Wang. Drift turbulence, particle transport, and anomalous dissipation at the reconnecting magnetopause. 2018. *Physics of Plasmas*. (6) 62103. (LA-UR-18-21459 DOI: 10.1063/1.5027086)

Liu, Y. H., A. Y. Le, M. Hesse, T. C. Li, and M. Kuznetsova. Orientation and Stability of Asymmetric Magnetic Reconnection X Line. 2018. *Journal of Geophysical*

Research: Space Physics. (6) 4908-4920. (LA-UR-18-26828 DOI: 10.1029/2018JA025410)

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Regulation of Intercellular Signaling

Christopher Neale
20160676PRD4

Project Description

G-protein coupling receptors (GPCR) are a large family of proteins that detect external signals (e.g., light or molecules) on a cell's surface and trigger a cell response. Cell responses can range from opening a channel that leads to a nerve system signal, or to trigger cell division. GPCRs are the target of over 50% of approved drugs in the market. However, the mechanisms of action of GPCRs are not known at the molecular level. Understanding the mechanism of action can help understand diseases at the molecular level, which in turn can help design new drugs. This project employs high performance computational tools to simulate the dynamics of GPCRs in environments that mimic the cell surface. The simulations are validated with experimental data available in the literature. A comparison of atomistic simulation data with in cell data enables the postulation and testing of hypotheses about the mechanism of action of these proteins.

Publications

Neale, C. A. Mechanistic insights into allosteric regulation of the A2A adenosine G protein-coupled receptor by physiological cations. 2018. *Nature Communications*.

(1) 1372. (LA-UR-18-20653 DOI: 10.1038/s41467-018-03314-9)

Building Full-scale Computational Models of Viruses

Tyler Reddy

20160677PRD4

Project Description

Viruses are effectively ancient self-replicating microscopic machines that infect living organisms (i.e. humans, important food crops) and coerce them for the purpose of self-propagation. A deadly self-replicating, self-spreading entity could threaten public health, safety, and security. While many scientists study the spread of viruses at a population level using epidemiology, we focus on looking at the physically realistic computer model of a single virus (a single self-replicating machine) to gain insight about its behavior on the microscopic scale. The primary target outcome is biophysical insight into the behavior of enveloped viruses (especially HIV-1), which may reveal structural susceptibilities pertinent to vaccine, drug, and chemical neutralization efforts. This project has applications to all emerging viral threats, both natural and engineered, and aligns with the Laboratory's biosecurity mission. It directly supports the Science of Signatures science pillar, specifically in threat reduction and global health security. Unlike conventional bioweapon threats, a natural or engineered high-fatality pandemic is the greatest national security threat because of its global reach. This work will help solidify local efforts that seek to revolutionize Deoxyribonucleic Acid (DNA)-sequence-based risk assessment of threats. Additionally, modeling of complex systems at the atomic scale builds our abilities for several other national security missions.

Quantifying Covalency in Californium and the Other +3 Actinides

Samantha Schrell
20170663PRD1

Project Description

Identifying methods to measure subtle differences in M–Cl orbital mixing could have broad impact in virtually every technologically relevant area associated with the f-elements. This spans from isotope production to advanced nuclear fuel cycle development, plutonium sustainment, and the national nuclear security administration's (NNSA) missions in nuclear science. For example, many claims have rationalized unusual actinide behavior by invoking 5f-covalency in actinide-ligand bonding. As such, this project represents a leap forward for characterizing covalency in transplutonium metal-ligand bonding. We are excited at the opportunity to correlate the impact of covalency on the chemical and physical properties of important compounds and materials. Finally, these results have potential to serve as inspiration to strategically interrogate other actinide compounds in an effort to identify mechanisms to further enhance 5f- and 6d-contributions to covalent bonding.

Impacts of Climate and Land Use on Global River Dynamics

Joel Rowland
20170668PRD1

Project Description

By using global datasets of remotely sensed imagery to quantify river dynamics, this project will directly improve our ability to predict and mitigate risks to infrastructure, agriculture, and navigation due to changing channels. Rivers and floodplains play an essential role in the storage and transport of water sediment and biogeochemical constituents. Quantifying the magnitude and controls on these fluxes and impacts to infrastructure helps support DOE science missions and the NNSA's national security missions. An improved predictive understanding of river responses to floods and droughts will aid in disaster planning and assessing risk to critical infrastructure.

Publications

Gran, K., C. Dolph, A. Baker, M. Bevis, S. Cho, J. Czuba, B. Dalzell, A. Hansen, S. Kelly, Z. Lang, J. P. Schwenk, P. Belmont, J. Finlay, P. Kumar, S. Rabotyagov, G. Roehrig, P. Wilcock, and E. Foufoula-Georgiou. Data synthesis for collaborative, multidisciplinary research in an intensively managed agricultural landscape: the Minnesota River Basin environmental observatory. Submitted to *Water Resources Research*. (LA-UR-18-29803)

Developing a Unique Technology to Control Emerging Threats of Antibiotic-resistant Pathogens

Patrick Chain
20170671PRD2

Project Description

The project goal is to control *C. difficile* infections (CDI), their re-occurrence, and the rise of antibiotic resistance.

C. difficile infections pose threats to our nation's public health and security. Our proposed work takes a systematic approach to utilize the normal human gut flora to naturally control CDI and antibiotic resistance.

Forecasting Failure

Paul Johnson
20170673PRD2

Project Description

A large earthquake in Cascadia or California would devastate the regional and potentially national economies. The primary national security challenge the project will address is attempting to characterize when a large earthquake may occur and how large it may be so that preparatory action may be taken. Our secondary security challenge is applying this same technology to anthropogenic ally induced seismicity, particularly in the mid west. Can we tell when a large, human induced earthquake will take place and how large it will be, so that we can take action to prevent it? That is the secondary goal. The novelty of our work is the use of machine learning to discover and understand new physics of failure, through examination of the full continuous time signal. The future of earthquake physics will rely heavily on machine learning to process massive amounts of raw seismic data. Our work represents an important step in this direction. The outcomes of this project are expected to have broad technical application. Not only does it have import to earthquake forecasting, but also the approach is far-reaching, applicable to potentially all failure scenarios including nondestructive testing, brittle failure of all kinds, avalanche, etc.

Publications

G. Rouet-Leduc, B. P., C. Hulbert, D. C. Bolton, C. Ren, C. Marone, R. A. Guyer, and J. A. Paul. Estimating Fault Friction From Seismic Signals in the Laboratory. 2018. *Geophysical Research Letters*. (3) 1321-1329. (LA-UR-17-29312 DOI: 10.1002/2017GL076708)

Prediction of Magnetic Properties of Actinide Complexes Using Ab Initio Methods

Ping Yang

20170677PRD2

Project Description

The U.S. National Energy Policy states the critical need for the expansion of nuclear energy to enhance energy security and reduce domestic dependence on foreign fossil fuels. Yet, comprehensive and innovative storage or reprocessing solutions hinge on physics and chemistry knowledge going far beyond what is currently available. Separation of the highly hazardous minor actinides from the rest of the waste would greatly facilitate disposal by drastically reducing the storage time of bulk waste and the volume of waste required for long-term storage. Unfortunately, due to the similarities between minor actinides and lanthanides, a procedure to isolate these elements is still missing. This work is the first systematic study of the magnetic properties of actinide molecular systems, which will enable us to draw structure/property correlations. This will not only improve our understanding of the subtle differences in the chemistry in transuranium elements, it will also help us identify, and potentially design, new molecular species capable of effecting the separation of minor actinides. The impact of having this predictability will advance us towards cleaner and more cost-effective reprocessing mechanisms to deal with spent nuclear fuel, which addresses Los Alamos missions in plutonium excellence, energy security, repository science, and long-term waste management.

Publications

Aguirre Castiblanco, N. F., J. C. A. O. Jung, and P. Yang. First-Principle Study of Structure and Stability of Thorium Dioxide Nanoclusters, $\text{Th}_n \text{O}_{2n}$ ($n = 1 - 8$). Submitted to *ACS Nano*. (LA-UR-18-29967)

Tandem Dehydrogenation of Formic Acid and Olefin Hydrogenation: Steps Towards a Self-Sustaining Pressure/Volume System

James Boncella
20170685PRD3

Project Description

The goal of this project is to generate the fundamental chemical understanding necessary to enable the fabrication of a chemical gas generation system that will replace large, heavy gas pressure bottles for performing pressure-based work. This will be accomplished through the generation of a tandem catalysis system that will perform two functions. It will decompose formic acid to hydrogen and carbon dioxide, and also use some of the hydrogen that is produced in the reaction to perform a separate reaction that will generate the heat necessary to drive the decomposition of formic acid at a practical rate. Such a reaction system would be an enormous advance to catalytic science because it would necessitate a detailed understanding of how to accomplish multi-step chemical transformations in a single reaction vessel.

Publications

Anderson, N. H., J. M. Boncella, and A. Tondreau. Reactivity of Silanes with (tbuPONOP)Ruthenium Dichloride: Facile Synthesis of Chloro-Silyl Ruthenium Compounds and Formic Acid Decomposition. 2017. *Chemistry - A European Journal*. (55) 13617-13622. (LA-UR-17-25821 DOI: 10.1002/chem.201703722)

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Epigenetic Control of Synchronized Proliferation in Harmful Algal Blooms (HABs)

Babetta Marrone
20170690PRD4

Project Description

The increased frequency of harmful algal blooms in regions in the United States affected by climate change has produced heightened scientific and regulatory attention; these blooms, by destroying the environment, cause economic instability, potential political unrest, and significant health issues. Research has focused on identifying harmful algal species and creating bloom prediction models; however, to date, little is known about the molecular and cellular physiology of these blooms. This knowledge is critical for predicting, suppressing, and controlling these deleterious events. The proposed research identifies important epigenetic processes that regulate harmful algal bloom formation and provides greater insight into critical mechanisms of action that could be harnessed to mitigate harmful algal blooms in coastal waters for increased regional and global security. Harmful algal blooms impact human health and economic stability as they ruin water quality, impact food safety, induce sickness and death from toxin exposure, and cause biothreats. Understanding regulation of harmful algal blooms directly contributes to program needs for the Department of Homeland Security (global security of bio-toxin production), the Department of Defense (sailor health and port environmental impacts), and the Department of Energy (bioenergy and environmental climate impacts).

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Publications

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Molecular Basis of RAS-related Cancers

Angel Garcia
20170692PRD4

Project Description

We will use high performance computer simulations to model the interactions of cancer related proteins in environments that mimic the cell environment. We study the interactions of oncogenes proteins with lipid membrane and with other proteins that upon binding activate the oncogenes. The nature of the interactions with the lipid bilayer and the activating proteins may offer opportunities to identify new targets for anti-cancer drug development. The computer simulations will be state-of-the-art atomistic molecular dynamics simulations. Larger scale models will also be used to study long time scale effects that are in time scales not accesible to atomistic simulations. Project collaborations include the National Cancer Institute and other National Laboratories.

Machine Learning the Physics of an Active Gold Mine

Daniel Trugman
20180700PRD1

Project Description

This work will address energy security and national security. Our work will advance earthquake forecasting, including human induced earthquakes. For instance, the energy storage site at Cushing Oklahoma is located in a highly earthquake-active region due to wastewater injection. This work will better predict if an earthquake near Cushing is imminent. In addition, it will tell us if a large tectonic quake is approaching, for instance in the Cascadia region. The high-level goals of this work are to advance our understanding of Earth faults and advance earthquake forecasting. This work will impact DOE/NNSA national security missions. For instance, a megaquake in Cascadia will have dramatic impact on the regional and national economy. A quake at Cushing, has the potential to disturb oil reserves or their distribution, and could have a negative impact on the national economy.

Shearer, P. M., R. E. Abercrombire, D. T. Trugman, and W. Wang. Comparing EGF Methods for Estimating Corner Frequency and Stress Drop from P-wave Spectra. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-18-30681)

Trugman, D. T., M. T. Page, S. E. Minson, and E. S. Cochran. Peak ground displacement saturates exactly when expected: Accounting for measurement time-dependence in earthquake early warning. Submitted to *Geophysical Research Letters*. (LA-UR-18-30809)

Trugman, D. T., and P. M. Shearer. Strong Correlation between Stress Drop and Peak Ground Acceleration for Recent M_w 1–4 Earthquakes in the San Francisco Bay Area. 2018. *Bulletin of the Seismological Society of America*. (LA-UR-18-20708 DOI: 10.1785/0120170245)

Publications

Koper, K. D., K. L. Pankow, J. C. Pechmann, J. M. Hale, R. Berclau, W. L. Yeck, H. M. Benz, R. B. Herrman, D. T. Trugman, and P. M. Shearer. Afterslip Enhanced Aftershock Activity During the 2017 Earthquake Sequence Near Sulphur Peak, Idaho. 2018. *Geophysical Research Letters*. (11) 5352-5361. (LA-UR-18-22721 DOI: 10.1029/2018GL078196)

Meade, B., P. Gerstoft, Z. E. Ross, M. J. Bianco, Q. Kong, and D. T. Trugman. Machine Learning in Seismology: Turning Data into Insights. To appear in *Seismological Research Letters*. (1) 3-14. (LA-UR-18-28089 DOI: 10.1785/0220180259)

Qin, Y., X. Chen, J. Haffener, D. T. Trugman, B. M. Carpenter, and J. I. Walter. Deciphering the stress state of seismogenic faults in Oklahoma and southern Kansas based on high-resolution stress maps. Submitted to *Earth and Planetary Science Letters*. (LA-UR-18-27043)

Ross, Z. E., D. T. Trugman, E. Hauksson, and P. M. Shearer. Searching for Hidden Earthquakes in Southern California. Submitted to *Science*. (LA-UR-19-20273)

Unusual Oxidation States and Covalency-Tuning in Transuranic Molecules

Andrew Gaunt
20180703PRD1

Project Description

The research will focus on using specialized and unique radiological capabilities at Los Alamos National Laboratory to synthesize unprecedented organometallic compounds with actinides, including highly radioactive isotopes of neptunium, plutonium and americium. The results will open up never before possible low oxidation state chemistry for these elements and define new bonding trends. This fundamental science will be published in top journals, be internationally recognized as world leading and of direct benefit to DOE-SC programs to solve basic research needs in their Heavy Element Chemistry program. The advance in fundamental chemical bonding knowledge fosters future 'basic science knowledge-driven' innovative creative solutions to applied needs in the DOE complex aimed at tackling challenges associated with radioactive waste/chemical processing arising from used nuclear fuel (energy security), and environmental remediation problems. In addition, plutonium science is central to the national security mission of Los Alamos, and any significant new understanding in the chemistry of this element is clearly important.

Publications

Windorff, C. J., J. M. Sperling, B. E. Klamm, C. A. P. Goodwin, D. N. Huh, A. N. Gaiser, D. E. Hobart, S. A. Kozimor, A. J. Gaunt, W. J. Evans, and T. E. Albrecht-Schmitt. Probing the Reactivity of Plutonium(II) with Cyclooctatetraene. Submitted to *Organometallics*. (LA-UR-18-29397)

Forest Ecosystems: Resilience or Tipping Point?

Rodman Linn
20180704PRD1

Project Description

Forest ecosystems, including the semi-arid forests of the Southwest, play key roles in regional meteorology, precipitation and hydrology. Disturbances such as drought, insect outbreaks, flooding, wildfires and harvesting as well as elevated carbon dioxide (CO₂) levels, rising temperatures and changing precipitation patterns can change the energy and resource balances that govern forest productivity as well as resilience and thus exacerbate or dampen vulnerability of these ecosystems. These effects have significant influence on energy, water and food security of a region and impact regional stability. A systems-based understanding of these disturbances and their impact will provide unprecedented insight into energy and water policy development as well as healthy forest management.

Publications

Banerjee, T., M. J. Holmes, and R. R. Linn. Effect of canopy architecture on wildfire behavior. Submitted to *Agricultural and Forest Meteorology*. (LA-UR-18-21622)

New First Row Transition Metal Based Catalysts for Sustainable Energy Production

John Gordon

20180705PRD1

Project Description

While several technologies capable of generating energy exist, including nuclear, wind, solar, or hydrogen, none of these power sources alone can reasonably sustain increasing population driven energy demands in their current forms. While petroleum has long been the fuel of choice for energy production, the declining availability of light and middle cut petroleum feedstocks threatens the energy security of the nation and thus necessitates the development of novel fuel and chemical production technologies from renewable sources. The scientific results of this project will potentially provide industrially applicable techniques capable of generating transportation fuels and higher value chemicals, ameliorate possible petroleum deficits within the U.S., and provide high quality publications and potentially new Intellectual Property for the Laboratory and the DOE.

Design of State-of-the-art Flow Cells for Energy Applications

Ivan Popov
20180710PRD1

Project Description

The current project is aimed to design price-competitive redox flow cells batteries that can effectively store and use greener electricity, with the overall aim of approaching the cost target on large-scale energy storage (\$150/kWh) set by Department of Energy. This project is expected to discover novel electrolytes, which can be used in environmentally friendly and economically affordable redox flow cells that are critical for the national security of the United States.

Popov, I. A., R. Mukundan, E. R. Batista, and P. Yang. Catalyst-Inspired Charge Carriers for High Energy Density Redox Flow Batteries. To appear in *Physical Chemistry Chemical Physics*. (LA-UR-18-28568 DOI: 10.3389/fphy.2018.00141)

Zhang, X., I. A. Popov, K. A. Lundell, H. Schnockel, H. Wang, K. H. Bowen, and A. I. Boldyrev. Realization of an Al₂Al Triple Bond in the Gas-Phase Na Al Cluster via Double Electronic Transmutation. 2018. *Angewandte Chemie International Edition*. (43) 14060-14064. (LA-UR-18-22726 DOI: 10.1002/anie.201806917)

Publications

Chao, L., Z. Chen, I. A. Popov, Z. M. Sun, and A. I. Boldyrev. Aromaticity and Antiaromaticity in Zintl Clusters. 2018. *Chemistry - A European Journal*. (55) 14583-14597. (LA-UR-18-23061 DOI: 10.1002/chem.201801715)

Davis, B. L., G. A. Andrade, I. A. Popov, E. R. Batista, P. Yang, B. L. Scott, and T. Chu. Linked Picolinamide Nickel Complexes As Charge Carriers for Non-Aqueous Flow Batteries. Submitted to *ChemSusChem*. (LA-UR-18-27470)

Davis, B. L., T. Chu, E. R. Batista, P. Yang, R. Mukundan, J. C. Gordon, N. C. Smythe, N. Mehio, and I. A. Popov. Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. To appear in *ACS Omega*. (11) 14766-14778. (LA-UR-18-22442 DOI: 10.1021/acsomega.8b01921)

Fedik, N., C. Mu, I. A. Popov, H. Wang, W. Wang, K. H. Bowen, A. I. Boldyrev, and X. Zhang. Boron-made N₂: the Realization of a B₂Al₃ Triple Bond in the B₂Al₃- Cluster via Double Electronic Transmutation. Submitted to *Angewandte Chemie International Edition*. (LA-UR-18-24865)

Kelley, M., I. A. Popov, E. R. Batista, and P. Yang. Unusual In-Plane π Back-Donation in AnIV Metallacycles. Submitted to *Nature Communications*. (LA-UR-19-21182)

Liu, C., N. V. Tkachenko, I. A. Popov, N. Fedik, X. Min, A. I. Boldyrev, and Z. M. Sun. An All-Metal Spherically Aromatic Pyritohedron [Sb@In₈Sb₁₂]³⁻. Submitted to *Journal of the American Chemical Society*. (LA-UR-19-21142)

Principles for Optimal Establishment and Resilience of Microbial Communities

John Dunbar
20180746PRD3

Project Description

Deciphering fundamental principles of microbial invasion will raise the probability of successfully engineering microbial communities for applications to address a number of national security challenges. For example, robust understanding of principles of microbial invasion will allow for 1) effective development and deployment of probiotics for soldier health 2) improvements in agricultural soil microbe manipulations for increased food and energy security and 3) remediation and restoration of degraded environments for climate impact management.

Remediation Process Simulation-Optimization Under Complex Uncertainties

Velimir Vesselinov
20150711PRD2

Project Description

This project will advance an interval-fuzzy subsurface modeling system (IIFMS) for addressing interval and fuzzy uncertainties quantification (UQ) in modeling of contaminant fate and transport. Groundwater contamination can lead to adverse impacts and risks to society and the environment. Remediation costs are typically high and there is a big need for cost-effective strategies. Uncertainties are inherently associated with conceptualization and modeling of the contaminant fate, transport, and remediation process. Site remediation management is composed of various interconnected components that exhibit more complexities than its individual parts do. Such interconnections may lead to various complexities such as uncertainties in parameters and parameter relations, associated with dynamic and multi-objective features. We anticipate this work will be directly useful for generating more cost-effective remediation management strategies with improved efficiencies and increased robustness. The developed methods/models can also be applicable to other research areas where complicated uncertainties exist such as energy systems planning and surface water resources management.

Technical Outcomes

The project achieved development of risk assessment methodology and computation framework accounting for fuzzy and probabilistic uncertainties. The framework allows for scientifically-defensible comparison of the robustness of alternative decisions. The framework was tested for groundwater contaminant problems and it is applicable for any real-world problem where uncertainties are impacting the decision processes.

Publications

Jeong, H., A. Y. Sun, and X. Zhang. Cost-optimal design of pressure-based leakage monitoring networks considering geological uncertainty. Submitted to *Applied Energy*. (LA-UR-17-23051)

Wang, H., and X. Zhang. A Decentralized Bi-Level Fuzzy Two-Stage Decision Model for Flood Management. 2018. *Water Resources Management*. (5) 1615-1629. (LA-UR-17-21139 DOI: 10.1007/s11269-017-1894-0)

Zhang, H., S. M. Gorelick, P. V. Zimba, and X. Zhang. A remote sensing method for estimating regional reservoir area and evaporative loss. 2017. *Journal of Hydrology*. 213-227. (LA-UR-17-24804 DOI: 10.1016/j.jhydrol.2017.10.007)

Zhang, X., A. Y. Sun, I. J. Duncan, and V. V. Vesselinov. Two-Stage Fracturing Wastewater Management in Shale Gas Development. 2017. *Industrial & Engineering Chemistry Research*. (6) 1570-1579. (LA-UR-16-27947 DOI: 10.1021/acs.iecr.6b03971)

Zhang, X., and V. V. Vesselinov. Energy-water nexus: Balancing the tradeoffs between two-level decision makers. 2016. *Applied Energy*. 77-87. (LA-UR-16-23511 DOI: 10.1016/j.apenergy.2016.08.156)

Zhang, X., and V. V. Vesselinov. Integrated modeling approach for optimal management of water, energy and food security nexus. 2017. *Advances in Water Resources*. 1-10. (LA-UR-15-28987 DOI: 10.1016/j.advwatres.2016.12.017)

Laboratory Study of Fracturing and Hydraulic Conductivity through Heterogeneous Materials in Compressive Stress Environments

Luke Frash
20160642PRD1

Project Description

Our primary focus is to understand how mechanical damage (due to stress, temperature, fatigue, aging, chemical attack, etc.) to materials manifests as a changing permeability to fluids. These experiments will provide the first-ever study and x-ray imaging of fracture-fluid interactions at high-pressure and temperature and significantly advance our understanding of the consequences of fracture damage. Our work considers the behavior of heterogeneous materials with a particular application to high explosives. Analysis of the impacts of aging and deterioration of these materials are critical to DOE missions in nuclear weapons and explosives.

Technical Outcomes

Luke Frash designed and built an effective and efficient experimental system for characterizing permeability of rocks fractured at subsurface conditions. This led to the discovery of a critical stress above which permeable fractures do not form and a critical stress above which reactivation of fractures does not increase permeability. These important findings impact methods of extracting hydrocarbon from the subsurface, sequestration of CO₂, and production of geothermal energy.

Publications

- Carey, J. W., L. Frash, M. L. Porter, T. L. Ickes, and H. S. Viswanathan. Permeability of fractures created by triaxial direct shear and simultaneous X-ray imaging. Presented at *51st U.S. Rock Mechanics/Geomechanics Symposium*. (San Francisco, California, United States, 2017-06-25 - 2017-06-28). (LA-UR-18-30568)
- Carey, J. W., and L. Frash. Laboratory Study of Fracturing and Hydraulic Conductivity through Heterogeneous Materials in Compressive Stress Environments. Unpublished report. (LA-UR-17-30659)
- Carey, J. W., and L. Frash. Engineering Prediction of Axial Wellbore Shear Failure Caused by Reservoir Uplift and

Subsidence. 2018. *SPE Journal*. (04) 1039-1066. (LA-UR-17-20934 DOI: 10.2118/189981-PA)

- Frash, L., J. W. Carey, and T. L. Ickes. Fracturing, fluid flowing, and x-ray imaging through anhydrite at stressed conditions. Presented at *52nd US Rock Mechanics/Geomechanics Symposium, 24-27 June 2018*. (Seattle, Washington, United States, 2018-06-24 - 2018-06-27). (LA-UR-17-31383)
- Frash, L., T. L. Ickes, H. S. Viswanathan, and J. W. Carey. Caprock integrity susceptibility to permeable fracture creation. 2017. *International Journal of Greenhouse Gas Control*. 60-72. (LA-UR-16-28685 DOI: 10.1016/j.ijggc.2017.06.010)
- Gutierrez, M., J. W. Carey, A. Ketan, L. Frash, and F. Pengcheng. Laboratory validation of fracture caging for hydraulic fracture control. Presented at *52nd US Rock Mechanics/Geomechanics Symposium, 24-27 June 2018*. (Seattle, Washington, United States, 2018-06-24 - 2018-06-27). (LA-UR-17-31384)
- Hampton, J., L. Frash, L. Matzar, and M. Gutierrez. Extended term monitoring of acoustic emissions post-laboratory hydraulic fracturing. Presented at *52nd US Rock Mechanics/Geomechanics Symposium, 24-27 June 2018*. (Seattle, Washington, United States, 2018-06-24 - 2018-06-27). (LA-UR-17-31382)
- Hampton, J., L. Frash, and M. Gutierrez. Predictions of macro-scale fracture geometries from acoustic emission point cloud data in a hydraulic fracturing experiment. To appear in *Journal of Petroleum Exploration and Production Technology*. (LA-UR-18-28364 DOI: 10.1007/s13202-018-0547-z)
- Hampton, J., M. Gutierrez, L. Matzar, D. Hu, and L. Frash. Acoustic emission characterization of microcracking in laboratory-scale hydraulic fracturing tests. 2018. *Journal of Rock Mechanics and Geotechnical Engineering*. (LA-UR-17-30661 DOI: 10.1016/j.jrmge.2018.03.007)
- Hood, J., M. Mokhtary, H. Huang, E. Mattson, J. Hampton, M. Gutierrez, A. Tutuncu, J. W. Carey, and L. P. Frash. Complex hydraulic fracture patterns observed in true-triaxial experiments. Submitted to *Journal of Petroleum Exploration and Production Technology*. (LA-UR-18-30572)

Welch, N. J., J. W. Carey, and L. Frash. Scalable en echelon shear-fracture aperture roughness mechanism: theory, validation, and implications. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-18-27419)

Climate, Hydrology and Forest Disturbances in Southern and Western Watersheds

Katrina Bennett
20160654PRD2

Project Description

This project will develop a novel approach to quantifying changes in extreme events, with the goal of identifying critical watersheds where the greatest flooding and drought are anticipated to occur. The projected increase in frequency and intensity of billion-dollar weather and climate disasters, including severe storms, drought, and fire, is a significant domestic and global threat. We will develop a hydrologic model for the entire Colorado River basin (where key infrastructure and industry are located) that will be used to project future streamflow changes. One result will be a ranking of critical basins to determine the probability of future changes in extreme floods and droughts. This novel assessment of potentially destabilizing impacts will provide notable science results and new climate impact assessment technology to the national security community.

Technical Outcomes

Our results highlight the impacts of changing disturbances and climate on water resources in the Colorado River basin. We found a) impacts of decadal-scale forest disturbances and climate can result in up to a 20% reduction in streamflow, b) hydrologic models run under climate change are sensitive to forest cover parameterizations, and, c) climate change is leading to strong impacts on hydrology that must be better understood to mitigate serious future water management challenges.

Publications

- Bennett, K. E., A. Cannon, and L. Hinzman. Historical trends and extremes in boreal Alaska river basins. 2015. *Journal of Hydrology*. 590-607. (LA-UR-15-21132 DOI: 10.1016/j.jhydrol.2015.04.065)
- Bennett, K. E., J. R. Urrego Blanco, A. Jonko, T. Bohn, A. L. Atchley, N. M. Urban, and R. S. Middleton. Global Sensitivity of Simulated Water Balance Indicators Under Future Climate Change in the Colorado Basin. 2018. *Water Resources Research*. (1) 132-149. (LA-UR-17-27608 DOI: 10.1002/2017WR020471)

- Bennett, K. E., T. Bohn, K. C. Solander, E. Vivoni, N. McDowell, C. Xu, and R. S. Middleton. Climate-driven disturbances in the San Juan River sub-basin of the Colorado River. To appear in *Hydrology and Earth System Sciences*. (1) 709-725. (LA-UR-17-27609 DOI: 10.5194/hess-22-709-2018)
- Clark, M. P., M. F. Bierkens, L. Samaniego, R. A. Woods, R. Uijlenhoet, K. E. Bennett, V. R. Pauwels, X. Cai, A. W. Wood, and C. D. Peters-Lidard. The evolution of process-based hydrologic models: historical challenges and the collective quest for physical realism. 2017. *Hydrology and Earth System Sciences*. (7) 3427-3440. (LA-UR-17-27603 DOI: 10.5194/hess-21-3427-2017)
- Huntsman, B. M., J. A. Falke, J. W. Savereide, and K. E. Bennett. The role of density-dependent and -independent processes in spawning habitat selection by salmon in an Arctic riverscape. 2017. *PLOS ONE*. (5) e0177467. (LA-UR-17-27606 DOI: 10.1371/journal.pone.0177467)
- Koster, R., A. Betts, P. Dirmeyer, M. Bierkens, K. Bennett, S. Dery, J. Evans, R. Fu, F. Hernandez, R. Leung, X. Liang, M. Masood, H. Savenije, W. Guiling, and X. Yuan. Hydroclimatic variability and predictability: a survey of recent research. 2017. *Hydrology and Earth System Sciences*. (7) 3777-3798. (LA-UR-17-27604 DOI: 10.5194/hess-21-3777-2017)
- McDowell, N. G., S. Michaletz, K. E. Bennett, K. C. Solander, C. Xu, R. M. Maxwell, C. Allen, and R. S. Middleton. Predicting Chronic Climate-Driven Disturbances and Their Mitigation. 2018. *Trends in Ecology & Evolution*. (1) 15-27. (LA-UR-17-31438 DOI: 10.1016/j.tree.2017.10.002)
- Smith, D. W., M. Welch, K. E. Bennett, J. Padgham, and R. Mohtar. Building a WEF Nexus Community of Practice (NCoP). 2017. *Current Sustainable/Renewable Energy Reports*. (3) 168-172. (LA-UR-17-27607 DOI: 10.1007/s40518-017-0080-6)
- Solander, K. C., K. E. Bennett, D. Gutzler, E. M. Hopkins, R. S. Middleton, and S. W. Fleming. Interactions between climate change and complex topography drive observed streamflow changes in the Colorado River Basin. Submitted to *Journal of Hydrometeorology*. (LA-UR-17-27512)
- Solander, K. C., K. E. Bennett, and R. S. Middleton. Shifts in historical streamflow extremes in the Colorado

River Basin. 2017. *Journal of Hydrology: Regional Studies*. 363-377. (LA-UR-16-29616 DOI: 10.1016/j.ejrh.2017.05.004)

Development and Application of Multi-scale Models for Disease Forecasting

Carrie Manore
20160662PRD2

Project Description

We will examine three specific examples of infectious disease outbreaks as case studies to develop science-based decision support, including model development, uncertainty quantification, and risk communication. As a result of this work, we will have a greater understanding of the lessons to be learned from three specific epidemics of enormous importance to global public health: the West African Ebola outbreak of 2014, the emergence of virulence and antibiotic resistance in high disease-burden environments, and the spread of vector-borne disease. From these studies, we will also gain insights into how demographics, climate change, and policy decisions can influence these and other cases of disease emergence. This work addresses the Laboratory's global security mission.

Manore, C. A., R. Ostfeld, F. Agosto, H. Gaff, and S. LaDeau. Defining the Risk of Zika and Chikungunya Virus Transmission in Human Population Centers of the Eastern United States. Submitted to *PLOS Neglected Tropical Diseases*. (LA-UR-18-29808)

Technical Outcomes

We developed methods to couple models of complex systems with heterogeneous data in order to better predict risk under current situations and under potential future scenarios or interventions. The systems modeled include drug resistant malaria and non-typhi salmonella; Ebola; the 2016 Zika virus outbreak; and used non-traditional data. This work has served as a foundation for several awarded proposals and submitted and in-progress grants and manuscripts, all of which are contributing to the Laboratory's mission.

Publications

Brown, M., C. Cain, J. Whitfield, E. Ding, S. Y. Del Valle, and C. A. Manore. Modeling Zika Virus Spread in Colombia Using Google Search Queries and Logistic Power Models. Submitted to *PLOS Computational Biology*. (LA-UR-18-23845)

Manore, C. A. Can Neighborhood Screening Help Control Zika in the US?. Submitted to *BMJ*. (LA-UR-17-22311)

Manore, C. A. Modeling Virus Coinfection to Inform Management of Maize Lethal Necrosis in Kenya. 2017. *Phytopathology*. (10) 1095-1108. (LA-UR-17-22310 DOI: 10.1094/PHYTO-03-17-0080-FI)

Physiological and Structural Acclimation to Climate Change in Forest Ecosystems

Sanna Sevanto
20160670PRD3

Project Description

The proposed work is to conduct studies of the plasticity and acclimation of forest trees in response to experimental reductions in precipitation and elevations in temperature. Multi-factor experiments are rare but invaluable for studying the response of trees to climate change. Furthermore, research on acclimation to climate change has often been conducted on tree seedlings in controlled growth chambers with few studies in natural settings. This project will use a Los Alamos field experiment where whole-tree chambers and rain exclusion systems have been established to control both soil moisture and atmospheric temperature for two tree species presenting contrasting physiological responses to drought. The knowledge of tree acclimation acquired through this project will provide valuable information for the calibration and validation of climate-vegetation models.

Technical Outcomes

The project developed experimental and analysis methods for quantifying the acclimation capacity of growth, photosynthesis and water uptake of trees to drought and atmospheric warming. The results show that acclimation even in time scales of a few years can protect trees against mortality under environmental stress. These studies are the first developed for quantifying mature tree acclimation responses to warming and drought.

Publications

- Grossiord, C., A. Gessler, S. C. Reed, I. Borrego, A. D. Collins, L. T. Dickman, M. G. Ryan, L. Schonbeck, S. A. Sevanto, A. Vilagrosa, and N. G. McDowell. Reductions in tree performance during hotter droughts are mitigated by shifts in nitrogen cycling. Submitted to *New Phytologist*. (LA-UR-18-23417)
- Grossiord, C., S. A. Sevanto, D. Bonal, I. Borrego, T. Dawson, M. G. Ryan, W. Wang, and N. McDowell. Prolonged warming and drought modify belowground interactions for water among coexisting plants. To appear in *Tree Physiology*. (LA-UR-18-25100 DOI: 10.1093/treephys/tpy080)
- Grossiord, C., S. A. Sevanto, D. Bonal, I. Borrego, T. E. Dawson, M. G. Ryan, W. Wang, and N. G. McDowell. Prolonged warming and drought modify belowground interactions for water among coexisting plants. Submitted to *Tree Physiology*. (LA-UR-18-23416)
- Grossiord, C., S. A. Sevanto, D. Todd, A. Henry, A. D. Collins, L. T. Dickman, B. D. Newman, E. A. Stockton, and N. G. McDowell. Warming combined with more extreme precipitation regimes modifies the water sources used by trees. 2017. *New Phytologist*. (2) 584-596. (LA-UR-16-24124 DOI: 10.1111/nph.14192)
- Grossiord, C., S. A. Sevanto, H. D. Adams, A. D. Collins, L. T. Dickman, N. A. McBranch, S. T. Michaletz, E. A. Stockton, M. Vigil, and N. G. McDowell. Precipitation, not air temperature, drives functional responses of trees in semi-arid ecosystems. To appear in *Journal of Ecology*. (1) 163-175. (LA-UR-18-30597 DOI: 10.1111/1365-2745.12662)
- Grossiord, C., S. A. Sevanto, I. A. Borrego, A. L. Chan, A. D. Collins, L. T. Dickman, P. Hudson, S. T. Michaletz, W. Pockman, M. G. Ryan, E. Stockton, A. Vilagrosa, and N. McDowell. Tree water dynamics in a drying and warming world. 2017. *Plant, Cell & Environment*. (9) 1861-1873. (LA-UR-17-22377 DOI: 10.1111/pce.12991)
- Grossiord, C., S. A. Sevanto, J. M. Limousin, P. Meier, M. Mencuccini, R. E. Pangle, W. Pockman, Y. Salmon, R. Zweifel, and N. G. McDowell. Manipulative experiments demonstrate how long-term soil moisture changes alter controls of plant water use. 2017. *Environmental and Experimental Botany*. (LA-UR-17-28179 DOI: 10.1016/j.envexpbot.2017.12.010)
- Grossiord, C., S. A. Sevanto, J. M. Limousin, P. Meir, M. Mencuccini, R. Pangle, W. Pockman, Y. Salmon, R. Zweifel, and N. McDowell. Manipulative experiments demonstrate how long-term soil moisture changes alter controls of plant water use. 2018. *Environmental and Experimental Botany*. 19-27. (LA-UR-18-24942 DOI: 10.1016/j.envexpbot.2017.12.010)
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Atom-Efficient Upgrading of Bio-Derived Isopropanol/Acetone Mixtures

Cameron Moore
20160671PRD3

Project Description

The project proposes to develop a chemical route to fuels and feedstocks using cheap abundant metal catalysts and low-energy input approaches to produce a cost-competitive process. We will take a bioderived building block and convert it to high-value chemicals and high-volume fuels. This dual-purpose approach allows for an agile strategy for replacing the whole barrel of oil with bioderived renewable sources. The result will be the development of catalyst systems to (1) efficiently dehydrogenate isopropanol to liberate dihydrogen and (2) upgrade the resulting acetone through self-condensation chemistry, targeting products with carbon chain lengths appropriate for fuel applications (C6 and greater).

Technical Outcomes

The project developed a fully heterogeneous catalyst system for the efficient upgrading of bioderived acetone to C6+ ketones. The system comprises an earth-abundant nickel hydrogenation catalyst and commercially available acidic ion-exchange resin. Products derived from the acetone upgrading methodology are useful as fuel additives for spark ignition engines, while select products are useful as paint additives and industrial solvents. The upgrading process can be tailored to provide product profiles that match market demand.

Publications

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Evolution of Water and Carbon Dioxide at Mars: Implications for Its Past and Future

Katherine Mesick
20160672PRD3

Project Description

Non-polar regions on Mars with near surface water deposits indicated by Mars Odyssey neutron data will be studied. Our work will provide key information in understanding the context for forming these equatorial water deposits on Mars, and what Mars' past climate was like. These answers will provide vital information on the history of water on Mars and the potential for future human exploration. This work also supports the nuclear nonproliferation mission area with space-based instruments capable of detecting nuclear explosions in the atmosphere and space.

Technical Outcomes

The project extended the processed data from the Mars Odyssey Neutron Spectrometer (MONS) to cover 8 Mars Years, doubling the amount of data previously published. This data set is valuable to future proposal opportunities. Under this project we started preliminary comparisons of equatorial water deposits derived from the MONS data with other measurement techniques and considered geological context. Future work will continue these efforts to improve the modeling and interpretation of MONS data.

Publications

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Design of New Materials for Energy Applications

Ping Yang

20170684PRD3

Project Description

The scientific results of this project will not only spark further experimental verification of the proposed redox flow cells, but will also be used as a general guideline towards the realization of novel inexpensive, safe, and high-performance flow cells, which could be implemented in electricity grids in the near future. This project directly responds to the aim of approaching DOE's cost target on large-scale energy storage, \$150/kWh. Having developed such systems, people will be able to effectively store and use greener electricity rather than relying on carbon energy sources, such as fossil fuels, which the world will run out of sooner or later.

Technical Outcomes

The project computationally predicted two novel Fe(iron)-based complexes with improved redox properties designed for redox flow cells. The proposed electrolytes were found to be stable at three oxidation states of Fe and exhibit four reduction potentials in the electrochemical window of acetonitrile. Proposed compounds have already been experimentally synthesized. Currently, the complexes undergo chemical characterization and cyclic voltammetry tests. One paper is close to the submission, while the second one is being prepared.



Information Science and Technology

Hybrid Quantum-Classical Computing

Rolando Somma
20160069DR

Project Description

This project will investigate the potential of hybrid quantum-classical computing to deliver significant gains in computing speed. Our findings will play a paramount role in the design of future computing architectures. Hybrid quantum-classical computing (HQCC) provides the potential for orders-of-magnitude faster computation than is possible by today's computers. The main goal is to investigate the computing power of physically realizable quantum annealers, exemplified by a D-Wave device. HQCC will deliver powerful algorithms for optimization, with potential applications that range from materials science to national security. These algorithms will be implemented in an available D-Wave quantum annealer and on conventional computers, using advanced numerical methods that simulate quantum annealers. HQCC will also conduct quantum annealing experiments, which will allow us to study the physical phenomena that can impact the efficiency of quantum annealers at very large scales.

Technical Outcomes

Among the results of HQCC, we successfully demonstrated significant quantum speedups for optimization problems. We developed improved tools to simulate quantum systems on quantum computers and investigated the role of physical phenomena in quantum computations. We executed numerous simulations in quantum annealers (Los Alamos' Ising supercomputer) that also allowed for a benchmark of the device. We invented techniques for mapping optimization problems to various quantum computing architectures that resulted in a "quantum program compiler".

Publications

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Real-time Adaptive Acceleration of Dynamic Experimental Science

James Ahrens
20170029DR

Project Description

This project aims to accelerate knowledge-to-discovery from experimental scientific facilities by combining computer and statistical science to produce an adaptive methodology and tool set that will analyze data and augment a scientist's decision-making so that the scientist can optimize experiments in real time. We will develop this capability in the context of dynamic compression experiments at advanced light sources, an area of core mission importance for Los Alamos and an area that is currently in the midst of substantial increases in the rate of data generation. This project will result in a data science focused information science and technology tool set that is optimized for and will revolutionize dynamic compression science experiments using X-ray user facilities. Our novel approach will strengthen national security by enabling scientific results from experimental facilities to be directly relevant to our stockpile stewardship mission.

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High-Order Hydrodynamic Algorithms for Exascale Computing

Nathaniel Morgan
20170051DR

Project Description

The objective of the research is to improve hydrodynamics algorithms, which are of great importance to science-based prediction in programmatic applications. Hydrodynamic simulations at Los Alamos are regularly used to (1) design hydrodynamic experiments where many exceed a million dollars to execute, (2) aid understanding of experiments, (3), interpolate between different experiments, (4) estimate margins and uncertainties, (5) investigate high strain-rate deformation of metals, and (6) extrapolate experiments into regimes and scales that are not readily accessible. This research will likely positively impact many key Laboratory programs such as the Advanced Simulation and Computing (ASC) program and the DoD/DOE joint munitions program. Developing high-order algorithms is also beneficial to computational fluid dynamics (CFD) codes that are used at Los Alamos to simulate flows in such applications as internal combustion engines, casting of metal parts, and climate models. The results from this research effort could radically transform the computer simulation capabilities at Los Alamos and beyond.

Publications

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Advancing Predictive Capability for Brittle Failure Using Dynamic Graphs

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Project Description

This project addresses the failure of brittle materials and fluid flow through fractures in brittle materials, in applications of interest to global and national security. The former is a concern for weapons performance where it is critical to predict how fractures propagate in materials leading to damage and eventually failure. Our algorithms will predict failure times quicker and more accurately under a wide range of commonly encountered scenarios, which increases confidence in our predictions. We will also model how gases flow through fractured medium below the surface in the aftermath of a chemical or nuclear explosion. It is critical to detect the nature of explosions based on identifying gases such as Xenon that migrate upward to the atmosphere through fractures that already exist in natural formations and those created by the blast. Being able to detect these gases is of utmost importance to our Nuclear Nonproliferation programs. We will also predict failure times and patterns in the case of brittle materials, which is a phenomenon of importance in nuclear weapons performance. The Advanced Simulation and Computing (ASC) program will benefit from more accurate models to predict failure for various weapons performance scenarios.

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Optimization and Physics Inspired Machine Learning Approaches

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Project Description

Physics Informed Machine Learning (PIML) merges cutting-edge computational and algorithmic ML tools with physical knowledge in the form of constraints, symmetries, and domain expertise regarding effective degrees of freedom. Our focus is to develop methodologies and algorithms for the optimization and control of power and infrastructure systems, automated model reduction and coarsening, and learning macro-scale models that capture relevant physics of micro-scale simulations. The resulting technologies are applicable to a wide range of mathematical structures that arise in practical applications related to control and operations of complex engineered network, such as natural gas and water systems.

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Robust Deep Unsupervised Machine Learning for Big-Data Analytics

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20180060DR

Project Description

Large datasets are being accumulated in almost every scientific field. Multidimensional data related to National and Global Security are collected every day by distributed sensor networks, large-scale experimental measurements, and computer simulations, amongst many others. Examples include: photos of people; time-lapse hyperspectral images; spatiotemporal sensor data of contaminant plumes, earthquakes and gas leaks caused by low-yield nuclear tests; Molecular Dynamics simulations of Los Alamos National Laboratory mission critical materials; and many others. The recent explosion of ultra-large multidimensional datasets---critical for scientific discoveries, decision-making, emergency response, and National and Global Security---mandates the development of the next-generation of machine learning tools that can be applied to Los Alamos National Laboratory and DOE's mission.

Technical Outcomes

We developed a novel unsupervised machine learning methodology for data analytics, based on Nonnegative Tensor Factorization, called NTFk. We showed that NTFk is capable of determining the (unknown) number of the basis hidden features (patterns) buried in the data. By analyzing various experimental and computer-generated real-world datasets we demonstrated the advantage and power of NTFk. The results obtained via NTFk secured our participation in NNSA 2019 program: Advanced Data Analytics for Proliferation Detection (ADAPD).

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- Vesselinov, V. V., D. Katzman, D. O'Malley, and B. Alexandrov. Evaluation of Potential Source Areas for the Chromium Plume Using Machine Learning Data Analyses of Geochemical Data. Submitted to *Journal of Contaminant Hydrology*. (LA-UR-18-21076)
- Vesselinov, V. V., M. K. Mudunuru, S. Karra, D. O'Malley, and B. Alexandrov. Unsupervised Machine Learning Based on

Non-Negative Tensor Factorization for Analyzing Reactive-Mixing. Submitted to *Water Resources Research*. (LA-UR-18-20868)

Neuromorphic Systems for Real-Time Data Understanding

Garrett Kenyon
20180142DR

Project Description

Information science and advanced computer technologies play a critical and growing role in essentially all aspects of national security science. They represent an essential component of the DOE/ NNSA portfolio of research and programmatic applications in weapons systems development and nonproliferation. This project will develop brain-inspired algorithms for data processing, encoding, and pattern recognition, to produce “neuromorphic systems” that work better than conventional computers for a range of tasks. Such algorithms will allow the use of brain-inspired chips for dramatic reductions of system size, weight and power. We will employ neuromorphic algorithms to interpret static or video imagery for reconnaissance, surveillance, and intelligent analysis tasks currently performed by humans. Related systems will provide drones, robots, or autonomous vehicles with improved onboard systems for navigation and avoidance of obstacles or threats. Similar algorithms will be used to learn and detect anatomical sources of dynamic patterns of brain activity seen in brain imaging studies. In addition to direct biomedical utility, this application is a prototype for national security systems that need to make inferences from multiple data sources that may be limited, noisy, or incomplete.

Technical Outcomes

Our results show that it is possible to learn spatiotemporal kernels using cortically-inspired algorithms that enable higher-quality reconstruction of images and video from low-power, low-bandwidth retinal event trains. Specifically, the images and video reconstructed by our cortically-inspired algorithm are of qualitatively higher-fidelity than could be obtained simply by directly summing retinal events.

Publications

Hayes, C., C. V. Schelle, G. Taylor, B. Martinez, Y. Yang, G. Kenyon, T. Lienert, and D. D. L. Mascarenas. Event-Based Imager-based Techniques for Analyzing Metallic Melt Pools

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Watkins, Y. Z., A. M. Thresher, P. F. Schultz, A. Wild, A. T. Sornborger, and G. Kenyon. Simulating Self-Organizing Neuromorphic Processors. Presented at *Neurally Inspired Computational Elements (NICE)*. (Albany, New York, United States, 2019-03-26 - 2019-03-29). (LA-UR-18-31521)

Watkins, Y. Z., A. M. Thresher, P. F. Schultz, A. Wild, A. T. Sornborger, and G. Kenyon. Towards Self-Organizing Neuromorphic Processors: Unsupervised Dictionary Learning via a Spiking Locally Competitive Algorithm. Presented at *IEEE International Symposium on Circuits and Systems (ISCAS)*. (Saporo, Japan, 2019-05-26 - 2019-05-29). (LA-UR-18-31520)

Watkins, Y. Z., G. Kenyon, D. Mascarenas, and A. M. Thresher. Sparse Coding Enables the Reconstruction of High-Fidelity Images and Video from Retinal Spike Trains. Presented at *ICONS '18 Proceedings of the International Conference on Neuromorphic Systems Article No. 8*. (Knoxville, Tennessee, United States, 2018-07-23 - 2018-07-26). (LA-UR-18-31509)

Watkins, Y. Z., O. Iaroshenko, M. Sayeh, and G. Kenyon. Image Compression: Sparse Coding vs. Bottleneck Autoencoders. Presented at *2018 IEEE Southwest Symposium on Image Analysis and Interpretation (SSIAI)*. (Las Vegas, Nevada, United States, 2018-04-09 - 2018-04-10). (LA-UR-18-31510)

Efficient Exploration of High-Dimensional Model Structural Uncertainties

Nathan Urban
20160189ER

Project Description

We propose to develop efficient techniques to measure uncertainties in computer model predictions that exist due to different choices of physical approximations. The goal is to automatically explore the computer-simulation uncertainties without having to rewrite and re-run the model for each new approximation. These uncertainties can be pervasive in many fields, such as climate science, fluid dynamics, material science, etc. We will test new automated uncertainty quantification techniques on a series of idealized problems from geophysical fluid dynamics to test the validity of the methods. If successful, this would revolutionize how computer model structural uncertainties are quantified. Currently, this work is done slowly, by hand, exploring only a narrow range of possible uncertainties.

Technical Outcomes

From the simulation output of simple numerical computer models, we statistically reconstructed the dynamical behavior of the computer models, and constructed computationally efficient reduced models of the numerical models. We applied these techniques to quantify structural or model-form uncertainties in the computer models. We developed a scalable form of dynamic mode decomposition, a dimension reduction method, that applies to high-dimensional data.

Publications

- DeGennaro, A. M. Model Structural Inference Using Local Dynamic Operators. Submitted to *International Journal for Uncertainty Quantification*. (LA-UR-18-21957)
- DeGennaro, A. M. LDO Inference from a Quantity of Interest using the Adjoint-Gradient Optimization. Unpublished report. (LA-UR-18-24884)
- DeGennaro, A. M., and N. M. Urban. Scalable Extended Dynamic Mode Decomposition using Random Kernel Approximation. Submitted to *SIAM Journal on Scientific Computing*. (LA-UR-17-29880)

Global Optimization Methods for Structural Bioinformatics

Hristo Djidjev
20160317ER

Project Description

This project develops algorithms for predicting the 3D structure of proteins, which helps understand their function. The results of this project can lead to a breakthrough in drug design and finding cures for diseases such as Parkinson's and cancer. The proposed work will result in algorithms and tools for structural bioinformatics, focusing on predicting the structural alignment of proteins. We will restrict our focus to versions of those problems that can be modeled as quadratically constrained quadratic problems. Such problems include multi-component protein assembly, side-chain positioning, inverse folding, and multiple structural alignment. In order to validate our models and test the efficiency of our algorithms, we will use data banks such as the Protein Data Bank (PDB). While this proposal focuses on bioinformatics, the global optimization framework that we develop could also impact the Laboratory's information science and technology capability and has the potential to be extended and applied to other areas such as cybersecurity and co-design.

Technical Outcomes

The results of this project demonstrate that combinatorial and global optimization methods combined with machine learning can be used to accurately solve problems in bioinformatics, where previously inexact heuristic-based methods have been mostly used. We have applied the methodology to predicting the structure of proteins given by their amino-acid sequences and for genome assembly based on next-generation sequencing (NGS) genomic data. Our algorithms produce results that are consistently better than the best methods previously available.

Publications

Akhter, N., G. Chennupati, H. N. Djidjev, and A. Shehu. ML-Select: Improved Decoy Selection via Machine Learning and Ranking. Presented at *2018 IEEE 8th International Conference on Computational Advances in Bio and medical*

Sciences ICCABS-2018. (Las Vegas, Nevada, United States, 2018-10-18 - 2018-10-18). (LA-UR-18-28188)

Akhter, N., G. Chennupati, H. N. Djidjev, and A. Shehu. Decoy Selection for Protein Structure Prediction Via Extreme Gradient Boosting and Ranking. Submitted to *BMC Bioinformatics*. (LA-UR-18-30854)

Andonov, R., H. N. Djidjev, S. Francois, and D. Lavenier. Complete Assembly of Circular and Chloroplast Genomes Based on Global Optimization. Submitted to *Journal of Bioinformatics and Computational Biology*. (LA-UR-18-25924)

Djidjev, H. N., L. Aleksandrov, and G. J. Chapuis. Parallel Shortest-Path Queries in Planar Graphs. Presented at *HPGP'16*. (Kyoto, Japan, 2016-05-31 - 2016-05-31). (LA-UR-16-21298)

Francois, S., R. Andonov, D. Lavenier, and H. N. Djidjev. Global optimization approach for circular and chloroplast genome assembly. Presented at *International Conference on Bioinformatics and Computational Biology*. (Las Vegas, Nevada, United States, 2018-03-19 - 2018-03-19). (LA-UR-18-20059)

Francois, S., R. Andonov, D. Lavenier, and H. N. Djidjev. Global Optimization for Scaffolding and Completing Genome Assemblies. Presented at *International Network Optimization Conference*. (Lisbon, Portugal, 2017-02-26 - 2017-02-26). (LA-UR-17-21184)

Francois, S., R. Andonov, H. Djidjev, and D. Lavenier. Global Optimization Methods for Genome Scaffolding. Presented at *12th International Workshop on Constraint-Based Methods for Bioinformatics*. (Toulouse, France, 2016-09-05 - 2016-09-05). (LA-UR-16-25623)

Francois, S., R. Andonov, H. N. Djidjev, M. Traikov, and N. Yanev. Mixed Integer Linear Programming Approach for a Distance-Constrained Elementary Path Problem. Presented at *Cologne-Twente Workshop on Graphs and Combinatorial Optimization*. (Paris, France, 2018-06-18 - 2018-06-18). (LA-UR-18-21323)

A Multiscale, Non-stochastic Approach to Model Collisions in Particle Systems

Luis Chacon
20160448ER

Project Description

This project aims at developing a noise-free collisional particle treatment for physical systems of relevance to the Los Alamos mission. This research will enable high-fidelity simulations with far fewer computational resources than ever before. We will demonstrate the feasibility, accuracy, and efficiency of deterministic (vs. stochastic) particle collisional treatments in two applications of relevance: thermal radiative transfer and semi-collisional plasmas. The successful conclusion of the research proposed in this project will enable unprecedented fidelity in the modeling of these two physical systems with far fewer computational resources, thus opening a new computational frontier. The methods proposed here will also conform naturally to modern architectures such as the Trinity supercomputer, thus opening the possibility of high utilization of modern computing architectures. The algorithms stemming from this research, once successfully demonstrated, will impact a variety of mission spaces including energy security and nuclear security defense.

Technical Outcomes

This project has delivered on all its milestones, and has demonstrated multidimensional, multiscale, non-stochastic collisional algorithms for both thermal radiative transfer (TRT) and collisional plasma systems. In TRT, we have produced an algorithm that outperforms Monte Carlo in accuracy and efficiency by orders of magnitude. In collisional plasmas, we have used Machine Learning tools to reconstruct continuum particle distribution functions with Gaussians, which are then efficiently evolved according to simple ordinary differential equations.

Publications

Chacon, L., H. Park, and H. R. Hammer. A multi-dimensional, moment-accelerated deterministic particle method for time-dependent, multi-frequency thermal radiative transfer problems. 2019. *Journal of Computational Physics*. (LA-UR-18-29197 DOI: 10.1016/j.jcp.2019.02.035)

Hammer, H. R., H. Park, and L. Chacon. A multi-dimensional, moment-accelerated deterministic particle method for time-dependent thermal radiative transfer problems. Presented at *ANS Winter Meeting*. (Orlando, Florida, United States, 2018-11-11 - 2018-11-15). (LA-UR-18-24473)

Hammer, H. R., J. E. Morel, and Y. Wang. A Weighted Least-Squares Transport Equation Compatible with Source Iteration and Voids. To appear in *Nuclear Science And Engineering*. 1-16. (LA-UR-18-23281 DOI: 10.1080/00295639.2018.1525977)

Hammer, H. R., J. E. Morel, and Y. Wang. Nonlinear Diffusion Acceleration of the Least-Squares Transport Equation in Geometries with Voids, Part 2: Numerical Results. Submitted to *Nuclear Science and Engineering*. (LA-UR-18-24017)

Hammer, H. R., J. E. Morel, and Y. Wang. Nonlinear Diffusion Acceleration of the Least-Squares Transport Equation in Geometries with Voids, Part 1: Iterative Analysis. Submitted to *Nuclear Science and Engineering*. (LA-UR-18-24016)

Park, H., L. Chacon, A. M. Matsekh, and G. Chen. A Multigroup Scale-bridging deterministic particle solver for time-dependent thermal radiative transfer problems. Submitted to *Journal of Computational Physics*. (LA-UR-17-30337)

Park, H., L. Chacon, H. R. Hammer, A. M. Matsekh, and G. Chen. Multigroup Deterministic Particle Solver for 1D Curvilinear Geometries. Presented at *2018 ANS Winter Meeting and Nuclear Technology Expo*. (Orlando, Florida, United States, 2018-11-11 - 2018-11-15). (LA-UR-18-24870)

Asynchronous Navier-Stokes Solver on 3-Dimensional Unstructured Grids for the Exascale Era

Jozsef Bakosi
20170127ER

Project Description

The project pioneers computer science technology required to use the largest future computers in an energy-efficient fashion to simulate physics problems. While the project concentrates on hydrodynamics, our software design is prepared for future multi-physics simulations, e.g., coupling with reactions, radiation, electrodynamics, and magnetism among non-ideal multiple materials. With such vision pointing well beyond this project, we anticipate an impact on multiple Los Alamos and DOE/NNSA programs, including high-energy-density hydrodynamics, global security, astrophysics, as well as atmospheric, climate, and fusion energy sciences. If successful, this project will put Los Alamos at the forefront of exascale real-world fluid dynamics; furthermore, by delivering not just a mini application (that only mimics certain aspects of production software) but a production-like open-source code, it may provide a fully asynchronous extensible software infrastructure for Los Alamos mission.

Publications

- Bakosi, J., A. K. Pandare, and H. Luo. An enhanced AUSM +-up scheme for high-speed compressible two-phase flows on hybrid grids. To appear in *Shock Waves*. (LA-UR-18-24062 DOI: 10.1007/s00193-018-0861-x)
- Bakosi, J., J. I. Waltz, and A. K. Pandare. A Reconstructed Discontinuous Galerkin method for Multi-Material Flows with Sharp-Interfaces. Unpublished report. (LA-UR-19-20312)
- Bakosi, J., O. Certik, J. Barnett, and G. Collins. Vectorize! Bridging the Performance-Productivity Gap of Vectorization. Unpublished report. (LA-UR-17-29524)

3-dimensional Structure from Drone and Stereo Video

Garrett Kenyon
20170155ER

Project Description

The main national security challenge this research addresses is the need to develop techniques that can learn useful representations from large, unlabeled datasets, such as drone video, infra-red "night-vision" video, etc. We adopt a biologically motivated approach to learning such representations by attempting to implement the self-organizing principles governing cortical development. Ultimately, we hope to enable intelligence and military analysts with the ability to annotate a relatively small number of examples of a given target in a particular video clip and to then search for that same target in additional clips.

Publications

- Carroll, J. A., N. T. Carlson, and G. Kenyon. Phase Transitions in Image Denoising via Sparsely Coding Convolutional Neural Networks. Presented at *NIPS*. (Long Beach, California, United States, 2017-12-04 - 2017-12-04). (LA-UR-17-30744)
- Springer, J. M., C. S. Strauss, A. M. Thresher, E. Kim, and G. Kenyon. Classifiers Based on Deep Sparse Coding Architectures are Robust to Deep Learning Transferable Examples. Presented at *CVPR*. (Long Beach, California, United States, 2019-06-15 - 2019-06-21). (LA-UR-18-31651)
- Watkins, Y. Z., O. Iaroshenko, G. Kenyon, and M. Sayeh. Image Compression: Sparse Coding vs. Bottleneck Autoencoders. Presented at *NIPS*. (Long Beach, California, United States, 2017-12-04 - 2017-12-04). (LA-UR-17-30743)
- Yoon, B. Machine Learning Estimators for Lattice QCD Observables. Submitted to *Physical Review*. (LA-UR-18-26411)
- Yoon, B., and T. Bhattacharya. Do not measure correlated observables, but train an artificial intelligence to predict them. Submitted to *Proceedings of Science*. (LA-UR-18-30761)

Next Generation Image Processing and Analysis Algorithms for Persistent Sky Surveillance

Przemyslaw Wozniak
20170183ER

Project Description

In the 21st century, space has become a competitive arena that demands constant innovation to meet the nation's security goals. Custody of Resident Space Objects (RSO) requires persistent monitoring on a global scale to extract rare and subtle signatures of important state changes and maneuvers. Looking everywhere all the time is expensive and requires substantial investments in hardware deployed around the world. It is therefore critically important to develop sophisticated algorithms that can achieve more with less hardware. Accurate direct pixel-by-pixel image subtraction based on convolution is an essential tool for processing crowded sky surveillance images. Our key objective is to develop an effective regularization method to stabilize the convolution kernel while preserving the required flexibility. Another problem is source confusion, i.e. unreliable image segmentation and light attribution for faint sources. We will develop new source extraction and point-spread function recovery algorithms based on modern exemplar models. This will lead to a dramatic reduction in artifacts, allow a much cleaner extraction of important signatures, and enable robust selection of events of interest. Image processing algorithms developed by this project have a potential to significantly enhance the detection sensitivity and coverage of the imaging sensors used for space object tracking.

Sun, Y., S. Xu, Y. Li, L. Tian, B. E. Wohlberg, and U. Kamilov. Regularized Fourier Ptychography using an online plug-and-play algorithm. Presented at *International Conference on Acoustics, Speech, and Signal Processing*. (Brighton, United Kingdom, 2019-05-12 - 2019-05-12). (LA-UR-18-30506)

Publications

Garcia Cardona, C., and B. E. Wohlberg. Convolutional dictionary learning for multi-channel signals. Presented at *Asilomar Conference on Signals, Systems, and Computers*. (Pacific Grove, California, United States, 2018-10-28 - 2018-10-28). (LA-UR-18-31323)

Sun, Y., B. E. Wohlberg, and U. Kamilov. An Online Plug-and-Play Algorithm for Regularized Image Reconstruction. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-18-28977)

Development of Computational Methods for Large-Scale Simulations of Heavy Elements in Solution Environments

Enrique Batista
20170198ER

Project Description

A computational methodology that can simulate thousands of atoms in solutions containing heavy elements and nuclear products is much needed to use computers in the design of remediation approaches. Such a capability would find application immediately not only at Los Alamos but in other areas of DOE such as environmental management (EM), NNSA, NE, and other agencies. Currently such a simulation is impossible. This project plans to address the development of techniques for large-scale simulations of chemical processes involving nuclear materials. The success of this proposal will provide the Laboratory with a first-of-its-kind capability, allowing us to carry out realistic solution chemistry simulations with multiple components.

A Polyhedral Outer-Approximation, Dynamic-Discretization Solver for Mixed-Integer Semi-Definite Programming (MISDP)

Russell Bent
20170201ER

Project Description

Analysis of critical infrastructure (electric power, natural gas, water, etc.) is a very important national security challenge. The socio-economic systems of the United States depend on the reliable delivery of energy, water, etc. in order to function. As a result, DOE and other stakeholders are tasked with ensuring these systems are safe and robust. However, the ability of policy makers to analyze and protect these systems is limited by the computational requirements of modeling these systems. This project is focused squarely on building the fundamental algorithms that reduce these computational burdens and facilitate the ability of policy makers to make informed decisions on how to best secure the nation's critical infrastructure.

Publications

Garcia, M. J., H. Nagarajan, and R. Baldick. Convex Hull Pricing for the AC Optimal Power Flow Problem. Submitted to *IEEE Transactions on Control of Network Systems*. (LA-UR-19-20365)

Hijazi, H. L. Gravity: A Modeling Language for Mathematical Optimization and Machine Learning. Presented at *CPAIOR*. (Delft, Netherlands, 2018-06-27 - 2018-06-29). (LA-UR-17-31097)

Lu, M., H. Nagarajan, R. W. Bent, S. Eksioğlu, and S. Mason. Tight Piecewise Convex Relaxations for Global Optimization of Optimal Power Flow. Presented at *Power Systems Computation Conference*. (Dublin, Ireland, 2018-06-11 - 2018-06-15). (LA-UR-17-30173)

Nagarajan, H., K. Sundar, H. L. Hijazi, and R. W. Bent. Convex Hull Formulations for Mixed-Integer Multilinear Functions. Presented at *15th International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Delft, Netherlands, 2018-06-26 - 2018-06-30). (LA-UR-17-31448)

Nagarajan, H., M. Lu, S. Wang, K. Sundar, and R. W. Bent. An Adaptive, Multivariate Partitioning Algorithm for Global

Optimization of Nonconvex Programs. Submitted to *Journal of Global Optimization*. (LA-UR-17-25666)

Sundar, K., H. Nagarajan, S. Misra, M. Lu, C. J. Coffrin, and R. W. Bent. Optimization-Based Bound Tightening using a Strengthened QC-Relaxation of the Optimal Power Flow Problem. Submitted to *IEEE Transactions on Power Systems*. (LA-UR-18-28769)

Sundar, K., H. Nagarajan, S. Wang, R. W. Bent, and J. Linderoth. Tight Piecewise Polyhedral Relaxations of Multilinear Terms. Submitted to *Operations Research Letters*. (LA-UR-18-22508)

Tasseff, B. A., R. W. Bent, and P. van Hentenryck. Optimization of Topography-based Flood Mitigation Strategies. Submitted to *Water Resources Research*. (LA-UR-18-21506)

Wang, S., R. W. Bent, C. J. Coffrin, S. Eksioğlu, and S. Mason. A Scenario-Based Algorithm for Joint Chance-Constrained Programs with Finite Support and Feasible Integer Recourse. Submitted to *INFORMS Journal of Computing*. (LA-UR-18-20297)

Computational Algorithms for Modeling Non-adiabatic Dynamics in Molecular Systems

Dima Mozyrsky
20170460ER

Project Description

Upon completion, this project will result in novel computational capabilities critical for understanding light-induced dynamics in many technologically relevant molecular systems and nanostructures. In particular our studies will boost our ability to model molecular dynamics that involves transitions between different electronic states in a molecule, which is the case, for example, when a molecule absorbs a photon (i.e. a quantum of electromagnetic radiation). Such physical processes are common in a multitude of situations of physical, chemical, biological and technological interest, ranging from light harvesting or photosynthesis to the physics of high-energetic materials (i.e., explosives). We believe that the numerical algorithms developed in the course of the project will enhance accuracy and thus our predictive power in modeling these materials and processes, which, in turn, will lead to further technological development and design of relevant materials and systems. Our new unique theoretical capability can immediately provide a substantial impact on a number of existing and future programs at Los Alamos and DOE.

Publications

- Baskov, R., A. J. White, and D. V. Mozyrsky. An Improved Ehrenfest Approach to Model Correlated Electron-Nuclear Dynamics. Submitted to *Physical Review Letters*. (LA-UR-18-26927)
- Bjorgaard, J. A., D. G. Sheppard, S. Tretiak, and A. M. Niklasson. Extended Lagrangian Excited State Molecular Dynamics. 2018. *Journal of Chemical Theory and Computation*. (2) 799-806. (LA-UR-17-27227 DOI: 10.1021/acs.jctc.7b00857)
- Chubukov, A., and D. V. Mozyrsky. Evolution of the dynamics of neutral superconductors between BCS and BEC regimes: The variational approach. To appear in *Low Temperature Physics*. (6) 528-533. (LA-UR-18-23263 DOI: 10.1063/1.5037555)
- Mozyrsky, D. V., and A. Chubukov. Dynamic properties of superconductors: Anderson-Bogoliubov mode and Berry phase in BCS and BEC regimes. Submitted to *Physical Review B*. (LA-UR-19-21884)
- Nelson, T. R., S. Tretiak, D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. Jalindo, V. Kleiman, S. Fernandez-Alberti, and A. Roitberg. Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. 2018. *Nature Communications*. (1) 2316. (LA-UR-17-30143 DOI: 10.1038/s41467-018-04694-8)
- Sifain, A. E., B. J. Gifford, L. A. Lystrom, D. W. Gao, T. R. Nelson, and S. Tretiak. NEXMD Modeling of Photoisomerization Dynamics of 4-Styrylquinoline. Submitted to *Journal of Physical Chemistry A*. (LA-UR-18-28405)
- Sifain, A. E., J. A. Bjorgaard, T. R. Nelson, B. T. Nebgen, A. J. White, B. J. Gifford, O. V. Prezhdo, S. Fernandez-Alberti, A. E. Roitberg, and S. Tretiak. Photoexcited Nonadiabatic Dynamics of Push-Pull Pi-Conjugated Oligomers. Submitted to *Journal of Chemical Theory and Computation* *Journal of Physical Chemistry A* *Journal of Chemical Physics*. (LA-UR-18-20388)
- Sifain, A. E., L. Wang, S. Tretiak, and O. V. Prezhdo. Numerical Tests of Coherence-Corrected Surface Hopping Methods Using a Donor-Bridge-Acceptor Model System. Submitted to *Journal of Chemical Physics*. (LA-UR-19-20761)
- Tretiak, S., S. Fernandez-Alberti, V. Freixas, D. Ondarse-Alvarez, D. Makhov, and D. Shalashilin. Photoinduced non-adiabatic energy transfer quantum pathways in dendrimer building blocks. Submitted to *Journal of Chemical Physics*. (LA-UR-18-31806)

Effects of Cosmic Ray Neutrons on Modern High Performance Computing (HPC) Components

Nathan Debardeleben
20180017ER

Project Description

Advanced supercomputer systems are using technologies and components of amazing scale and complexity. As we push into these extreme regions, we also greatly push the envelope in the reliability of the systems both in terms of productive use of the machine (utilization, throughput, uptime, etc.) but also in the integrity (correctness) of the calculations done on these systems. It is imperative that we fully understand the causes of interruptions on these extreme-scale systems so that we can better understand how to build and operate them not only for the next generation systems but also the computing industry. Today's extreme-scale supercomputers become tomorrow's corporate supercomputers for technical and economic innovation. To accomplish this, we will use historical data from LANL supercomputers to attribute causes to effects, particularly environmental effects, which are believed to be the primary cause for errors on these systems. Based on preliminary work by the team, we will deploy neutron detectors, correlate the rate with system events, model, and simulate the expected neutron impacts on the supercomputer using advanced software simulation tools. We will also study the effects of solar events (coronal mass ejections) and evaluate the efficacy of shielding the supercomputer from a variety of error sources.

Publications

Bowen, C. M., and F. Liu. Comparative Study of Differentially Private Data Synthesis Methods. Submitted to *Statistical Science*. (LA-UR-18-31132)

Snoke, J., and C. M. Bowen. What is Differential Privacy, and Why Should Statisticians Care?. Unpublished report. (LA-UR-18-31767)

Enabling Fast Disaggregation of Large Parameter Spaces

Kary Myers
20180097ER

Project Description

We propose an entirely new way to address the fundamental scientific goal of disaggregation, or estimation of the components of an unknown measured target. Disaggregation problems appear in national security problems such as nuclear forensics and power grid analysis. Our approach combines forward models with measurements to estimate a target's component proportions while accounting for uncertainty. This work will advance both computer model calibration (to make disaggregation possible) and emulation (to make disaggregation fast). Compared to a brute force approach that can require a year of computation to estimate a single target's composition, our strategy will create a fast estimation procedure that could ultimately support processing of data on board a sensor.

Publications

Bhat, K. G., K. L. Myers, E. C. Lawrence, J. P. Colgan, and E. Judge. Using computer model calibration to estimate instrument response parameters. Submitted to *Technometrics*. (LA-UR-19-20033)

Synthesizing Fokker-Planck and Navier-Stokes Methods for Strongly Coupled Hydrodynamics and Material Fields in Turbulent Mixing

Raymond Ristorcelli
20180154ER

Project Description

The project develops a new statistical/engineering treatment of the coupled physics of hydrodynamics and turbulent mixing, involving materials with very different properties, e.g., gaseous iron and hydrogen. This requires approximations for problems where the numerical resolution of all relevant physical scales is not economical. We do this by ensuring mathematical and statistical constraints and thus enforce physical realizability constraints, required for correctness and code stability. We anticipate an impact on multiple Los Alamos National Laboratory and DOE/NNSA programs, including high-energy-density hydrodynamics, global security, astrophysics, as well as atmospheric, climate, and fusion energy sciences.

Hamiltonian on Demand for Computational Materials Using Machine Learning

Sergei Tretiak
20180213ER

Project Description

Computational materials methods have become an indispensable counterpart of experiments. To overcome our current limitations we will construct Machine Learning based algorithms for producing effective Hamiltonian parameters for molecular materials. The developed scalable, general (applicable to any molecular or material system), transferrable and robust algorithms will be able to predict an assortment of quantum mechanical properties of a system with quantitative accuracy. The range of materials include organic semiconductors, bio-molecules, transition metals, actinides and lanthanides. Success in predicting properties of such materials will strongly contribute to the Lab core missions and will provide new capabilities in a range of DOE Office of Science targets.

Publications

Nebgen, B. T., N. E. Lubbers, J. S. Smith, A. E. Sifain, A. Lokhov, O. Isayev, A. Roitberg, K. M. Barros, and S. Tretiak. Less is more: Sampling chemical space with active learning. 2018. *Journal of Chemical Theory and Computation*. (24) 241733. (LA-UR-18-22005 DOI: 10.1021/acs.jctc.8b00524)

Sifain, A. E., N. E. Lubbers, B. T. Nebgen, J. S. Smith, A. Lokhov, O. Isayev, A. E. Roitberg, K. M. Barros, and S. Tretiak. Discovering a Transferable Charge Assignment Model Using Machine Learning. 2018. *The Journal of Physical Chemistry Letters*. (16) 4495-4501. (LA-UR-18-24683 DOI: 10.1021/acs.jpcllett.8b01939)

Smith, J. S., B. T. Nebgen, N. E. Lubbers, O. Isayev, and A. E. Roitberg. Less is more: Sampling chemical space with active learning. 2018. *The Journal of Chemical Physics*. (24) 241733. (LA-UR-18-30171 DOI: 10.1063/1.5023802)

Smith, J. S., B. T. Nebgen, R. Zubatiuk, N. E. Lubbers, C. Devereux, K. M. Barros, O. Isayev, S. Tretiak, and A. E. Roitberg. Outsmarting quantum chemistry through transfer learning. Submitted to *Science*. (LA-UR-18-25687)

Preprocessing Algorithms for Boosting Quantum Annealing Scalability

Hristo Djidjev
20180267ER

Project Description

Quantum annealing is recognized by many in the scientific community as one of the promising exascale and “beyond Moore’s law” computing technologies. While there are commercially available quantum annealing computers by D-Wave that currently have as many as 2048 quantum bits (qubits), significant innovative research is needed before such computers demonstrate quantum supremacy and become a viable alternative. Taking advantage of the D-Wave 2X computer available at Los Alamos National Laboratory and the expertise of the project team in solving optimization problems using D-Wave, this project addresses some of the biggest challenges to ultimately improve the efficiency and accuracy of quantum annealing computers.

Publications

Djidjev, H. N., E. A. R. Pelofske, and G. Hahn. Solving large Maximum Clique problems on a quantum annealer. Presented at *First International Workshop on Quantum Technology and Optimization Problems (QTOP’19)*. (Munich, Germany, 2019-03-18 - 2019-03-18). (LA-UR-18-30973)

Djidjev, H. N., T. Vyskocil, and S. D. Pakin. Embedding inequality constraints for quantum annealing optimization. Presented at *First International Workshop on Quantum Technology and Optimization Problems (QTOP’19)*. (Munich, Germany, 2019-03-18 - 2019-03-18). (LA-UR-18-30972)

Djidjev, H. N., and T. Vyskocil. Simple constraint embedding for quantum annealers. Presented at *International Conference on Rebooting Computing*. (Washington, District Of Columbia, United States, 2018-11-07 - 2018-11-07). (LA-UR-18-24168)

Djidjev, H. N., and T. Vyskocil. Optimization approach to constraint embedding for quantum annealers. Presented at *Integer Programming and Combinatorial Optimization*. (Ann Arbor, Michigan, United States, 2019-05-22 - 2019-05-22). (LA-UR-18-30971)

Hahn, G., and H. N. Djidjev. Reducing Binary Quadratic Forms for More Scalable Quantum Annealing. Presented at *IEEE International Conference on Rebooting Computing*. (Washington, District Of Columbia, United States, 2017-11-08 - 2017-11-08). (LA-UR-17-27401)

Pakin, S. D., and S. P. Reinhardt. Programming a D-Wave Annealing-Based Quantum Computer: Tools and Techniques. Submitted to *Quantum Information & Computation*. (LA-UR-19-20660)

R. Pelofske, E. A., G. Hahn, and H. N. Djidjev. Solving large minimum vertex cover problems on a quantum annealer. Presented at *ACM International Conference on Computing Frontiers*. (Alghero, Italy, 2019-04-30 - 2019-04-30). (LA-UR-19-21008)

Prajapati, N., S. Rajopadhye, and H. N. Djidjev. Analytical Cost Metrics : Days of Future Past. Unpublished report. (LA-UR-18-21279)

Vyskocil, T., and H. N. Djidjev. Embedding Equality Constraints of Optimization Problems into a Quantum Annealer. Submitted to *Algorithms*. (LA-UR-19-20224)

Vyskocil, T., and H. N. Djidjev. Constraint embedding for solving optimization problems on quantum annealers. Presented at *21st Workshop on Advances in Parallel and Distributed Computational Models*. (Rio de Janeiro, Brazil, 2019-05-20 - 2019-05-20). (LA-UR-19-21107)

Rapid Response: Novel Computing

Stephan Eidenbenz
20180719ER

Project Description

The computational scalability of traditional computer hardware has stalled because miniaturization has reached a level, where quantum mechanical effects can no longer be ignored. Developing novel computing technologies, such as quantum computing, neuromorphic computing, and application-specific designs is crucial to retain the nation's technological edge. Our rapid response project will explore the near-term opportunities that these technologies offer.

Publications

- Hijazi, H. L. Perspective Envelopes for Bilinear Functions. Presented at *LeGO 2018 - Int. Workshop on Global Optimization*. (Leiden, Netherlands, 2018-09-17 - 2018-09-17). (LA-UR-18-27814)
- Mniszewski, S. M., R. Shaydulin, H. M. Ushijima-Mwesigwa, I. Safro, and Y. Alexeev. Community Detection Across Emerging Quantum Architectures. Presented at *3RD INTERNATIONAL WORKSHOP ON POST-MOORE'S ERA SUPERCOMPUTING (PMES) - Supercomputing 2018*. (Dallas, Texas, United States, 2018-11-11 - 2018-11-16). (LA-UR-18-28413)
- Mniszewski, S. M., R. Shaydulin, H. M. Ushijima-Mwesigwa, I. Safro, and Y. Alexeev. Network Community Detection On Small Quantum Computers. Submitted to *Physical Review Letters*. (LA-UR-18-30364)
- A. Negre, C. F., H. M. Ushijima-Mwesigwa, and S. M. Mniszewski. Community detection using quantum annealing on the D-Wave system. Submitted to *Quantum Information & Computation*. (LA-UR-18-30760)

Microstructure Sensitive Radiation Effects

Laurent Capolungo
20170615ER

Project Description

Typical models transcribing the response and microstructure evolution of metals are weakly connected to materials chemistry. The novel hybrid model proposed will, for the first time, address this issue in the context of radiation-induced damage. In the long term, this work should yield a path towards materials selection for nuclear environments.

predicting defect accumulation, defect energetics, and irradiation conditions. 2018. *Computational Materials Science*. 272-285. (LA-UR-17-29959 DOI: 10.1016/j.commat.2018.02.048)

Technical Outcomes

The internal strain state in a material interacts with point defects in ways that determine how metals respond to radiation, eventually influencing the physical properties, mechanical properties and engineering performance of the metal. This project has developed new capabilities to quantify these effects for three dimensional dislocation microstructures representative of the strain environment of real materials, including analysis of spatial localization of radiation damage and statistical distributions in radiation response.

Publications

- Kohnert, A. A., L. Capolungo, and B. D. Wirth. Modeling microstructural evolution in irradiated materials with cluster dynamics methods: A review. 2018. *Computational Materials Science*. 442-459. (LA-UR-17-29965 DOI: 10.1016/j.commat.2018.02.049)
- Kohnert, A. A., and L. Capolungo. A novel approach to quantifying the kinetics of point defect absorption at dislocations. 2019. *Journal of the Mechanics and Physics of Solids*. 98-115. (LA-UR-18-24458 DOI: 10.1016/j.jmps.2018.08.023)
- Kohnert, A. A., and L. Capolungo. Effect of Spatial Correlation Between Dislocations on the Kinetics of Point Defect Absorption. Submitted to *Physical Review B*. (LA-UR-17-30812)
- Kohnert, A. A., and L. Capolungo. The Sink Strength and Dislocation Bias of Three Dimensional Microstructures. Submitted to *Physical Review Materials*. (LA-UR-19-20656)
- Stewart, J. A., A. A. Kohnert, L. Capolungo, and R. Dingreville. Design and analysis of forward and reverse models for

Machine Learning Emulators for Turbulence

Michael Chertkov
20180478ER

Project Description

Machine Learning capabilities are in a phase of tremendous growth, and there is great opportunity to point these tools toward physical modeling. The challenge is to incorporate domain expertise from traditional scientific discovery into next-generation machine learning models. We propose to develop new algorithms that extend cutting-edge computational and algorithmic machine learning tools and merge them with physical knowledge in the form of constraints, symmetries, and domain expertise regarding effective de-grees of freedom. Our focus is on developing algorithms for efficient emulation of physical phenomena for which direct experimental or numerical studies are prohibitive. Building upon our substantial preliminary studies in statistical learning, we employ state-of-the-art machine learning, large-scale optimization, and validation techniques to enable further use and development of these new methods in weapons related fluid dynamics problems and other physics application of relevance to Los Alamos National Laboratory and the Department of Energy.

at *The 21st International Conference on Artificial Intelligence and Statistics*. (Lanzarote, Spain, 2018-04-09 - 2018-04-11). (LA-UR-17-29804)

Technical Outcomes

The project developed physical tests for acceleration and automation with Deep Learning (DL) of hydrodynamic codes in the regime of developed turbulence. We have observed that even though the static DL scheme fails to reproduce intermittency of turbulent fluctuations at small scales and details of the turbulence geometry at large scales, the dynamic DL schemes are capable to correct for the small-scale caveat of the static schemes.

Publications

Chertkov, M., O. A. Hennigh, and R. King. From Deep to Physics-Informed Learning of Turbulence: Diagnostics. Presented at *Thirty-second Conference on Neural Information Processing Systems*. (Montreal, QC, Canada, 2018-12-03 - 2018-12-08). (LA-UR-18-29576)

Chertkov, M., S. Ahn, J. Shin, and A. Weller. Gauged Mini-Bucket Elimination for Approximate Inference. Presented

Finding a Needle in a Haystack: Physics-Constrained Discrete Optimization by Coupling HPC and Quantum Annealing

Daniel O'Malley
20180481ER

Project Description

We will develop methods and tools that enable us to solve a class of problems that are currently intractable: physics-constrained discrete optimization problems. These problems are hard because the best algorithms for classical computers are not much better than exhaustively checking every possibility in an exponentially large set of possibilities; additionally, physical constraints make checking each possibility computationally expensive. These problems arise in a number of critical DOE/NNSA mission areas. The one that we target for application is gas migration from subsurface nuclear tests, wherein gas flows through a discrete fracture network and the process is constrained by the physical laws governing flow through a porous medium. In addition to the impact on this application, our innovation will be to productively use quantum annealing as a missing piece in the scientific enterprise. We are transitioning to a "beyond Moore's Law" era where we can no longer rely on rapid improvements in classical computing technology; methods, such as the ones proposed here, that utilize alternative computational architectures are needed. This research represents a significant step forward for beyond Moore's Law computing.

Technical Outcomes

The project combined quantum computing (realized by a quantum annealer) and High Performance Computing to solve challenging optimization problems with physical constraints. This project resulted notable success on several fronts: a significant publication in a high-impact journal, numerous of invited talks, and follow-on programmatic funding for FY19 alone that exceeds LDRD's investment in this research. This work and follow-on work with programmatic funding paves the way toward utilizing post-classical computing in key LANL scientific computing workflows.

Publications

- Battiato, I., P. T. Ferrero, D. O'Malley, C. T. Miller, P. S. Takhar, F. J. Valdes-Parada, and B. D. Wood. Theory and Applications of Macroscale Models in Porous Media. Submitted to *Transport in Porous Media*. (LA-UR-18-26414)
- O'Malley, D. An approach to quantum-computational hydrologic inverse analysis. 2018. *Scientific Reports*. (1) 6919. (LA-UR-17-29924 DOI: 10.1038/s41598-018-25206-0)

Towards Optimal Adaptive Control of Particle Accelerators using Deep Reinforcement Learning

Sunil Thulasidasan
20180491ER

Project Description

The LANSCE particle accelerator is the premier experimental facility at Los Alamos National Laboratory and supports a wide variety of our DOE/NNSA missions including stockpile stewardship as well as basic and applied research. The proton beam also supports the DOE Office of Science Isotope Production Facility enabling approximately 30,000 patients a month to receive positron-emission tomography scans in the United States. Reliable and dependable operation of the accelerator is therefore key to the success of these programs, the Laboratory and the nation. Presently, the accelerator is operated with a team of people that must watch over several hundred parameters while trying to achieve and maintain good beam performance. The goal of this research is to transform the way particle accelerators such as LANSCE and others in the DOE complex are tuned and optimized by using the power of modern artificial intelligence techniques. The adaptive artificial intelligence system would learn complex patterns and correlations and can be used to control the accelerator with the goal of achieving higher performance and reliability than is presently realized with just human operators. These improvements would translate into more user beam time, which directly translates into higher output for the user programs at LANSCE.

Technical Outcomes

We implemented and successfully tested a simulation-based prototype trained on a virtual LANSCE test-bed concentrating on the first few modules of the LANSCE accelerator. The framework consists of an AI controller module which uses deep neural nets and learns via reinforcement learning. Our system learns optimal policies (as opposed to just optimal parameters) and we were able to achieve better-than-human level performance in terms of beam current and phase distribution.

Publications

Pang, X., S. Thulasidasan, and L. J. Rybarcyk. Autonomous Accelerator Control with Deep Reinforcement Learning. Unpublished report. (LA-UR-18-27905)

Analyst-Driven Machine Learning for Image Segmentation

Diane Oyen
20180496ER

Project Description

Nuclear forensics analysis uses morphology, the sizes and shapes of particles, in microscope images to investigate potential sources of discovered nuclear material. The first step in this analysis is to segment the image to delineate the particles. In support of morphological signature science, materials analysts collect thousands of images and would like to process 1000 images per day. Each image takes about 2 hours for an analyst to fully process using current software due to the amount of human involvement required to hand-fix the automated segmentation. A transformational advance in our image segmentation technology is needed to scale to the rate of data analysis that materials morphology analysts expect. Image segmentation technology has advanced enormously in the past few years by using machine learning. This analyst-driven machine learning project will improve the accuracy of image segmentation by orders of magnitude to reduce analyst time from hours to about a minute per image, and it will provide a methodology to continually improve analytics as more data arrives.

Technical Outcomes

We applied and evaluated machine learning algorithms for segmenting images of materials with limited amount of human input. Using machine learning with only about 30 images that have been annotated by hand, foreground is better discriminated from background compared with traditional methods. Further research and development is needed to separate overlapping foreground particles in materials images.

Publications

Canning, J., D. A. Oyen, and K. Sentz. Deep Learning Image Segmentation for Nuclear Forensics. Unpublished report. (LA-UR-18-27966)

Lanza, N. L., D. A. Oyen, and R. Yousefzadeh. Learning Diverse Gaussian Graphical Models and Interpreting Edges. Presented at *SIAM Data Mining*. (Calgary, Canada, 2019-05-05 - 2019-05-05). (LA-UR-18-29840)

Multiscale Relational Analytics for Weapons of Mass Destruction (WMD) and Proliferation Activity Monitoring

Lakshman Prasad
20180555ER

Project Description

Our primary mission impact areas are Nuclear Nonproliferation and Intelligence, and Data Analytics at Scale. Our motivation for this proposal is the discernment of events from multiple, inconclusive signals by leveraging temporal context. This is a need that cuts across several areas of Global Security and Threat Reduction. Indeed, a capability for detection and early warning of an emerging threat, be it from hostile entities, terrorism, disease, or environment is critical to Laboratory's execution of its National Security mission and science to safeguard the nation. The generality of our approach enables its adaptation to diverse sentinel technologies where observations are time-sensitive. Also, while individually the observations may carry some information, their contextual leverage greatly enhances their information content and value towards detecting an event. This also makes analysis more tolerant to partial information loss. When applied to physical sensors and pattern-of-life information, our approach can benefit nuclear proliferation and detonation detection. When applied to web data and multi-Int feeds, it can benefit counterterrorism, epidemiology, and predicting/anticipating hostile nation actions. When applied to computer networks it can benefit Cybersecurity. Our approach enables dynamic triage for predictive monitoring of emerging events based on scale-adaptive clustering and process modeling.

Technical Outcomes

This project has resulted in a new Los Alamos capability for multi-phenomenology sensor fusion and event detection & characterization, with algorithms and prototype software that has been demonstrated to be capable of analyzing real-world data. In particular, a novel, robust relational pattern detection method tolerant to missing and interfering data in event detection has been developed for application in real-world noisy scenarios. This work achieved a follow-

on programmatic DOE NNSA project on low-profile proliferation detection.

Publications

Prasad, L. Multiscale graph-based framework for efficient multi-sensor integration and event detection. Presented at *SPIE Defense + Security Symposium*. (Orlando, Florida, United States, 2018-04-15 - 2018-04-19). (LA-UR-18-22413)

Development of Variational Data Sets for the Study of Radiographic Data (U)

Garry Maskaly
20180722ER

Project Description

This work is an initial effort to develop a capability to better extract information from radiographic data. If successful, these approaches could make both DARHT surrogate and Enhanced Capability for Subcritical Experiments (ECSE) data more useful for future certification and assessment efforts. In this introductory study, we will start analysis of a training dataset. These studies will help move radiographic data comparisons into a more quantitative space allowing a more thorough extraction of the information. The team's experience in weapons physics also helps incorporate expert knowledge into these assessments. As part of this work, we are also developing a validation and uncertainty quantification plan to test the algorithms and approaches we are studying.

Technical Outcomes

This work provides a first assessment of machine learning capabilities applied toward a training dataset. The research has three main sections. First, we detailed ideas we have produced for applying machine learning to radiographic data. Next, we examined the results for correlations between metrics with performance quantities. Finally, results from an application of machine learning approaches was successfully performed.

Integrating MAGPIE and (Functional UNcertainty Constrained by Law and Experiment) F_UNCLE

Andrew Fraser
20180727ER

Project Description

One needs an accurate model of the gases produced by detonating an explosive in order to address several national security challenges including the following: To design and forecast the performance of conventional weapons; To characterize sensitivity of our munition magazines to hostile or accidental detonations; Nuclear stockpile stewardship. This project fosters collaboration between an existing first principals theoretical modeling effort called "MAGPIE" and an empirical Data Science project called "F_UNCLE". It will enable calibrating the MAGPIE models to fit experimental data, and it will enable the F_UNCLE to extrapolate to regimes that are difficult to explore experimentally.

Technical Outcomes

Applications of explosives use energy transferred to the immediate environment by the expansion of the high pressure gasses produced by detonation to achieve their effects. Predicting effects accurately requires a good model of pressure as the gas expands. Our project compared several such models for the gasses produced by detonating the high explosive PBX-9501. Ultimately we combined aspects of Magpie (based on fundamental physical theory) with F_UNCLE (empirically based on experiments).

Publications

Fraser, A. M., and S. A. Andrews. Estimating physics models and quantifying their uncertainty using optimization with a Bayesian objective function. Submitted to *ASME Journal of Verification, Validation, and Uncertainty Quantification*. (LA-UR-18-27132)

Fusing Hard and Soft Data for Activity-Based Intelligence in Denied Areas (U)

Geoffrey Fairchild
20180730ER

Project Description

The threat landscape is increasingly complex and uncertain, particularly as it relates to weapons of mass destruction. Los Alamos National Laboratory's Intelligence Capability Exchange workshop in Sept. 2017 highlighted the urgent need for fundamentally new approaches for automated detection, tracking, and targeting of road-mobile forces and related activities, especially in the face of sophisticated denial and deception techniques. Because of this evolving threat and identified capability gap, this need continues to persist and magnify. This project enables development of an innovative automated analysis approach that leverages hard and soft non-traditional data streams that can provide secondary (proxy) indicators that: 1) may not be obviously linked to the activities of interest and, as such, are more robust to traditional denial and deception measures; and 2) are weak indicators within each of the single modalities but when combined may provide a fuller picture of the situation. In short, this project addresses an urgent need by providing a concept demonstration of a high impact new approach; this will establish credibility for potential intelligence community sponsors who have expressed the immediate need to fully develop and operationalize such a method.

Technical Outcomes

This study assessed the potential applicability of satellite imagery and social media data to characterize activities within a 100km radius over a region of interest in 2017. Results show that we can identify changes in the landscape, but these changes do not necessarily correspond to known events – further research is required to categorize those changes. In addition, the social media analysis shows that we can identify topics of interest, volume, and overall trends.

Neuromorphic Implementation of Back-propagation Algorithm

Andrew Sornborger
20180737ER

Project Description

Low power computing is crucial to drones, satellites, and other autonomous systems. Neuromorphic chips have been shown to run data intensive algorithms using three orders of magnitude less power than on a standard computer. This project will provide a machine learning algorithm capable of running on a neuromorphic chip.

Technical Outcomes

The goal of this 3 month project was to implement the forward propagation step of the backpropagation algorithm for a neuromorphic system. This algorithm is crucial to modern deep machine learning methods. This step was completed in full. We made additional progress that will help us move forward in implementing the complete algorithm.

Detection of Fake, Complex, Automatically-generated Signals via Bayesian Compressed Signaling

Juston Moore
20180742ER

Project Description

This research project aims to distinguish real images from images automatically generated by state-of-the-art artificial intelligence (AI) algorithms. Adversaries could conceivably use these AI algorithms today both to spread false narratives in the public media and to hide content in open-source intelligence by generating a large amount of fake data that is hard to distinguish from signal. The fundamental inability to visually or forensically distinguish real from fake content will alter accepted standards of evidence, and thus have widespread impacts on society and government. If related techniques were deployed to spoof sensor measurements, such attacks could lead to devastating effects when combined with traditional cyber warfare. These attacks could make it hard to distinguish whether a cyber system is operating normally, or alter measurements without leaving a digital trace. These impacts on the reliability of sensor measurements makes detection especially important for the NNSA mission.

Technical Outcomes

The goal of this project was to prove the feasibility of detecting fake, AI-generated images via sparse coding algorithms. We have successfully demonstrated the detection of fake images from a known generative network. Ongoing work is being conducted to show that our classifiers are more robust to adversarial machine learning attacks than current detection frameworks based on deep learning.

Publications

Moore, J. S., G. Kenyon, P. T. Hrabec, E. S. Michalak, and N. T. T. Nguyen. Final Report: Detection of Fake, Complex, Automatically-generated Signals via Bayesian Compressed Sensing. Presented at *Naval Applications of Machine Learning*. (San Diego, California, United States, 2019-02-11 - 2019-02-14). (LA-UR-18-31880)

Convolutional Compressive Sensing for Scientific Imaging

Cristina Garcia Cardona
20170549ECR

Project Description

Converting large amounts (terabytes) of observational data into meaningful information about the sample under study (morphology, composition, phase distribution, etc.) is extremely challenging. Inverse modeling is one of the analytical techniques that tries to facilitate the conversion of measurements into interpretable knowledge by formulating a mathematical model to explain the data and estimating the parameters of the model that best fit the observations. Ideally, the fewer measurements needed to characterize the sample, the greater the potential to maximize the performance and to reduce operation costs, since less time is required for experiment execution and less data has to be stored and processed. We are developing a novel inverse modeling technique that enables the accurate reconstruction of signals from incomplete sets of observations by learning a mathematical model that exploits intrinsic properties of the physically measured data (e.g. sparseness: few active components). Being able to assimilate information and extract knowledge from large experiments and to increase the performance (accuracy and speed) for sample reconstruction is crucial for the success of future facilities such as MaRIE and other DOE facilities producing high rates of imaging data.

(Pacific Grove, California, United States, 2018-10-28 - 2018-10-28). (LA-UR-18-31323)

Liu, J., C. Garcia Cardona, B. E. Wohlberg, and W. Yin. Online Convolutional Dictionary Learning. Presented at *International Conference on Image Processing (ICIP)*. (Beijing, China, 2017-09-09 - 2017-09-09). (LA-UR-17-20865)

Liu, J., C. Garcia Cardona, B. E. Wohlberg, and W. Yin. First- and Second-Order Methods for Online Convolutional Dictionary Learning. 2018. *SIAM Journal on Imaging Sciences*. (2) 1589-1628. (LA-UR-17-27611 DOI: 10.1137/17M1145689)

Skau, E. W., and C. Garcia Cardona. TOMOGRAPHIC RECONSTRUCTION VIA 3D CONVOLUTIONAL DICTIONARY LEARNING. Presented at *2018 IEEE Image, Video, and Multidimensional Signal Processing (IVMSP) Workshop*. (Zagori, Aristi Village, Greece, 2018-06-10 - 2018-06-12). (LA-UR-18-21364)

Publications

Garcia Cardona, C., and B. E. Wohlberg. Convolutional Dictionary Learning: A Comparative Review and New Algorithms. Submitted to *IEEE Transactions on Computational Imaging*. (LA-UR-17-27612)

Garcia Cardona, C., and B. E. Wohlberg. Subproblem Coupling in Convolutional Dictionary Learning. Presented at *International Conference on Image Processing (ICIP)*. (Beijing, China, 2017-09-17 - 2017-09-17). (LA-UR-17-20864)

Garcia Cardona, C., and B. E. Wohlberg. Convolutional dictionary learning for multi-channel signals. Presented at *Asilomar Conference on Signals, Systems, and Computers*.

Large-Scale Nonlinear Optimization via Cloud Computing

Carleton Coffrin
20170574ECR

Project Description

The proposed work will develop a world-leading algorithm for large-scale nonlinear distributed optimization. This capability will advance our understanding of the fundamental challenges inherent in optimizing infrastructure systems, large-scale machine learning, and dynamical systems. The resulting general-purpose nonlinear optimization software is applicable to a wide-range of large-scale simulation and optimization tasks faced by the Department of Energy and others.

Publications

Coffrin, C. J., M. R. Kelly-Gorham, and A. K. Barnes. Large Scale Network Vulnerability Study Results. Unpublished report. (LA-UR-18-27694)

Hijazi, H. L., C. J. Coffrin, and P. Van Hentenryck. Convex quadratic relaxations for mixed-integer nonlinear programs in power systems. 2017. *Mathematical Programming Computation*. (3) 321-367. (LA-UR-18-21065 DOI: 10.1007/s12532-016-0112-z)

Kroger, O., C. J. Coffrin, H. L. Hijazi, and H. Nagarajan. Juniper: An Open-Source Nonlinear Branch and Bound Solver in Julia. Presented at *15th International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Delft, Netherlands, 2018-06-26 - 2018-06-29). (LA-UR-17-31300)

Advancing Discrete Fracture Matrix Models using Topologically Driven System Reduction

Jeffrey Hyman
20180579ECR

Project Description

The model resulting from this project will allow Laboratory researchers to probe fundamental science questions concerning subsurface transport in fractured media. It is of interest to DOE's Offices of FE and Energy Efficiency & Renewable Energy (EERE) programs as well as the DOE initiatives SubTER and Energy-Water Nexus. In particular, the model will help predict how much hydrocarbon remains in unconventional reservoirs after production has ceased (by some estimates up to 70% is left behind), accurate calculations of when trace chemicals from an underground explosion will reach the surface, and promote successful environmental management strategies. This project also supports mission pillars of energy security (subsurface hydrocarbon acquisition, geothermal energy extraction, carbon sequestration), global security (DTRA gas migration from underground low yield nuclear weapons testing), and stockpile stewardship (brittle material failure prediction).

Srinivasan, G., N. Makedonska, D. Bolster, T. J. Sherman, and J. D. Hyman. Characterizing the impact of particle behavior at fracture intersections in three-dimensional discrete fracture networks. 2019. *Phys. Rev. E.* (1) 013110. (LA-UR-18-29382 DOI: 10.1103/PhysRevE.99.013110)

Publications

- Dentz, M., J. D. Hyman, A. A. Hagberg, and P. K. Kang. Linking structural and transport properties in three-dimensional fracture networks. To appear in *Journal of Geophysical Research: Earth Surface*. (LA-UR-18-27717 DOI: 10.1029/2018JB016553)
- Hyman, J. D., H. M. Ushijima-Mwesigwa, A. A. Hagberg, I. Safro, S. Karra, C. W. Gable, and G. Srinivasan. Multilevel Graph Partitioning for Three-Dimensional Discrete Fracture Network Flow Simulations. Submitted to *SIAM Journal on Scientific Computing*. (LA-UR-19-21113)
- Hyman, J. D., M. Dentz, A. A. Hagberg, and P. Kang. What Controls Asymptotic Transport Properties in Fractured Media? Uncovering a Connection Between Fracture Network Properties and Particle Behavior. Submitted to *Geophysical Research Letters*. (LA-UR-18-29270)

Robust Anomaly Detection in Complex Networks: Data Fusion and New-Link Prediction

Melissa Turcotte
20180607ECR

Project Description

Cybersecurity is one of the most important challenges that the U.S. Government currently faces, as indicated by Presidential Policy Directive 20 and the Comprehensive National Cybersecurity Initiative. Detection of cyber-attacks traditionally relies heavily on rule-based (or signature-based) intrusion detection systems, which are powerful tools but require specific threat signatures previously observed from attacks. As a result, they are fragile and are easily subverted by attacks with previously unknown or unidentified signatures. In contrast, anomaly detection systems offer an orthogonal defense; by dynamically learning models of normal behavior and detecting deviations to identify new variants of attacks. In spite of more than two decades of research on anomaly detection for cyber defense, operational use is still nascent primarily because of high false positive rates and un-interpretable alerts. This work aims to tackle these two problems by developing models for new links (previously unobserved relationships between network entities) in relational network data thereby reducing false alarms to practical levels and building causal relationship graphs of malicious behavior by combining "weak" signals crossing multiple cyber data sets both reducing false alarms and providing key event context enhancing the usefulness of anomaly detection in operational cyber defense.

Real-Time, Real-World Time Series Forecasting Using Internet Data

Reid Priedhorsky
20160595ECR

Project Description

Tracking disease with internet searches and social media can improve public health response, but this field (despite wide reporting) has shown mixed success, due in part to a lack of theory and controlled experiments. The proposed work will make critical progress toward a deployed science of reliable disease forecasting with quantitative uncertainty, as well as in the broader data science of large-scale, real-world forecasting. While many of the individual tools are standard, their emergent behavior in a combined setting is novel. Deliverables include a mathematical description of the information pipeline that transforms human observations into actionable knowledge via internet systems; validation of this pipeline using controlled experiments in a simulated setting; validation of this pipeline in diverse real-world settings; and quantification of the value of internet data for disease forecasting. This work addresses the Laboratory's global security mission.

Technical Outcomes

This work (1) created a mathematical model of disease surveillance based on information theory, including a new metric for risk of error called "deceptiveness"; (2) tested the value of deceptiveness knowledge using both simulated and real data; and (3) showed that a good flu forecasting model can in fact be improved by adding internet data, but there are limitations on this improvement.

Publications

Daughton, A. R., R. Priedhorsky, and D. A. Osthus. Even a good influenza forecasting model can benefit from internet-based nowcasts, but those benefits are limited. 2019. *PLOS Computational Biology*. (2) e1006599. (LA-UR-18-24343 DOI: 10.1371/journal.pcbi.1006599)

Priedhorsky, R., A. R. Daughton, M. Barnard, F. O'Connell, and D. A. Osthus. Estimating influenza incidence using search query deceptiveness and generalized ridge regression. Submitted to *PLOS Computational Biology*. (LA-UR-18-24467)

Priedhorsky, R., D. A. Osthus, A. R. Daughton, K. R. Moran, and A. Culotta. Deceptiveness of internet data for disease surveillance. Unpublished report. (LA-UR-18-27274)

Priedhorsky, R., D. A. Osthus, A. R. Daughton, K. R. Moran, and A. Culotta. Deceptiveness of internet data for disease surveillance. Submitted to *PNAS*. (LA-UR-17-24564)

Assimilation Algorithms for Data Fusion in Large-scale Non-linear Dynamical Systems

Humberto Godinez Vazquez
20160599ECR

Project Description

Complex dynamical systems, such as space weather, climate, and energy grids, are plagued by noise and uncertainty, which severely hampers their accurate forecasting. Using recent mathematical breakthroughs we will significantly reduce forecasting error. We will develop a new method that greatly enhances the efficiency of assimilating data into large-scale models while still preserving the nonlinear dynamics. It will initially be tested on a 2D shallow water model, followed by a realistic space weather model. We will implement our methodology to a magnetohydrodynamic model, to correctly specify Earth's magnetosphere. We will study its applicability to the Los Alamos space infrastructure, which will add critical forecasting to space awareness capabilities. A software library with the relevant assimilation method will be produced, tested, and released.

Technical Outcomes

This work developed new data assimilation methods that capture non-linear behavior over time and space to improve model forecasts. Furthermore, our assimilation methods were developed to make them easy to implement. Our assimilation methods were tested on a toy but physically relevant model, the two-dimensional shallow water model, where it showed significant reduction in forecast error. A number of journal publications are being prepared for submission, as well as an open source software package.

Publications

- McLaughlin, C. A., H. C. Godinez Vazquez, A. Sizemore, K. Barton, and P. Toledo. The Effects on Density and Orbit Propagation of Assimilating Various Data into General Circulation Models. Presented at *AIAA/AAS Astrodynamics Specialist Conference*. (Long Beach, California, United States, 2016-09-13 - 2016-09-16). (LA-UR-16-26431)
- Mehta, P., A. C. Walker, and H. C. Godinez Vazquez. Iterative Data Assimilation for Improved Upper Atmosphere

Modeling. Presented at *2016 AIAA/AAS Astrodynamics Specialist Conference*. (Long Beach, California, United States, 2016-09-13 - 2016-09-16). (LA-UR-16-26339)

Schiller, Q., W. Tu, A. Ali, X. Li, H. C. Godinez Vazquez, D. Turner, S. K. Morley, and M. G. Henderson. Simultaneous event-specific estimates of transport, loss, and source rates for relativistic outer radiation belt electrons. *Journal of Geophysical Research: Space Physics*. (LA-UR-17-29820 DOI: 10.1002/2016JA023093)

Godinez Vazquez, H. C. Assimilation Algorithms for Data Fusion in Large-scale Nonlinear Dynamical Systems. Unpublished report. (LA-UR-16-28949)

Godinez Vazquez, H. C., and C. A. McLaughlin. AFOSR white paper. Unpublished report. (LA-UR-16-24078)

Tensor Networks and Anyons: Novel Techniques for Novel Physics

Lukasz Cincio
20160643PRD2

Project Description

The main goal of the project is to create a scalable, numerical tool that will enable insights into two-dimensional quantum systems. In particular we plan to apply it to study topologically ordered phases and, more importantly, identify experimentally realizable systems that may serve as platforms for quantum computation. Our results will help in the design of quantum computers, which has immediate implications for national security. More generally, we anticipate that our tool will enable subsequent theoretical and experimental research.

Roberts, D., L. Cincio, A. B. Saxena, A. Petukhov, and S. Knysh. Environment-Enhanced Tunneling at Computational Bottlenecks of Quantum Annealing. Submitted to *arXiv*. (LA-UR-18-22769)

Somma, R. D., P. J. Coles, R. B. Porter, A. T. Sornborger, L. Cincio, Y. Subasi, A. Ch Narayan Chowdhury, E. Crosson, E. Rieffel, D. Venturelli, and S. Hadfield. Task-oriented discovery and optimization of hybrid algorithms. Unpublished report. (LA-UR-18-25484)

Publications

Cincio, L., B. Yan, and W. H. Zurek. Information Scrambling and Loschmidt Echo. Submitted to *Physical Review Letters*. (LA-UR-19-21861)

Cincio, L., P. J. Coles, and Y. Subasi. Entanglement spectroscopy with a depth-two quantum circuit. To appear in *arXiv.org Journal of Physics A: Mathematical and Theoretical*. (4) 44001. (LA-UR-18-25483 DOI: 10.1088/1751-8121/aaf54d)

Coles, P. J., A. T. Arrasmith, L. Cincio, A. T. Sornborger, and W. H. Zurek. Variational Consistent Histories: A Hybrid Algorithm for Quantum Foundations. Submitted to *Nature Physics*. (LA-UR-18-31704)

Hickey, C., L. Cincio, Z. Papic, and A. Paramekanti. Emergence of chiral spin liquids via quantum melting of noncoplanar magnetic orders. 2017. *Physical Review B*. (11) 115115. (LA-UR-17-23909 DOI: 10.1103/PhysRevB.96.115115)

Khatri, S., R. LaRose, A. Poremba, L. Cincio, A. T. Sornborger, and P. J. Coles. Quantum assisted quantum compiling. Submitted to *arXiv, Phys. Rev. A*. (LA-UR-18-25861)

LaRose, R., \. O'Neel-Judy, A. Tikku, L. Cincio, and P. J. Coles. Variational Quantum State Diagonalization. Submitted to *arxiv*. (LA-UR-18-29266)

Rams, M., P. Czarnik, and L. Cincio. Precise Extrapolation of the Correlation Function Asymptotics in Uniform Tensor Network States with Application to the Bose-Hubbard and XXZ Models. 2018. *Physical Review B, arXiv*. (4) 041033. (LA-UR-18-20465 DOI: 10.1103/PhysRevX.8.041033)

Trace Elements in Martian Rocks and Soils as Observed by ChemCam in Gale Crater, Mars, and Preparation for Los Alamos National Laboratory's Next Mars Mission

Ann Ollila
20160650PRD2

Project Description

This project will consist of performing calibrations of minor and trace elements for laser-induced breakdown spectroscopy (LIBS), expanding the capability of LIBS for space and ground missions. The rover will go to several regions that define the main goals of the mission, particularly a clay-rich region identified from orbit. Having better trace-element capabilities will be very helpful in the overall goals of the rover mission. LIBS can be applied in a wide variety of rugged environments, so it is potentially practical for detecting explosive residues, detecting transuranic elements and uranium isotope ratios, detecting contamination (e.g., beryllium, lead), and even for making some medical detections.

Neuromorphic Memcomputing via Interacting Nanomagnets

Francesco Caravelli
20170660PRD1

Project Description

The brain is estimated to perform up to $E+14$ TEPS (Traversed Edge Per Second) at a cost of approximately 20-25 Watts. The DOE BlueGene performs roughly $E+13$ TEPS, at a cost of roughly $E+6$ Watts. We propose to overcome that limitation via memcomputing. The concept of mem-computing is a more general approach to beyond-Turing-machine computation that has been identified by DOE as an essential national security challenge.

Statistical Mechanics and its Applications. 1507-1522. (LA-UR-17-26648 DOI: 10.1016/j.physa.2017.11.077)

McNerney, J., F. Caravelli, C. Savoie, and J. D. Farmer. The network structure of the economy amplifies secular growth. Submitted to *Nature*. (LA-UR-17-22598)

Publications

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- Caravelli, F., and A. Zegarac. Memristive Networks: from Graph Theory to Statistical PhysicsA.. Submitted to *European Physics Letters*. (LA-UR-18-31372)
- Caravelli, F., and C. Nisoli. Computation via Interacting Magnetic Memory Bites: Integration of Boolean Gates. Submitted to *Physical Review X*. (LA-UR-18-23268)
- Caravelli, F., and J. P. Carbajal. Memristors for the curious outsiders. Submitted to *MDPI Technologies*. (LA-UR-18-27766)
- Caravelli, F., and P. Barucca. A mean-field model of memristive circuit interaction. To appear in *EPL (Europhysics Letters)*. (4) 40008. (LA-UR-17-23729 DOI: 10.1209/0295-5075/122/40008)
- Cooper, F. M. Universal scaling and ferroelectric hysteresis regimes in the giant squid axon propagating action potential: a Phase Space Approach. Submitted to *Physical Review E*. (LA-UR-17-30245)
- Cuy, T., F. Caravelli, and C. Ududec. Correlations and clustering in wholesale electricity markets. 2018. *Physica A*:

Optimal Control of Quantum Machines

Wojciech Zurek
20180702PRD1

Project Description

The goal of the project is to reach a full understanding of the correlation structures in many-body quantum systems, and employ this knowledge to control quantum devices in realistic conditions. Quantum devices are expected to revolutionize data processing. Specifically, quantum computers will outperform the most powerful supercomputers in terms of speed. The project will study how to improve their efficiency, making them more robust to noise sources. A potential application of this new kind of device is the ultrafast simulation of nuclear experiments, made possible by exploiting the peculiar properties of quantum systems. This will help to efficiently maintain and steward the nuclear stockpile, a key challenge of relevance for national security. Another potential use of the project results may be in efficient long-distance quantum communication networks, enabling the transfer of sensitive data shielded from non-authorized access.

Publications

Girolami, D. How Difficult is it to Prepare a Quantum State?. To appear in *Physical Review Letters*, *arxiv*. (1) 010505. (LA-UR-18-27400 DOI: 10.1103/PhysRevLett.122.010505)

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Machine Learning of Membrane Transport of Signals and Drugs

Sandrasegaram Gnanakaran
20180745PRD3

Project Description

This project builds foundational capability for designing next-generation antibacterial drugs; with a focus on countermeasure development for treating pathogen infection; the understanding gained in this project will have broad applications in biosecurity. At present, we rely on antibiotics for the treatment of bacterial infections encountered in public health and bio-threat scenarios; however, the rapid emergence of antibiotic resistance poses a major hurdle to effective treatment. Our inability to design novel drugs for antibiotic applications is in part due to a lack of understanding of the mechanisms of multi-drug resistance. This project will provide molecular-level understanding of the operating principles governing how antibiotics move across membranes. The combined approach of multi-scale mathematical models and machine learning proposed in this project is not limited to biological system, but rather can be applied to understand other multi-scale problems of interest to DOE/NNSA. For example, the biological membrane for which the model is being developed have complexities very similar to those found in the properties of materials and our modeling procedure could be applied to detect defects in materials. The integration of above approach with high performance computing help solidify DOE's exascale computing initiatives, thereby strengthening the key NNSA goal of stockpile stewardship.

Publications

Mansbach, R. A., T. Travers, B. H. McMahon, J. M. Fair, and S. Gnanakaran. Snails in Silico: a Review of Computational Studies on the Conopeptides. Submitted to *Marine Drugs*. (LA-UR-19-21315)

Travers, T., R. A. Mansbach, B. H. McMahon, J. M. Fair, and S. Gnanakaran. Evaluating the evolutionarily-optimized combinatorial peptide libraries of cone snails from a structural perspective. Unpublished report. (LA-UR-18-25722)

Controlling Quantum Information by Quantum Correlations

Wojciech Zurek
20170675PRD2

Project Description

The main goal of the project is to design protocols to control quantum systems, which outperform any known classical strategies. In particular, we plan to determine how quantum correlations can decrease the time and the energy for driving a system into the optimal state to run a quantum computation. We will design experimental demonstrations of quantum correlation-boosted control, implementable e.g. in optical lattices and atom traps. The project will pave the way for achieving optimal control of complex quantum systems, which is essential to deliver scalable quantum technologies. The proposal fully aligns with the Laboratory's commitment to be a strong player in developing quantum science and technologies, which has been recognized as a strategic priority by the National Science and Technology Council and the National Security Agency. Quantum devices are expected to dramatically change big data processing, solving computational problems beyond the capability of the best classical machines, and leading to innovative solutions in critical sectors as environmental sustainability, energy provision, and national security.

157-161. (LA-UR-17-29411 DOI: 10.1016/j.optcom.2017.12.050)

Technical Outcomes

This work developed computational study of complexity measures in multipartite quantum systems and quantification of the dynamical sensitivity of quantum systems to general quantum transformations.

Publications

Girolami, D. Final Technical Report of the project "Controlling

Quantum Information by Quantum Correlations".
Unpublished report. (LA-UR-18-20317)

Girolami, D. Information Geometry of
Quantum Resources. To appear in *Springer
Proceedings in Mathematics & Statistics*. (LA-
UR-17-27861 DOI: 10.1007/978-3-319-97798-0_17)

Susa, C. E., and D. Girolami. Weaving and neural complexity in
symmetric quantum states. 2018. *Optics Communications*.



Materials for the Future

Foldamers: Design of Monodisperse Macro-Molecular Structure by Selection of Synthetic Heteropolymer Sequence

Charlie Strauss
20160044DR

Project Description

We propose to design, create, and identify polymers with defined 3D structure and function to provide a new class of materials for catalysis, chem-bio threat reduction, and optical electronics. Control over synthetic polymer 3D architecture ("foldamers") remains a grand challenge in material science. We are creating a fundamentally new class of engineered material with inherently broad impact across many application domains. This is seen by analogy to the bio-materials, proteins, whose unique folding ability enable materials with extreme performance. Our new class of folding material will have similar capabilities but will withstand harsh environmental conditions and can incorporate non-biological dynamic functional materials. This work impacts energy security objectives by establishing novel catalyst materials suited for high-temperature and strong pH in biofuel reactors for the efficient use, generation, storage, and impacts mitigation of energy derived from fossil fuels or renewables entails an energy production/delivery/utilization system. Foldamers can also supply the sophisticated molecular recognition required for hierarchical molecular self-assembly spanning millimeter scales, impacting national advanced manufacturing objectives.

Technical Outcomes

We have developed breakthroughs in the synthesis, computational modeling, and high throughput selection of structured polymer materials that will impact Los Alamos National Laboratory missions and Department of Energy sponsors. Applications include actinide, Pu, and Lanthanide chelators for multiple mission areas. Follow-ons of these applications are already incorporated in multiple funded projects.

Publications

Chakraborty, A., W. C. Lin, H. Y. Tang, C. C. Chang, Y. H. Lee, P. Y. Wang, T. C. Chen, J. D. Luo, C. S. Tung, Y. T. Lin, C. T. Yeh, M. L. Cheng, T. Y. Lin, S. C. Huang, M. S. Shiao, J. S. Yu, J. L. Liu,

L. Y. Sung, Y. S. Chang, and L. M. Pai. Histidine-Dependent Protein Methylation Is Required for Compartmentalization of CTP Synthase. 2018. *Cell Reports*. (10) 2733-2745. (LA-UR-17-30644 DOI: 10.1016/j.celrep.2018.08.007)

Fenimore, P. W. A wave-mechanical model of neutron scattering II. Role of the momentum transfer Q. Submitted to *Physical Review E*. (LA-UR-16-20751)

Lappala, A., P. W. Fenimore, C. S. Tung, and C. Strauss. Conformational states of structured peptoids and peptide-peptoid hybrids. Submitted to *Journal of Computational Chemistry*. (LA-UR-17-31450)

Manore, C. A., B. H. McMahon, J. R. Mourant, and P. W. Fenimore. Decision Support for Mitigation of Livestock Disease: Rinderpest as a Case Study. To appear in *Frontiers in Veterinary Science*. (LA-UR-17-29923 DOI: 10.3389/fvets.2018.00182)

Miner, J. C., J. Berendzen, G. Chen, I. Stroe, and P. W. Fenimore. Eigen & Zundel-like water geometries revealed in protein crystal structures.. Submitted to *Nature*. (LA-UR-18-31707)

Peterson, P. W., R. D. Gilbertson, J. C. Miner, R. F. Williams, and C. E. Strauss. Controlled Cyclization of Peptoid Dimers to form N,N'-2,5-Diketopiperazines. Submitted to *Journal of the American Chemical Society*. (LA-UR-18-24785)

Strauss, C. E. LDRD DR Foldamers Final report. Unpublished report. (LA-UR-18-31099)

Topology and Strong Correlations: A New Paradigm

Filip Ronning
20160085DR

Project Description

This project proposes to identify new materials and new functionalities as a consequence of combining the concepts of topology and electron correlations. We will develop a "materials by design" approach using state-of-the-art theory combined with new and existing experimental capabilities to rapidly identify correlated topological materials with new functionalities. We will explore f-electron based insulators - a natural choice due to their inherent strong electronic correlations and large spin-orbit coupling, which will lead to new topological orders. Our success will lay the foundation for the discovery of new states of correlated topological matter and control over the protected conducting surface states, which are promising candidates for future technologies. With high tenability, reduced dimensionality and large mobilities, these materials can address national security needs in many impact areas including: sensing, metrology, quantum information, nuclear fuels, and spintronics.

Technical Outcomes

We made significant progress in establishing a theoretical capability that could predict whether an f-electron material was topological, and validated this procedure experimentally on the compound PuB₄. State of the art tools including Kerr effect, angle resolved photoemission (ARPES), and quantum oscillations were used to probe single crystals of potentially topological materials with novel signatures. The discovery of the ²³⁹Pu nuclear magnetic resonance (NMR) for only the second time was prepared serendipity.

Publications

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Dioguardi, A., H. Yasuoka, S. M. Thomas, S. K. Cary, S. A. Kozimor, J. H. Choi, J. Zhu, J. D. Thompson, T. E. Albrecht-Schmitt, E. D. Bauer, and F. Ronning. Discovery of ²³⁹Pu nuclear magnetic resonance in plutonium tetraboride. Submitted to *Nature Materials*. (LA-UR-18-21953)

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Additive Manufacturing of Mesoscale Energetic Materials: Tailoring Explosive Response through Controlled 3-dimensional Microstructure

Alexander Mueller
20160103DR

Project Description

High explosive (HE) structures will be produced via 3-Dimensional printing techniques to enable studies on detonation science. The understanding gained and capabilities developed by this work will provide the ability to tailor HE performance through structure. This effort will lay the groundwork necessary to fabricate additive manufacturing (AM)-HE with novel controlled initiation and reaction zone characteristics by attaining prompt reactive burn through control of the internal structure of the HE part. We aim to tailor shock sensitivity and detonation performance, and envision AM-HE that exhibits better corner-turning capabilities for applications such as more effective HE boosters. Once detonating, the effects of the tailored chemical reaction zone dynamics on detonation critical diameter, confinement edge angles, and failure characteristics will be quantified. A combination of mesoscale-to-continuum scale data will be used to construct a new mesoscale informed reactive burn model.

Technical Outcomes

This effort laid the groundwork necessary to fabricate AM-HE with controlled initiation and reaction zone characteristics by attaining prompt reactive burn through control of the internal structure of the HE part. We developed structure-based methods to tailor shock sensitivity and detonation performance, and showed that AM-HE exhibits tunable corner-turning capabilities. A combination of mesoscale-to-continuum scale data were used to inform our reactive burn model to include micro and mesoscale structural variation within the modeled charge.

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Hybrid Photonic-Plasmonic Materials: Toward Ultimate Control Over the Generation and Fate of Photons

Jennifer Hollingsworth
20170001DR

Project Description

21st-century communication, quantum information and energy-efficient lighting technologies depend on our ability to create, manipulate and detect the basic unit of light: photons. We are developing novel hybrid materials for unprecedented control over these processes. Technological competitiveness in these areas is a national security challenge, as the enabled applications address defense, industrial, and energy security needs, including advanced photodetectors and sensors, secure communications, next-generation computing, and efficient lighting/display technologies. In this way, the fundamental science questions being addressed are "use-inspired," driven by a need to make better and unprecedented use of light in advanced technologies that will underpin our physical and economic security in the coming century. Beyond foundational science, we are developing new tools and capabilities for designing and creating functional hybrid materials. The latter enable precision integration and advanced manufacturing over a range of lengthscales from the nanoscale, where many new important properties emerge, to the macroscale, where real-world applications happen. For example, we are developing techniques for placing single light-emitters into metallic antenna to create novel single and entangled-photon sources for secure communication or sensor qualification, and optical circuitry to remove bottlenecks in communication networks. Integration is at the nanoscale but effects are realized in micro/mesoscale networks.

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Material Processing to Performance: A Path to Physically-Based Predictive Capability

George Gray
20170033DR

Project Description

The ability to numerically represent and accurately predict damage and failure in materials remains elusive, despite its importance to the mission of the Laboratory and the defense complex, as well as many industrial applications. Our lack of predictive capability is related to a poor scientific understanding and quantification of the correlations between material processing, microstructure, properties, and performance (PSPP). The novelty and goal of this project is to understand the complex relationship between material processing and microstructure, specifically its affect on key damage nucleation sites like grain, twin, and solidification boundaries. We will determine where and when material failure initiates through the development of innovative statistical models to represent extremes and tails in distributions. Newfound knowledge about the underlying physics and extreme-value modeling will be the basis for a mechanistic based toolset for predicting failure at the macro-scale as function of processing. Los Alamos has a leadership responsibility for understanding and quantifying the scientific basis and predictive modeling capability to support material performance under high strain rate, stress, complex stress states, and shock-loading conditions. This project will directly contribute to advancing the Laboratory's capabilities in the Materials for the Future focus areas of defects and interfaces, manufacturing, and extreme-loading environments.

Publications

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Shocked Chemical Dynamics in High Explosives

Shawn Mcgrane
20170070DR

Project Description

The research team is performing time resolved measurements of chemical changes in shocked explosives to validate molecular level simulations. This will enable better prediction of explosive performance and safety through improved modeling of the underlying physics. The goal is to change how explosive modeling is performed, starting at the level of chemical response and predicting hydrodynamics. Currently, the research team starts with large-scale hydrodynamics, and fits artificial underlying chemical models. Changing this will increase predictive capability, allowing us to change materials, geometry, and conditions to increase explosive performance.

Publications

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Uncovering the Role of 5f-electron Magnetism in the Electronic Structure and Equation of State of Plutonium (U)

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20180025DR

Project Description

Accurate simulations of plutonium under extreme conditions require an accurate knowledge of the electronic structure and equation of state. Magnetism is presently a missing component of the electronic structure and equation of state that is known to have a significant influence on the equilibrium volume, bulk modulus and other properties. The goal of the present project is to determine primarily by way of experiment, accompanied by advanced theoretical modeling tools, the correct way of incorporating the effects of magnetism in the electronic structure and equation of state of plutonium. The end result will be an accurate understanding of the mechanism at play when delta-plutonium undergoes its initial volume collapse at low pressure. Such an understanding is crucial for accurate estimates to be made of plutonium's physical quantities under reduced volume, and also by extrapolation into more extreme environments where accurate or safe measurements are presently not possible.

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Rational Design of Halide Perovskites for Next Generation Gamma-ray Detection

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20180026DR

Project Description

This project will address two key national security challenges: (i) we will establish the scientific understanding and the design principles for a new halide perovskite materials technology for the fabrication of radiation detectors, critical for several Los Alamos National Laboratory and NNSA missions; (ii) we will demonstrate a proof-of-concept room temperature (RT) operated gamma ray detector with sensitivity and energy resolution exceeding that of cadmium-zinc-telluride (CZT) detectors, which represent the state-of-the-art for RT Gamma-ray detection.

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Boom or Bust? Predicting Explosive Safety under Impacts

Kyle Ramos
20180100DR

Project Description

High explosives are a component of conventional and nuclear weapons. We seek to understand the fundamental origins of the impact safety of explosives over a wide range of loading rates. Impacts on explosives generate localized deformation and fracture which can lead to ignition. Our ability to accurately predict how deformation occurs has been limited both by the complexity of these materials and the challenges of interrogating the structural responses of these materials under violent loading. We have made huge strides toward overcoming both of these obstacles in recent years. First, in situ, time-resolved x-ray imaging and diffraction at the Advanced Photon Source have provided new insights into how materials deform. Developments in theory and simulation have led to truly predictive models of explosives responses under shock loading. Moreover, the coupling between deformation and temperature can now be measured directly with vibrational spectroscopy. We will greatly extend our proof-of-concept work so we can understand and predict the impact responses and hence safety of cyclotrimethylene trinitramine (RDX) and cyclotetramethylene tetranitramine (HMX) single crystals and composites, two explosives of importance to DOD and DOE. Finally, we will apply our modeling framework to computationally design new energetic materials with microstructures tailored for impact safety.

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Properties, Theory, and Measurements for Understanding the Function of Heavy Elements

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20180474DR

Project Description

The study of heavy elements continues to be essential to the United States and central to the missions of the DOE and its NNSA laboratories, including nuclear weapons, global security, environmental restoration, and radioactive waste management. Of real concern is the recognition that academic degree programs and research opportunities in heavy-element science are small so that the field is becoming subcritical at a crucial time for our nation. Research performed by competitively selected Seaborg supported postdoctoral Fellows and students in nuclear science has provided exceptional return on investment in both science and acquisition of new hires.

Publications

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Theoretical Studies of Strongly Correlated Electron Systems

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20180717DR

Project Description

We will explore how strong electronic correlations can give rise to a new powerful family of topological materials. The consideration of such materials requires new algorithms and measurement techniques, both of which we will improve and develop in this project. On the algorithm front, we will investigate quantum annealing algorithms, electronic structure algorithms, and quantum electrons coupled to classical spins. We propose the exploration of fundamental interactions arising from the emergence of non-Fermi liquid behavior that is the grand challenge problem of condensed matter physics. This behavior is emergent in systems with strong electronic correlation involving competing orderings such as exotic magnetism and unconventional superconductivity. One of the fundamental questions of modern condensed matter physics is about the origin of non-Fermi liquid behavior near quantum critical points. Although transport measurements reveal strong deviations from conventional Fermi liquid behavior near antiferromagnetic quantum critical points, we still do not know what is the corresponding low-energy effective theory (the new fixed point). Because fermionic quantum critical points are ubiquitous in f-electron materials, it is a topic of central interest to the physical systems of relevance to the Laboratory with experimental work being carried out at the National High Magnetic Field Laboratory, and elsewhere.

Frontiers in Quantum Science

Angel Garcia
20160587DR

Project Description

This project addresses fundamentals of the electronic properties of materials, from actinides to photovoltaics, with emphasis on computational algorithms. We will apply concepts and algorithms of quantum computation to (1) understand the electronic structure of materials from complex correlated systems (2) explore novel functionality in topologically protected states such as skyrmions, and (3) bridge concepts of fluctuation-induced forces with new meta-material technology. This work has relevance in developing new materials for energy applications such as photovoltaic materials, modeling and predicting properties of f-electron matter, including plutonium, for NNSA mission objectives, and developing materials for quantum computing applications.

Technical Outcomes

This project studied quantum phase transition in materials. These transitions are relevant for developing materials that can be used in quantum computing and sensors. We discovered a Casimir force phase transitions in systems belonging to the graphene family. The graphene family are 2D materials formed with C, Is, Ge, and Sn. We studied topological phase and quantum anomalous Hall effect in quadratic band touching systems. In addition we developed new software to study nonadiabatic quantum dynamics.

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Brighter, Faster, Denser: Adaptive Co-design of Next-Generation Radiation Detector Materials

Blas Uberuaga
20180009DR

Project Description

Our goal is to develop and demonstrate an experimentally-informed machine learning model that can predict scintillator performance targeted to specific applications. Ultimately, we are primarily motivated by the radiographic imaging needs of the Enhanced Capabilities for Subcritical Experiments (ECSE) facility. In this project, we will show proof-of-principle of the proposed development and how we can use an integrated loop between modeling, synthesis and characterization to discover new materials. If this work is successful, follow-on work would develop models targeting the discovery of new materials with enhanced performance for the ECSE radiographic camera.

Technical Outcomes

Efficient materials discovery for scintillators and radiation detection application requires coupling theory, modeling, synthesis and characterization. This project undertook a proof-of-principle research effort to develop models to screen materials with promising performance and to identify the consequences of less-than-perfect materials for quick synthesis and characterization on the experimental side. Our results show that such models can be developed and that we can understand how microstructure impacts performance, allowing for high-throughput screening of new materials.

Publications

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Predicting High Temperature Dislocation Physics in Hexagonal Close Packed (HCP) Crystal Structures

Abigail Hunter
20160156ER

Project Description

The primary goals of this project are to use a novel mesoscale model framework to investigate high temperature deformation mechanisms, and predict their effect on the mechanical response of hexagonal close packed metals during manufacturing processes. We will advance a 3D mesoscale code unique to Los Alamos called phase field dislocation dynamics (PFDD). The model aims to bridge the atomic to meso-scale gap, and produce predictive multiscale simulations crucial for understanding dislocation structure evolution under extreme conditions. Continuum-scale material models used in weapons codes lack physically based descriptions of mechanisms that many atomic, nano, and microscale models have shown to be important. The information gained during this project will be used to develop physically based constitutive models to describe strength and damage.

Technical Outcomes

Our mesoscale code now accounts for dislocation motion in body-centered cubic and hexagonal close-packed metals, and also dislocation-grain boundary interactions. It was restructured to be sufficiently versatile for further advancements. The code was successfully open-sourced making it a pathway to start/continue external collaborations. Following warm rolling experiments, we discovered re-bonding phenomena occurred at reductions far below that required for room temperature bonding. This may make it possible to roll materials that we could not before.

Publications

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Mianroodi, J. R., A. Hunter, I. J. Beyerlein, and B. Svendsen. Theoretical and computational comparison of models for dislocation dissociation and stacking fault/core formation in fcc crystals. 2016. *Journal of the Mechanics and Physics of Solids*. 719-741. (LA-UR-17-21493 DOI: 10.1016/j.jmps.2016.04.029)

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Quantum Optics of Solitary Covalent Dopants in Carbon Nanotubes

Han Htoon
20160172ER

Project Description

With this project, we aim to establish doped carbon nanotubes that can be synthesized at a very low cost as a new transformational material for making light sources that emit one photon at a time (single photon sources) and switches that could control a stream of single photons: two fundamental building blocks needed for the realization of eavesdropping proof quantum communication technology. In addition, single photon sources can also enable quantum meteorology technology, in which absorption of the light can be measured beyond the shot-noise limit of typical laser light sources. Such technology could enable novel ultra-sensitive sensing platforms. Results of this project could help protect information critical for national security. The work directly addresses information collection, surveillance and reconnaissance, and national defense missions.

Technical Outcomes

This project achieved room temperature single photon generation at 1.55 μ m telecommunication from covalent defect states of carbon nanotubes. Single nanotube field effect transistor device capable of electroluminescence and possibly electrically driven single photon generation is also demonstrated. This project has resulted in peer-reviewed 12 publications and an intellectual property. This project has also enabled us to secure future funding for two new projects in the area of quantum information science.

Publications

Doorn, S. K. Photoluminescence Dynamics of Aryl sp³ Defect States in Single-Walled Carbon Nanotubes. 2016. *ACS Nano*. (9) 8355-8365. (LA-UR-17-24661 DOI: 10.1021/acsnano.6b02986)

Doorn, S. K., K. Shayan, X. He, Y. Luo, C. Rabut, X. Li, N. F. Hartmann, J. L. Blackburn, H. Htoon, and S. Strauf. Suppression of exciton dephasing in sidewall-functionalized carbon nanotubes embedded into metallo-

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Ishii, A., X. He, N. F. Hartmann, H. Machiya, H. Htoon, S. K. Doorn, and Y. K. Kato. Enhanced Single-Photon Emission from Carbon-Nanotube Dopant States Coupled to Silicon Microcavities. 2018. *Nano Letters*. (6) 3873-3878. (LA-UR-18-22596 DOI: 10.1021/acs.nanolett.8b01170)

Kwon, H., M. Kim, M. Nutz, N. F. Hartmann, V. Perrin, B. Meany, M. S. Hofmann, C. W. Clark, H. Htoon, S. K. Doorn, A. Hoegeler, and Y. Wang. Ultra-bright Trions Observed at Fluorescent Quantum Defects. Submitted to *Nature Photonics*. (LA-UR-17-30363)

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Transient Thermal Conduction in Nonlinear Molecular Junctions

Dmitry Yarotski
20160180ER

Project Description

We will apply a unique integration of chemical synthesis, advanced ultrafast optical techniques, and theoretical modeling of nonlinear vibrational dynamics to reveal the mechanisms and test the dynamic limits of thermal transport in Deoxyribonucleic Acid (DNA) molecules. The close communication between the new dynamic thermal probes and theoretical modeling should enable us to resolve the controversy between existing coarse-grained models (that reproduce equilibrium properties of DNA equally well but differ by orders of magnitude in the estimates of the non-equilibrium response) and develop predictive description of complex thermal conductivity of DNA oligomers. The results of this work will strongly impact national security missions that rely on complex systems, nanotechnology and, especially, nanoelectronics, because better understanding of nonlinear heat transfer in molecular-scale systems is an enabling ingredient for technological applications of novel molecular electronic and heattronic/phononic devices.

Technical Outcomes

Advances in new dynamic thermal probes and theoretical modeling enabled us to resolve the controversy between existing coarse-grained models (that reproduce equilibrium properties of DNA equally well but differ by orders of magnitude in the estimates of the non-equilibrium response) and develop predictive description of complex thermal conductivity of DNA oligomers. The results of this work will strongly impact national security missions that rely on complex systems, nanotechnology and, especially, nanoelectronics.

Publications

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Velizhanin, K. A., S. Sahu, C. C. Chien, Y. Dubi, and M. Zwolak. Crossover behavior of the thermal conductance and Kramers' transition rate theory. 2015. *Scientific Reports*. (1) 17506. (LA-UR-18-28759 DOI: 10.1038/srep17506)

Rigorous Development of Atomic Potential Functions in Terms of Strain Functionals

Edward Kober
20160220ER

Project Description

This project will develop a robust method for capturing the deformation properties of metals at an atomistic level. The resulting functions will be used in extreme scale simulations of those materials to enable the manufacture of improved materials. The overall goal is to develop atomic potential functions for the molecular dynamics (MD) simulations of metals that capture the very broad range of behavior including mechanical deformation, phase transitions and shock-loading. These will be calibrated to a combination of experimental data and electronic structure calculations. This will enable predictive MD simulations that will accurately capture the behavior of irregular atomic structures found around defects and grain boundaries in metals. This will allow us to more completely understand how the mesoscale structure of a metal affects its response characteristics, and enable the design of improved materials. Understanding the performance properties of metals and developing accurate models that can predict that behavior under a wide variety of circumstances is of critical importance to energy and defense missions, and also of significance to general manufacturing capability.

Technical Outcomes

The Strain Functional method was developed and demonstrated to be a robust and rigorous method for describing atomistic geometries in a physically appropriate framework. It was shown that this framework provides a path for incorporating more physical data (elastic constants, phonon modes) into the development of potential forms. We did not develop a separate potential function form, but provided paths to improve the existing MEAM and SNAP formulations.

Stimuli-Responsive Coordination Polymersomes

Reginaldo Rocha
20160284ER

Project Description

This project aims to create next-generation nanocarriers for controlled transport and triggered release of diagnostic/therapeutic agents in nanomedicine. The proposed systems can also be further applied into emerging self-healing materials technologies. The successful demonstration of functional metallo-polymersomes in this capacity will also have important implications as stimuli-responsive carriers of catalysts and reactants in the realm of electronic, photonic, and energy materials (e.g. damage self-repair and corrosion remediation). Because the broad field encompassing dynamic metallo-supramolecular polymers and functional metal-organic composite materials is still in its infancy, our research undertaking has a great potential for technical leadership and programmatic growth in areas of relevance to Los Alamos missions. There is potential for applications in optically and electronically responsive devices, as well as materials healing and treatment, including nuclear/weapon components.

Technical Outcomes

This ER project developed next-generation nanocarriers based on metal-stitched polymers that can self-assemble into vesicles and potentially burst on command to deliver the macromolecular cargo. Besides controlled transport and triggered release of diagnostic or therapeutic agents in nanomedicine, functionalities imparted into the demonstrated stimuli-responsive metallo-polymer assemblies can find applications in various areas, especially emerging self-healing materials technologies. This research has resulted in several presentations and two journal publications (with another in preparation).

Publications

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Nonequilibrium Dynamics and Controlled Transport in Skyrmion Lattices in Nanostructures

Charles Reichhardt
20160369ER

Project Description

This project aims to understand how a very small magnetic object called a skyrmion can be dynamically controlled. Skyrmions could act as smaller, more robust, more energy-efficient information carriers for computers. We will model and understand how to precisely control skyrmion motion in nanostructured geometries for the most effective way to move, write, read, and pack skyrmions in dense patterns that remain stable for long times. We will use a combination of continuum and particle-based simulations to model these geometries and driving protocols. The potential to create low-power, high-density magnetic storage devices and other magnetic-based logic devices would have a wide range of applications relevant for national security, including making smaller, more compact, lighter, and less energy costly devices for use by soldiers, aerial vehicles, and drones.

Technical Outcomes

Skyrmions are nanoscale magnetic particles that show great promise for a variety of nanoscale devices due to their size scale and mobility. This work demonstrated and confirmed in various experiments that skyrmions move at a velocity-dependent angle relative to a driving force in the presence of a substrate. This drive dependence must be considered when building skyrmion devices or interpreting electrical transport measures. We also demonstrated accurate control of skyrmion motion using various nanostructures.

Publications

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Connecting Interface Structure and Functionality in Oxide Composites

Blas Uberuaga
20160501ER

Project Description

Using atomistic and mesoscale modeling, combined with experimental synthesis and characterization, we will determine the relationship between interfacial atomic structure and ionic conductivity in complex oxide heterostructures. Many technologically important applications, ranging from solid-oxide fuel cells, to supercapacitors, rely on materials that exhibit high ionic conductivity -- these are referred to as superionic. Despite the promise of these materials and the intensive research accompanying them, they still fall short of expectations. Not only will our work enable improved materials for applications such as fuel cells and supercapacitors, it will also enable control of mass transport in complex materials via interfacial properties. This will be a first for Los Alamos, leading to a new ability to design materials for advanced applications involving superionics.

Technical Outcomes

Composite materials with a high density of interfaces are attractive due to enhanced functionality, such as higher ionic conductivity. However, it is still unknown how interfaces impact the conductivity. Using model materials with varying interfacial structure, we have interrogated how defects and dopants interact with that structure. We conclude that properties are sensitive to interface structure and that carrier mobility is lower at these interfaces, raising questions about what drives the enhancement observed in experiments.

Publications

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Controlling the Functionality of Materials through Interfacial Colloidal Gelation

Matthew Lee
20160519ER

Project Description

This project will develop new synthetic routes for high-performance materials utilizing nano-scale particles as building blocks for complex structures vital to many modern technologies, including catalytic and energy systems (e.g. batteries). The project goal is a rational design of porous and composite solids with controlled interfacial functionality using an emerging class of soft matter known as bicontinuous interfacially jammed emulsion gels, or Bijels. Because Bijels are a recent invention, our fundamental understandings of their physical assembly, aging, and mechanical properties are at an early stage. Moreover, Bijels have vast untapped potential in an array of current engineering applications, including interfacial catalysis and renewable energy systems. Successful realization of the proposed research objectives will provide critical advances in both theoretical modeling of multi-phase soft materials and novel materials synthesis techniques, paving the way for new generations of functional porous and composite solids for a diverse array of applications, including optimized energy storage devices and waste management and remediation technologies.

Technical Outcomes

This project successfully achieved several key R&D outcomes related to Bijel materials and their engineering applications. First, our team conceived and developed a new theoretical model to guide the formation of future Bijel materials, wherein their complex physics may be captured through simple equations. Second, we developed new bijels made from metallic nanoparticles that have promise in catalytic systems and energy storage. Lastly, we successfully utilized bijels to create new classes of ultra-light aerogel materials.

Publications

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Emergent and Adaptive Polymers

Antonietta Lillo
20160528ER

Project Description

This project aims to provide multifunctional materials for next-generation polymer light-emitting electrochemical cells (PLECs) and organic light-emitting diodes (OLEDs) used in implantable and wearable electronics. We will create libraries of genetically encoded and optically active polymers, and through a technique akin to evolution, sort for those polymers that exhibit a defined optical or adaptive response. Use of genetically encoded polymers (GEPs) allows us to create large libraries of stimuli-responsive polymers (far eclipsing current synthetic techniques) and to identify, en masse, those polymers with a defined function or physical property in a matter of days instead of decades.

Technical Outcomes

This project developed methodology to produce elastin-like polymers with controlled structural elements (rods and springs), as well as developing efficient methods to conjugate those polymers to optical moieties. We have also developed composite materials that exhibit stimuli-responsive optical changes. We have learned how to integrate these genetically encoded optical polymers into devices and to control their color and fluorescence using electrical stimulation.

Publications

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Rocha, R. C., J. Martinez, K. C. Elbert, K. Ghosh, and E. R. M. Balog. A metallo-biopolymer conjugate of elastin-like polypeptide: photoluminescence enhancement in the coacervate microenvironment. To appear in *JBC Journal of Biological Inorganic Chemistry*. (7) 1153-1157. (LA-UR-18-21561 DOI: 10.1007/s00775-018-1580-6)

Exotic States in Uranium-based Superconductors

Roman Movshovich
20160572ER

Project Description

This project aims to determine the symmetry of the superconducting order parameter in a number of uranium-based superconductors with different magnetically ordered ground states, and correlate that symmetry with the nature of those related magnetic state. Uranium (U) -based heavy fermion compounds offer a particularly fertile area to look for an emergent behavior, as they present a large variety of magnetically ordered ground states that seem to be connected to superconductivity. We will correlate the order parameter symmetry with the nature of magnetic fluctuations, accessing the microscopic origins of superconductivity in selected U-based superconductors. These results will help understand the origins of unconventional superconductivity in a wider range of materials, including high temperature cuprate and pnictide superconductors.

Technical Outcomes

This project developed a capability to measure thermal conductivity in rotating magnetic fields, at dilution refrigerator and magnetic field up to 14 T. This capability is particularly useful for investigating the nature of a superconducting state, where charge transport tools are not applicable, as resistance turns to zero. We discovered a ubiquitous nature of triply intertwined orders: a d-wave superconductivity, magnetic spin density wave (SDW), and a spatially inhomogeneous superconducting p-wave pair density wave (PDW).

Publications

- Kim, D. Y., S. Lin, D. F. Weickert, E. D. Bauer, F. Ronning, J. D. Thompson, and R. Movshovich. Resonances in the Field-Angle-Resolved Thermal Conductivity of CeCoIn₅. 2017. *Physical Review Letters*. (19) 197001. (LA-UR-16-29172 DOI: 10.1103/PhysRevLett.118.197001)
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Interfacial Structure Transfer for Direct Band Gap Wurtzite Group-IV Semiconductors

Jinkyung Yoo
20170121ER

Project Description

The research enables us to prepare a novel phase of group-IV semiconductors, such as silicon (Si) and germanium (Ge), which are dominant materials for most semiconductor device applications. The novel phase has hexagonal crystal structure and direct electronic band gap according to decades-long theoretical predictions. Furthermore, direct band gap group-IV semiconductors are the ideal building blocks for monolithic optoelectronic integrated system because the highly efficient light-emitting characteristics of direct band gap materials make it possible to fabricate an integrated system encompassing light-emitter, transmitter, detector, and processor with a single material. Direct band gap group-IV semiconductor is the "holy grail" of semiconductor-based optoelectronic devices because it hasn't been realized in reproducible and production-compatible manner. The research is being conducted by an integrated approach of predictive materials design led by quantum mechanical modeling and intensive experimental methods, such as chemical vapor deposition of two-dimensional (2D) materials and Si/Ge, nanocharacterizations, and nanofabrications for multi-scale analyses. Our progress has demonstrated that production-compatible thin film hexagonal Si and Ge can be prepared on 2D materials. The project is closely relevant to the DOE grand challenges to "control at the level of electrons" and "energy and information on the nanoscale."

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Publications

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- Yoo, J., T. Ahmed, R. Chen, A. Chen, Y. H. Kim, K. C. Kwon, C. W. Park, H. S. Kang, H. W. Jang, Y. J. Hong, W. S. Yang, and C. H. Lee. Enhanced nucleation of germanium on graphene

Designing Emergent Behavior in the Collective Dynamics of Interacting Nano-Magnets

Cristiano Nisoli
20170147ER

Project Description

Magnetism is critical to areas of national security, from magnetic sensing/control, to information technology, to energy-efficient devices. However, magnets with useful properties at room temperature are rare overall, found serendipitously, and their supply depends on foreign countries. A far greater set of magnetic functionality could be unlocked if we could implement artificial, topologically complex magnetism. Magnetic technology generally concerns itself with manipulation of localized dipolar degrees of freedom, artificial materials containing delocalized monopolar charges, and generally controllable emergent behaviors at room (or desired) temperature is scientifically very exciting but also a possible technological game-changer.

Publications

Lao, Y., C. Nisoli, F. Caravelli, M. Sheikh, P. Schiffer, J. Sklenar, D. Gardezabal, J. Watts, A. Albrecht, A. Scholl, and K. Dahmen. Classical topological order in the kinetics of artificial spin ice. 2018. *Nature Physics*. (7) 723-727. (LA-UR-17-29552 DOI: 10.1038/s41567-018-0077-0)

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Nisoli, C. Inner Phases of Colloidal Hexagonal Spin Ice. 2018. *Physical Review Letters*. (2) 027204. (LA-UR-18-29684 DOI: 10.1103/PhysRevLett.120.027204)

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Continuous In-situ Tuning and Nuclear Magnetic Resonance (NMR) Spectroscopy of Correlated Matter

Eric Bauer
20170204ER

Project Description

This project aims to perform nuclear magnetic resonance measurements under continuous in-situ strain to understand the exotic quantum states of matter, such as superconductivity. These unusual states of matter elucidated by our experiments may be used in future energy-saving technologies. For instance, some of the superconducting materials we will study in this project are already being planned for use as the main component, the magnet, in new and improved Magnetic Resonance Imaging machines, which operate at a fraction of the costs of today's machines. The knowledge that we generate in our project may also lead to improved devices under strain conditions that make up the DOE x-ray User Facilities and other high-energy colliders (such as the Large Hadron Collider, which led to the discovery of the Higgs Boson and a Nobel Prize) used throughout the US and the world.

Publications

Luo, Y., P. Guzman, A. Dioguardi, A. Pustogow, S. M. Thomas, F. Ronning, N. Kikugawa, D. Sokolov, F. Jerzembeck, A. Mackenzie, C. Hicks, E. D. Bauer, I. I. Mazin, and S. Brown. Normal state ^{17}O NMR studies of Sr_2RuO_4 under uniaxial stress. Submitted to *Physical Review X*. (LA-UR-18-30163)

Dynamics of Nonequilibrium Phase Transitions and Universality

Wojciech Zurek
20170211ER

Project Description

This project is basic research into the fundamental mechanisms of phase transitions: how one phase of matter transforms into another. The theory being developed has implications for atomic and materials physics, and is a unique application of quantum annealing, which is an early and promising form of quantum computing. The experimental tests being developed involve the nanoscale structure of ferroelectric and magnetic materials. These material systems have many applications in electromagnetic sensing, and optoelectronic devices.

Publications

Zurek, W. H. Eliminating Ensembles from Equilibrium Statistical Physics: Maxwell's Demon, Szliard Engine, and Thermodynamics via Entanglement. Presented at *Hybrid Qantum- Classical Computing*. (Krawkow, Poland, 2017-04-17 - 2017-05-30). (LA-UR-17-22953)

Harnessing Dark Excitons in Carbon Nanotubes through Covalent Doping Chemistry

Stephen Doorn
20170236ER

Project Description

The defect-state emission we will study presents a unique photon source for optically based quantum information processing and data encryption of interest for global security needs that also offers interesting potential for sensing, imaging, and energy conversion applications. This represents new functionality for carbon nanotubes and results from localization of emitting "excitons" at the new defect sites. Localization in turn provides brighter photoluminescence, longer-lived excited states, and single-photon emission behavior. In order to better harness these behaviors, in this project we aim to probe the electronic structure of the new emitting states using low-temperature spectroscopy techniques. Additionally, the dynamic behavior of these states will be probed to understand relaxation mechanisms, provide additional information on electronic structure and to evaluate how optically generated excitons become trapped at defect sites. Each of these behaviors will be correlated to related nanotube structure and defect surface chemistry to drive new strategies for optimizing the chemical functionalization of carbon nanotubes that is the ultimate origin of this new functionality of significant interest.

Publications

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- Doorn, S. K., K. Shayan, X. He, Y. Luo, C. Rabut, X. Li, N. F. Hartmann, J. L. Blackburn, H. Htoon, and S. Strauf. Suppression of exciton dephasing in sidewall-functionalized carbon nanotubes embedded into metallo-dielectric antennas. *Nanoscale*. (26) 12631-12638. (LA-UR-18-24661 DOI: 10.1039/C8NR03542C)
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"Zero-Threshold Gain" and Continuous-Wave Lasing Using Charged Quantum Dots

Victor Klimov
20170279ER

Project Description

This project is relevant to the Los Alamos Science of Signatures science pillar; by introducing a novel type of highly flexible and versatile gain media, it can lead to the development of new types of lasers for sensing and diagnostics. Solution-processed quantum-dot lasers are uniquely suited for incorporation into various lab-on-a-chip platforms, such as those specifically for detection of chemical and biological threats. This work can potentially lead to the development of inexpensive, ultra-bright light sources, which can be used for the practical implementation of ideas of laser lighting, a topic of direct relevance to the Los Alamos energy security mission.

Publications

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- Wu, K., Y. S. Park, J. Lim, and V. I. Klimov. Zero-threshold optical gain using charged semiconductor quantum dots. Submitted to *Nature Nanotechnology*. (LA-UR-17-20412)
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Hetero-Interfaces of Novel 2-Dimensional Dirac Semiconductors

Nikolai Sinitsyn
20170328ER

Project Description

Bi-layer transition-metal dichalcogenides materials are extremely interesting for the variety of tunable optical, thermal, and electric properties that they can have depending on relative orientation of different single atomic layers. Los Alamos has the world's highest magnetic field setup to study characteristics of these systems. We want to place the Laboratory as the leading institution to study physical properties of these materials. We hope to observe so-called indirect excitons that are electron-hole bound states. In bilayers, such quasi-particles can have unusually long life-times. Since they carry energy and since they are created by light, there are potential applications in photovoltaics and other optoelectronic and energy efficient applications.

Journal of Physics A: Mathematical and Theoretical. (24) 245201. (LA-UR-17-26367 DOI: 10.1088/1751-8121/aac3b2)

Publications

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Chemical Approaches to Stable, Narrow-Bandgap Perovskite Materials

Nathan Smythe
20170393ER

Project Description

This project aims to address national security challenges in the area of energy security, which is an important DOE mission. A recent Basic Energy Science Advisory Committee (BESAC) report entitled “Basic Research Needs to Assure a Secure Energy Future” clearly emphasized the need to rapidly develop new materials that resist degradation due to various conditions, including temperature effects. This report highlights the need to develop methods for solar energy conversion for the production of fuels and electricity. The report also points out, “inorganic materials science today is critically lacking in the knowledge of predictive reaction pathway mechanisms that would allow the design and synthesis of materials with specified reactivity and properties.” Furthermore, the report goes on to say that “a truly integrated basic research approach of theory, modeling, synthesis, validation and testing is required” in order to facilitate “unprecedented control and predictability of properties and reactivity of technically relevant materials.” Within the scope of this project, we will focus on this integrated approach in order to develop more robust materials capable of supporting light-driven chemical transformations and solar energy conversion.

Quantum Molecular Dynamics of Strongly Correlated Materials

Kipton Barros
20170450ER

Project Description

Molecular dynamics (MD) simulations have become a powerful and widely used predictive tool in computational materials science, chemistry and biology. MD is also a capability required for a large number of DOE/NNSA missions. Examples include the design of next-generation energy harvesting materials, modeling high-energy explosives, modeling decay of weapons systems, etc. The validity of MD simulations is limited by the accuracy of the potential energy function. An emerging research area is quantum-MD, in which first principle quantum mechanical equations determine the electronic states, from which ionic forces are calculated at every MD time-step. This project better incorporates quantum mechanical effects into MD simulation.

Publications

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Suwa, H., J. S. Smith, N. E. Lubbers, C. D. Batista, and G. W. Chern. Machine learning for molecular dynamics with strongly correlated electrons. Submitted to *Physical Review Letters*. (LA-UR-18-31198)

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Wang, Z., K. M. Barros, G. W. Chern, D. L. Maslov, and C. D. Batista. Resistivity Minimum in Highly Frustrated Itinerant Magnets. To appear in *Physical Review Letters*. (20) 206601. (LA-UR-18-31202 DOI: 10.1103/PhysRevLett.117.206601)

Driven Quantum Matter

Alexander Balatsky
20170665ER

Project Description

The hypothesis that drives this research is that the highly tunable quantum matter (electronic liquid, spins, lattice) will develop qualitatively different responses depending on the nature of the time dependent drives. The ideal outcome of this project would be the test of the central hypothesis: the nature of the induced states in driven quantum matter depends on the nature of external drive: scalar, vector or tensorial. As an intermediate goal we expect to have a catalogue of possible collective instabilities, such as transient excitonic and superconducting instabilities in Dirac Materials (DM) and in Majorana states. We expect the following efforts and results over the project lifetime: 1) Investigation of the mass quench in Dirac materials and Quantum mechanical modeling of the Majorana states quench in topological superconductors. 2) Development of the models to test the role of the dynamics of DM in response to vector fields like magnetic and electric field and modeling of the Dynamical Quantum Phase transitions in Majorana and Dirac states. 3) Demonstration of control of collective instabilities and emergent new collective states in drive DM and Majorana states.

Truncation. 2018. *Physical Review Letters*. (1) 016403. (LA-UR-17-24060 DOI: 10.1103/PhysRevLett.120.016403)

Huang, Z., and A. V. Balatsky. Complexity and geometry of quantum state manifolds. Submitted to *Physical Review A*. (LA-UR-18-30745)

Publications

Arovas, D. P., W. Zhu, J. Zhu, Z. Huang, and A. V. Balatsky.
Invariance of Topological Indices Under Hilbert Space

Quantitative Understanding of Electronic Correlations in F-Electron Quantum Matter

Shizeng Lin
20180098ER

Project Description

Understanding and ultimately predicting the properties of complex materials is required to secure US energy independence and bolster national security. This project, in particular, addresses the DOE priority of realizing controlled functionality by employing quantum materials that exhibit tunable and emergent properties driven via collective behavior of electrons. This class of materials holds strong promise for future applications for future applications ranging from power management and transmission, to quantum computation, to novel versatile sensors as emphasized in the recent DOE/BES Basic Research Needs reports “Quantum Materials for Energy Relevant Technology”. Our approach combines advanced neutron scattering methods with new approaches in modeling to quantitatively understand the link between collective electron behavior and materials properties, thus laying the scientific foundation that will enable predictive quantum matter design. The use of neutron scattering at high pressure as we will employ here, and science enabling material by design capabilities is of particular interest to the DOE/Office of Basic Energy Sciences. Finally, we note that properties of plutonium metal, which are of relevance to the NNSA stockpile stewardship and nuclear weapons missions, are also determined by collective electronic behavior. The research performed here will provide insights relevant to the understanding of plutonium.

Publications

Halsbeck, F., S. Saeubert, M. Seifert, C. Franz, M. Schulz, A. Heinemann, T. Keller, P. Das, J. D. Thompson, E. D. Bauer, C. Pfleiderer, and M. Janoschek. Interplay of Itinerant and Localized Spin Fluctuations in the Ferromagnetic Superconductor UGe₂. Submitted to *Physical Review Letters*. (LA-UR-18-20542)

Kim, T., C. C. Chien, and S. Lin. Re-entrant Fulde-Ferrell-Larkin-Ovchinnikov State in Small-Sized Superconductors. Submitted to *Physical Review B*. (LA-UR-18-30667)

Lin, S., J. Zhu, and A. B. Saxena. Kelvin modes of a skyrmion line in chiral magnets and the associated magnon transport. Submitted to *Physical Review B*. (LA-UR-19-20239)

Lin, S., and Y. Su. Pairing symmetry and spontaneous vortex-antivortex lattice in superconducting twisted-bilayer graphene: Bogoliubov-de Gennes approach. 2018. *Physical Review X*. (19) 195101. (LA-UR-18-26090 DOI: 10.1103/PhysRevX.9.195101)

Su, Y., and S. Lin. Nontrivial topology and localization in the double exchange model with possible applications to perovskite manganites. 2018. *Phys. Rev. Lett.* (23) 235116. (LA-UR-18-29965 DOI: 10.1103/PhysRevB.98.235116)

Making the Unmakeable: Nanostabilized Magnetic Alloys

Sergei Ivanov
20180114ER

Project Description

In recent years, there has been an explosion in recognizing the need for new low-cost rare-earth-free magnetic materials for various applications: hard ferromagnets, as ideal active components for a broad range of energy generating/converting devices, multiferroic (e.g., ferromagnetic and magnetoelectric) and ferromagnet/antiferromagnet composites for advanced electronic and spintronic circuitry components. Combination of light magnetic metals with electron-rich heavy elements, such as Tl, Pb, or Bi, has long been considered a lucrative goal in the search for such magnetic materials. The unfortunate problem of complete immiscibility of these metals at ambient pressures precluded the synthesis of such alloys. We propose a general path to overcome the miscibility limitation that will lead to the formation of those “forbidden” alloys of Mn, Fe, or Co with Pb or Bi and their oxides via nanoscale synthesis. Once successful, the project will demonstrate the low-cost, general, and facile approach to hard-to-synthesize metal alloys for multiple applications. In particular, it will open up a path toward unique magnetic materials necessary for efficient energy generation and new generation of circuitry components for electron spin manipulation. The latter would lead to novel secure computing approaches, sensors, and other magnetoelectronics-based devices.

Utilizing Crystalline Sponges to Perform Single Crystal X-ray Determination on Trace Amounts of Actinium Compounds

Brian Scott
20180128ER

Project Description

Actinium shows great promise as a cancer radioimmunotherapy agent. However, its scarcity has hindered chemical structure characterization with X-rays. Chemical structure is vital to understanding how actinium will behave in biological systems and also for designing therapeutic agents. This work will develop techniques to perform X-ray single crystal characterization using trace amounts of actinium absorbed into porous crystals. These porous crystals, known as metal-organic-frameworks (MOF's), are composed of metal centers linked together with organic molecules to form a three-dimensional structure with open pores. Microgram quantities of actinium are not sufficient to grow crystals for X-ray studies, but do provide ample material for an actinium-MOF crystal that can be used for X-ray structure determination. An MOF crystal large enough for X-ray studies can absorb micrograms of actinium into its pores. An X-ray crystal structure of the actinium containing MOF crystal will yield the structure of the MOF and the absorbed actinium species. Besides informing radioimmunotherapy development using actinium, this technique could also be used to determine chemical structure of trace amounts of chemical weapons agents, explosives, and other actinides and molecules of importance to national security.

Publications

Wolfsberg, L. E., G. Rodriguez, D. A. Yarotski, P. C. Dowden, B. L. Scott, and G. S. Goff. Experimental Signatures for Dynamic Plutonium Hydriding. Unpublished report. (LA-UR-19-20942)

Electronic Structure of Putative Topological Kondo Insulators

Mun Chan
20180137ER

Project Description

We will develop the capability to study electronic and magnetic properties of materials under simultaneous ultra-high pressures and high-magnetic fields. This will be applied to the study of topologically correlated electron materials, a field that promises significant technological implications, including ultra-fast quantum computation and spintronics. It is of vital importance to the Los Alamos mission to understand the properties of materials under pressure. Crystalline properties are routinely tracked with x-rays. Our new experimental capability will allow for a determination of the electronic properties. This will foster new collaborations at the high-magnetic field laboratory at the Laboratory.

Visualizing Nanoscale Spatio-Temporal Dynamics in Single Quantum Systems

Peter Goodwin
20180189ER

Project Description

This project is responsive to the Laboratory mission in the Materials for the Future Focus area in that it strives, through the development of novel characterization methods for the visualization of excited state dynamics in nanoengineered structures, for 'linking across length and time scales ... to achieve a multi-scale understanding, and ultimately control, of materials structure, dynamics and function.' These studies will uncover detailed aspects of quantum dot (QD) interparticle interactions that will be relevant toward designing and improving QD optoelectronic devices, displays, solar cells, biological labels, and other technologies, and will enable the discovery of new properties and unanticipated applications and devices involving QDs. These studies will also reveal features of electronic energy interactions unique to QDs and other nanoparticles, as well as features common to molecular systems in which excited state electronic interactions are important, such as organic molecule Förster resonance energy transfer (FRET), conjugated polymers, and biological photosynthetic complexes. Finally, this research will introduce new experimental methods and capabilities that can be exploited to investigate a wide variety of molecular and nanoscale systems, in which multiple emitters cluster, aggregate, or associate to transport electronic energy in a manner that is greater than the sum of its parts.

Publications

Ryan, D. P., P. M. Goodwin, C. J. Sheehan, K. J. Whitcomb, M. Gelfand, and A. Van Orden. Mapping Emission from Clusters of CdSe/ZnS Nanoparticles. 2018. *The Journal of Physical Chemistry C*. (7) 4046-4053. (LA-UR-18-20821 DOI: 10.1021/acs.jpcc.7b10924)

Improved Biologically Friendly Polymer Drag Reducers From Novel Architectures

Paul Welch
20180220ER

Project Description

The research described in this proposal will directly address the Objective Capability Area of Mitigating Impacts of Global Energy Demand Growth called out in the Los Alamos Energy Security Strategy. Specifically, we will address the objective of "Integrating multi-scale measurements, modeling, and uncertainty quantification to validate predictions to support decisions and investments in energy systems with a goal of anticipating risks, disruptions, impacts, and consequences." This project will produce a series of polymers designed to reduce drag in aqueous flows. The project will study the molecular physics involved in the polymer interactions in turbulent environments over a range of length and time scales using a novel combination of experimental and modeling techniques. Success in this project will produce new insight into the importance of molecular architecture in drag reduction, facilitating the design of new materials. In particular, we will learn: 1) whether intrinsically multi-time scale materials perform better in typical drag reduction applications; 2) how best to design the distribution of molecular time scales to optimally impact realistic flow fields; and 3) the biologically friendly chemical architectures that most likely satisfy that distribution.

Ultrafast X-ray Imaging Using Slow, Visible Cameras

Pamela Bowlan
20180242ER

Project Description

New bright sources of femtosecond (10-15 seconds) X-ray pulses are revolutionizing materials science giving atomic-scale snap shots of how materials behave in extreme conditions like high pressure or temperature. A major impediment in these experiments are the detectors which have temporal resolutions up to six orders of magnitude slower than the X-ray pulses, smearing out the dynamics being studied, and making it challenging to even diagnose the X-ray source. Future X-ray Free Electron Lasers, aimed to directly address DOE/NNSA mission goals like manufacturing science or dynamics in explosives, will use even higher X-ray photon energies and operate at higher X-ray pulse frequencies, for which no detector exists. Our work offers a novel, potentially transformative solution, where interacting an X-ray and visible light pulse in the right medium encodes the X-ray pulse's spatial and temporal information (i.e., the X-ray image and its femtosecond temporal evolution) in the visible light, making it possible to measure femtosecond time resolved X-ray images with standard visible cameras. This technology will both improve the capabilities at current DOE X-ray sources, and also help to motivate and build new sources optimized specifically for NNSA mission-relevant applications.

Publications

Bowlan, P. R. Ultrafast Control of Material Properties through Core Electrons. Unpublished report. (LA-UR-18-21644)

Next Generation Discrete Dislocation Dynamics Modelling for Materials Science Applications

Laurent Capolungo
20180250ER

Project Description

Having the ability to model microstructure-sensitive behavior of materials is essential to predict performance and to design new materials. The proposed work will improve the physics underlying polycrystalline materials models and, at the same time, provide a robust method to quantify defect content with non destructive evaluation (NDE). NDE methods are typically used to probe the state of material systems in service conditions. These approaches are particularly pertinent in scenarios in which the material is subjected to harsh environments (pressure, radioactivity, etc.). The project will largely contribute to vetting NDE based assessment of the material state and performance in harsh conditions.

Publications

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- Lebensohn, R. A., and A. D. Rollett. Spectral Methods for Full-Field Micromechanical Modelling of Polycrystalline Materials. Submitted to *Annual Review of Materials Research*. (LA-UR-18-28795)

Dopant Profiling in Semiconductors by Scanning Frequency Comb Microscopy

Dmitry Yarotski
20180283ER

Project Description

Moore's Law is a techno-economic model describing the tendency of nearly doubling the performance and functionality of digital electronics every two years within a fixed cost and area. Within a decade, it predicts that novel lithographic processes will bring characteristic device dimensions into the 3 nanometer (nm)–5 nm realm. This range corresponds to a dozen or fewer dopant atoms across critical circuit features, thus leading to the strong dependence of the device performance on the location of each impurity. Therefore, the progress in fabrication demands adequate characterization tools as it is no longer possible with current instrumentation for the semiconductor industry to satisfy the rule-of-thumb that the resolution in charge carrier profiling should be finer than 10% of the lithographic feature dimension, i.e. better than 1 nm. We will leverage recent Los Alamos National Laboratory breakthroughs in the development of nanoscale microwave sources, as well as extensive Laboratory capabilities in scanning probe microscopy and ultrafast laser spectroscopy to achieve non-destructive low-noise carrier profiling with unprecedented (~ 0.1 nm) resolution using newly-developed Scanning Frequency Comb Microscopy (SFCM). The primary benefit of our project would be improved semiconductor metrology that will facilitate further advances in semiconductor fabrication technologies and consumer electronics and computing.

Publications

Hagmann, M., M. Mousa, and D. A. Yarotski. Resolution in Carrier Profiling Semiconductors by Scanning Spreading Resistance Microscopy and Scanning Frequency Comb Microscopy. 2017. *Applied Microscopy*. (3) 95-100. (LA-UR-18-29738 DOI: 10.9729/AM.2017.47.3.95)

Scalable Dielectric Technology for Very Low Frequency (VLF) Antennas

John Singleton
20180352ER

Project Description

Very low frequency (VLF) transmitters use frequencies from 3 to 30 kilohertz (kHz). The technology is old and “state-of-the-art” stations date from the 1960s. Since VLF penetrates about 40 meter(m) of saltwater, it is our means of communication with nuclear-deterrent submarines. Other strategic uses include military navigation systems employed during/after global disaster or nuclear war and detection of hostile facilities deep underground. Current VLF transmitters are 200-300 m high and often >1 km across; a central tower is linked to surrounding masts by a network of cables in an attempt to increase efficiency. Additionally, a “carpet” of copper cables reduces power dissipated in the ground. Despite this complexity/cost, VLF transmitters are inefficient, radiating only 10-50% of transmitter power. Their size makes them very expensive, impossible to hide, vulnerable to attack and difficult to replace. We will study three new types of VLF antenna proposed at Los Alamos National Laboratory, and enabled by recent advances in materials science and electromagnetic theory. From these, the two best candidates will be selected to provide smaller, cheaper, more efficient and more easily concealed (and possibly portable) replacements for current VLF transmitters. Scale models of these will be built and tested rigorously using Navy protocols.

Two-dimensional Nanostructure-Engineered Durable Supercapacitors

Sergei Ivanov
20180360ER

Project Description

Supercapacitors are emerging energy storage devices complementary to conventional batteries, due to their shorter charging times, long lifetime, and wider temperature operational ranges. In addition, recent incidents have highlighted safety concerns surrounding the use of high energy density batteries due to the presence of highly reactive components. Supercapacitors are uniquely poised for applications such as regenerative braking in cars, static random access memory, motor starters, and various electronics. However, current materials used in supercapacitors have inherent technical limitations. We propose structural modifications to ubiquitous layered molybdenum disulfide (MoS_2) that will lead to the increase in performance of supercapacitors and to the improvement of the material's durability to prolonged used and handling. Specifically, our project will result in: (1) synthesis of nanocrystalline mix-metal layered copper sulfides or selenides with group VI metals or antimony (Sb) with molecular spacers between layers, (2) complete structural/electrochemical characterization of synthesized materials to establish the influence of composition, size and interlayer distance on their properties, and (3) fabrication of a durable supercapacitor prototype. Project success will lead to a new area of supercapacitor development using high performance low-cost materials coupled with ease of device manufacturing.

Switchable Spin Crossover Explosives: Nitrogen-rich Iron (Fe II) Complexes for On-Demand Initiation Sensitivity

Jacqueline Veauthier
20180369ER

Project Description

We seek to develop explosive materials that can switch from an insensitive (safe) phase to a more sensitive (less safe) phase when exposed to the appropriate stimuli. In the insensitive state, these materials would greatly reduce the potential for accidental detonation, while in the sensitive state they could be reliably detonated. This proposal addresses a long-standing goal within the Department of Energy (DOE) and the Department of Defense (DOD) communities for explosive materials with on-demand sensitivity and successful development of these materials would put Los Alamos National Laboratory at the forefront of the insensitive munitions efforts. Technologies derived from the proposed research will contribute to National R&D needs for the prediction and control of explosive initiation and Laboratory core missions in stockpile stewardship and energetic materials science. Our materials by design approach will not only advance the fundamental science of explosives, but will also have a broad impact in designing other molecularly switchable photonic materials. Our work will produce high impact results, train the next generation of energetic materials scientists and theorists and will put the Laboratory at the forefront of explosives science.

Breaking the Efficiency Limits in Quantum Dot Emitters Using Dual-Band Metamaterials

Houtong Chen
20180372ER

Project Description

Development of energy efficient materials and device architecture is one of the central missions of the Laboratory and our nation. Rational design of mesoscale and nanoscale materials and creation of transformative device concepts are critical to address some grand challenge questions regarding key technological gaps in photonics and optoelectronics (2012 National Research Council report). The success of this work will impact many quantum dot and thin-film optoelectronic applications, including thin film solar cells, high efficiency light emitting diodes (LEDs), ultrafast and sensitive detectors, to name a few. This project also leverages the fabrication, integration, and characterization capabilities at the Center for Integrated Nanotechnologies (CINT), a DOE national user facility.

Publications

Chen, H., C. C. Chang, A. J. Taylor, Z. Zhao, and S. Fan.
Achromatic linear-to-circular polarization conversion based on off-resonance reflective metasurfaces.
Submitted to *Science*. (LA-UR-18-31108)

Novel Algorithms for Large-Scale Ab-Initio Materials Simulations: Extending the Reach of Quantum Mechanics

Ondrej Certik
20180428ER

Project Description

The project significantly advances the capabilities of large-scale quantum mechanical materials calculations by developing, implementing, and applying a new class of real-space methods for solving the Kohn-Sham (KS) equations of Density Functional Theory (DFT). They will have broad applicability in condensed matter physics and molecular quantum mechanics by enabling ab initio quantum mechanical simulations of a wide range of large scale materials systems. They will also have the potential to be more efficient than the algorithms implemented in standard production codes like VASP and ABINIT, which are used for large-scale quantum-mechanical simulations using pseudopotentials. This would extend the applicability of Kohn-Sham pseudopotential DFT calculations to longer length and time scales in molecular dynamics, hence permitting new fundamental understanding and reliable prediction of macroscopic physical properties from ambient to extreme conditions. As such it advances mission challenges for agencies such as NNSA and has mission relevance to the Stockpile Stewardship Program, Explosives, lithium-ion batteries simulations (Commerce and Transportation and Renewable Energy) and others.

Publications

Benvenuti, E., A. Chiozzi, G. Manzini, and N. Sukumar. The eXtended Virtual Element Method for the Laplace equation with discontinuities and singularities. Formulation and preliminary results.. Unpublished report. (LA-UR-19-20877)

Certik, O., F. Gardini, G. Manzini, L. Mascotto, and G. Vacca. Design, analysis and numerical experiments for the virtual element p and hp approximations of elliptic eigenvalue problems. Unpublished report. (LA-UR-18-31762)

Gardini, F., G. Manzini, and G. Vacca. The nonconforming virtual element method for eigenvalue problems. Unpublished report. (LA-UR-18-20850)

- Manzini, G., E. Benvenuti, A. Chiozzi, and N. Sukumar. Numerical experiments with the extended virtual element method for the Laplace problem with strong discontinuities. Unpublished report. (LA-UR-18-23443)
- Manzini, G., G. Maguolo, and M. Putti. The high order mixed mimetic finite element method for time dependent diffusion problem. Submitted to *SIAM Journal on Numerical Analysis*. (LA-UR-17-28535)
- Manzini, G., L. Beirao da Veiga, and L. Mascotto. A posteriori error estimation and adaptivity in hp virtual elements. Submitted to *Numerische Mathematik*. (LA-UR-18-23445)
- Manzini, G., O. Certik, F. Gardini, and G. Vacca. The virtual element method for eigenvalue problems with potential terms on polytopal meshes. Submitted to *Applications of Mathematics*. (LA-UR-18-21436)
- Manzini, G., O. Certik, J. Droniou, and N. Sukumar. The gradient discretization framework for virtual element and partition of unity methods for the Schrodinger equation. Unpublished report. (LA-UR-18-29148)
- Manzini, G., P. F. Antonietti, and M. Verani. Design and convergence analysis of the conforming virtual element method for polyharmonic problems. Unpublished report. (LA-UR-18-29151)
- Manzini, G., and G. Vacca. Design, analysis and preliminary numerical results for the nonconforming VEM for parabolic problems. Unpublished report. (LA-UR-18-29150)

Methods and Algorithms to Account for Field Fluctuations Obtained by Homogenization in Solid Mechanics

Ricardo Lebensohn
20180441ER

Project Description

Los Alamos National Laboratory is a world leader in the theoretical formulation and numerical implementation of physically-based materials models of plasticity and failure of crystalline materials. We have pioneered the coupling of these models with numerical solutions based on Finite Elements (FE), resulting in numerical models at the engineering scale with sensitivity to the material's microstructure. These capabilities are part of the long-term objective of the Laboratory, critical to its stewardship mission. This project will explore one possible avenue to realize the theoretical and numerical counterparts of critical experiments related to the science of matter in extremes, crystalline material deformation with the goal of parameterizing and validating multiscale models. We will advance existing numerical tools, enabling mid-term practical applications to present problems faced by different experimental and modeling groups within the Laboratory.

Publications

- Knezevic, M., R. A. Lebensohn, R. J. McCabe, and M. Zecevic. Modeling of intragranular misorientation and grain fragmentation in polycrystalline materials using the viscoplastic self-consistent formulation. 2018. *International Journal of Plasticity*. 193-211. (LA-UR-18-23679 DOI: 10.1016/j.ijplas.2018.06.004)
- Lebensohn, R. A. Polycrystal plasticity models based on Green's functions: mean-field self-consistent and full-field Fast Fourier Transform formulations. To appear in *Handbook of Materials Modeling*. 1-27. (LA-UR-17-31125 DOI: 10.1007/978-3-319-42913-7_15-1)
- Lebensohn, R. A., E. Zepeda-Alarcon, N. Barton, and M. Messner. A Method for Including Diffusive Effects in Texture Evolution. To appear in *Journal of the Mechanics and Physics of Solids*. (LA-UR-18-23915 DOI: 10.1016/j.jmps.2019.01.016)
- Lebensohn, R. A., and A. D. Rollett. Spectral Methods for Full-Field Micromechanical Modelling of Polycrystalline Materials. Submitted to *Annual Review of Materials Research*. (LA-UR-18-28795)
- Luscher, D. J., and K. Bennett. Effective Thermoelasticity of Polymer-Bonded Particle Composites with Imperfect Interfaces and Thermally Expansive Interphases. To appear in *Journal of Elasticity*. (LA-UR-17-31014 DOI: 10.1007/s10659-018-9688-z)
- Pantleon, W., M. Zecevic, R. J. McCabe, R. A. Lebensohn, and M. Knezevic. Predicting intragranular misorientation distributions in polycrystalline metals using the viscoplastic self-consistent formulation. 2017. *Acta Materialia*. 398-410. (LA-UR-18-22506 DOI: 10.1016/j.actamat.2017.08.056)
- Ran, H., T. Riese, L. Evans, M. Finch, E. Gomez-Rivas, A. Griera, R. A. Lebensohn, M. Jessell, M. G. Llorens, S. Piazzolo, and P. Bons. Time for anisotropy: The significance of mechanical anisotropy for the development of deformation structures. 2018. *Journal of Structural Geology*. (LA-UR-18-23499 DOI: 10.1016/j.jsg.2018.04.019)
- Segurado, J., R. A. Lebensohn, and J. Llorca. Computational Homogenization of Polycrystals. 2018. *Advances in Applied Mathematics*. (LA-UR-18-23540 DOI: 10.1016/bs.aams.2018.07.001)
- Zecevic, M., R. A. Lebensohn, R. J. McCabe, and M. Knezevic. Modelling recrystallization textures driven by intragranular fluctuations implemented in the viscoplastic self-consistent formulation. To appear in *Acta Materialia*. 530-546. (LA-UR-18-27030 DOI: 10.1016/j.actamat.2018.11.002)

(U) Additive Re-Manufacturing Guided by Process and Hydrodynamic Modeling

John Carpenter
20180551ER

Project Description

This research is focused on understanding the applicability of additive techniques such as thermal spray for the remanufacture of non-nuclear material components within nuclear weapons. The application directly addresses current challenges in the safety, security, and reliability of nuclear weapons. Briefly, a simulation-based effort related to dynamic performance will inform the design of test objects built using thermal spray techniques. While performing the thermal spray trials, new data sets for the material-of-interest will be collected at conditions utilized in additive manufacturing. This will increase our understanding of this material and the data will also be used to form predictive process models. These predictive models will have impact both inside and outside the Laboratory by providing a more efficient route to the realization of the use of thermal spray on materials and applications. In addition to the novel materials science aspects, it is important to note that the work also will provide a window in a previously unexplored space in nuclear weapons design.

Publications

- Hollis, K. J., D. R. Jones, and B. M. Morrow. Gas Gun Flyer Plate Impact Testing of Stainless Steel Deposited by Low Pressure Plasma Spraying and Cold Gas Dynamic Spraying. Presented at *2019 International Thermal Spray Conference*. (Yokohama, Japan, 2019-05-26 - 2019-05-26). (LA-UR-19-20690)
- I. Stockman, T. J., J. Schneider, B. Walker, and J. S. Carpenter. A 3D Finite Difference Thermal Model Tailored for Additive Manufacturing. Submitted to *JOM*. (LA-UR-18-29322)

New Methods for Producing Stockpile Equivalent High Explosive Components

Gary Windler
20180605ER

Project Description

At present, the United States produces high energy (HE) components through a time- and labor-intensive process. A new process for HEs allows for enormous time and labor savings and provides an agility to prepare hundreds to thousands of parts with quick turnaround, a capability that does not exist now. The overall goal of this project is to prepare HE parts and demonstrate their equivalence to those made by current processes, through process parameterization and optimization. Based on preliminary tests on mock materials, we expect to be able to parameterize, better model, and optimize this process for HE. This innovation directly addresses the main DOE-NNSA mission of stockpile stewardship and surety, as it will provide the basis for rapid, agile production of non-nuclear HE weapon components in the future.

Target Projects in Theoretical and Experimental Materials Science: Novel Structural Models, Materials Imaging and Informatics, and Strength/Sensing Capabilities Integrated During Manufacturing

Filip Ronning
20160651ER

Project Description

We focus on developing new materials and design principles to enable better performance of batteries, computer memory, solar devices, and ultra light weight armor. Goals we aim to accomplish include: utilize adaptive feedback for faster 3D measurements of mesoscale materials; develop the computation capabilities to predict layered materials with emergent properties; develop methodologies to create 3D-printed fuel cell electrodes; develop techniques to create lighter than air solids; and develop novel memristors at vertical nanointerfaces with ultrahigh storage density.

Technical Outcomes

The rapid response program provides an agile response to capitalize on opportunities quickly, and in cases where funding is occasionally constrained. LDRD support provided training opportunities for new staff, and the ability to develop new capabilities in the area of materials science.

Publications

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Seo, S., E. D. Bauer, J. D. Thompson, P. Ferrari Silveira Rosa, S. M. Thomas, F. F. Balakirev, J. B. Betts, and M. Jaime. An FBG Optical Approach to Thermal Expansion Measurements under Hydrostatic Pressure. 2017. *Sensors*. (11) 2543. (LA-UR-17-28944 DOI: 10.3390/s17112543)

Depleted Uranium Oxides Photodiode

Igor Usov

20170143ER

Project Description

The project aims to address national security challenges and impact the DOE mission in several areas. First, discovery of a novel application for depleted uranium oxide (DUO), accumulated as part of the nuclear fuel cycle and nuclear weapons manufacturing, could significantly reduce the large stockpile of low-level nuclear waste and associated costs of its storage. In addition, it would position not only Los Alamos, but also US DOE and NNSA as leaders in innovative nuclear fuel cycle technologies and innovative utilization of nuclear materials. Our preliminary results also indicate that optoelectronics and electronics applications based on DUO have the potential to address numerous limitations of devices based on conventional semiconductors, such as poor stability and performance in high radiation and high temperature environments. This can lead to development of new technologies for national security (e.g., military, intelligence, reconnaissance, etc.) as well as other specialty applications, such as space exploration, robust electronics for nuclear and accelerator facilities, etc.

Technical Outcomes

This project brought about resurrection of the depleted uranium dioxide (DUO₂) thin film capability, expansion of the expertise in DUO₂ thin film fabrication, and advancement of the ion beam assisted thin film deposition process for semiconductor doping. This project also advanced our understanding about DUO₂ thin films properties and demonstrated a process suitable for fabrication of DUO₂ optoelectronic devices.

Meta-surface Enabled Passive Radiative Cooling

Matthew Reiten
20170357ER

Project Description

The "Meta-Cooler" concept will address national energy security by reducing resources and costs for maintaining a cooled environment for people, electronics, and possibly solar panels in locations exposed to the open sky. A low-cost radiative meta-surface cooler ("Meta-Cooler") will use low-cost engineered materials to reduce the temperature of structures below ambient temperature by enhancing thermal emission while reducing solar spectrum absorption. To circumvent the green house effect, which normally traps and reradiates thermal energy back at hot surfaces, the Meta-Cooler's thermal emissions will be vented into atmospheric "infrared windows." The extra heat will be radiated away into space. Low-cost materials and additive manufacturing will ultimately enable the scale-up of this proof-of-concept to widespread applications. The Meta-Cooler will have broad impact and a wide customer base, including commercial and residential structures and vehicle exteriors. It could assist in force sustainment and humanitarian efforts by reducing the logistics demands of cooling deployable shelters. External heat exchange units coated with Meta-Cooler surfaces could operate with increased efficiency generating significant cost savings.

Technical Outcomes

Initial lack of fabrication support pushed the meta-cooler team in new directions. Broader absorption from amorphous silica relaxes meta-surface tolerances. Photolithographic MC prototypes demonstrated enhanced absorbance in a laboratory setting and demonstrated cooling (~0.5 C) although not to anticipated levels (~10 C). Micro-contact transfer printing did not yield effective structures, but demonstrated the proof-of-concept. Two patent disclosures were initiated through the Feynman Center and a paper is under review for publication.

Publications

Azad, A. K., W. J. de Melo Kort-Kamp, S. Kramadhati, M. T. Reiten, and D. A. R. Dalvit. Passive Radiative "Thermostat" Enabled by Phase-Change Photonic Nanostructures. To appear in *ACS Photonics*. (11) 4554-4560. (LA-UR-18-25694 DOI: 10.1021/acsp Photonics.8b01026)

Pellet Cracking during Fabrication of Plutonium-238 Oxide Fuel

Adam Parkison
20170531ER

Project Description

The fabrication process currently utilized for the production of $^{238}\text{PuO}_2$ fuel pellets for radioisotope thermoelectric generators (RTG) has a 20-30% pellet failure rate, largely a result of pellet cracking during the fabrication process. This study will produce a MOOSE/BISON simulation of an off-stoichiometric surrogate system as well as the stoichiometric $^{238}\text{PuO}_2$ pellet/clad system.

Technical Outcomes

A computer model, PUMA, has been developed based on the MOOSE framework to simulate the fabrication process of $^{238}\text{PuO}_2$ heat source pellets. This development was aided by simultaneous experimental investigations, resulting in a rapid understanding of pellet behavior during fabrication. The results from this work will be applied to improving the fabrication process of $^{238}\text{PuO}_2$ pellets.

Publications

Matthews, C., and M. W. D. Cooper. PUMA: Plutonium Modeling and Analysis Theory Manual Rev 1.0. Unpublished report. (LA-UR-18-30520)

Parkison, A. J., A. D. R. Andersson, U. Carvajal-Nunez, F. A. Carver, M. W. D. Cooper, J. R. Harter, C. Matthews, H. M. Milenski, A. T. Nelson, S. S. Parker, M. J. Wilkin, N. Wozniak, and J. T. White. DEVELOPMENT OF THE PLUTONIUM MODELING AND ASSESSMENT (PUMA) SIMULATION THROUGH THE COUPLING OF EXPERIMENTS AND MOLECULAR DYNAMICS. Presented at *Nuclear and Emerging Technologies for Space*. (Richland, Washington, United States, 2019-02-25 - 2019-02-28). (LA-UR-18-31018)

Parkison, A. J., U. Carvajal Nunez, F. A. Carver, C. Matthews, and A. T. Nelson. UNDERSTANDING THE CAUSE OF PELLET FRACTURE DURING PRODUCTION OF PU-238 OXIDE HEAT SOURCES THROUGH THE COUPLING OF EXPERIMENTATION AND MODEL DEVELOPMENT. Presented at *Nuclear and Emerging Technologies for Space 2018*. (Las Vegas, Nevada, United States, 2018-02-26 - 2018-03-01). (LA-UR-18-21304)

Direct Electrolytic Reduction of Plutonium Oxide Surrogates

Jay Jackson
20170558ER

Project Description

We are developing an electrochemical method to produce plutonium metal in support of a laboratory mission. Our less labor intensive, more efficient and safer process will result in large cost savings and contaminated waste reduction. This project will simultaneously provide valuable data to programs interested in characterization and detection, as well as science of signatures. Additionally, developing the capability in the plutonium facility will facilitate future safeguard studies that can assist with safeguard development in molten salt reprocessing flowsheets, and molten salt reactor designs.

Technical Outcomes

This effort resulted in advances with regards to fundamental understanding, and practical implementation of electrolytic oxide reduction technology. Milestones included the commissioning of a molten salt electrolytic cell capable of collecting precise cyclic voltammetry measurements as well as performing bulk electrolysis experiments. Technology viability was determined through the successful reduction of tin oxide, and optimized through ceria reduction experiments. Progress was made towards plutonium trials, currently slated for execution next year supported by programmatic funding.

Publications

Chen, C. F., D. A. T. Rodriguez, K. R. Weisbrod, M. J. Monreal, E. L. Tegtmeier, and J. M. Jackson. Processing and Characterization of Polycrystalline CaRuO₃ Ceramic. Submitted to *ECS Journal of Solid State Science and Technology*. (LA-UR-18-29205)

Jackson, J. M., M. J. Monreal, K. R. Weisbrod, D. A. T. Rodriguez, and M. F. Simpson. Electrolytic Oxide Reduction of Plutonium Oxide Surrogates. Unpublished report. (LA-UR-18-29391)

Weisbrod, K. R. Electrolytic Oxide Reduction Process / Small Scale EOR Cell. Unpublished report. (LA-CP-18-20051)

Insensitive High Explosives using 3-picrylamino-triazole (PATO)

Philip Leonard
20170587ER

Project Description

The development of insensitive high explosives (IHE) that can replace existing explosives in nuclear and other weapon systems is essential in order to improve the safety of US assets without compromising effectiveness. The challenge of generating consistent explosive formulations over decades from domestic materials has driven us to explore new explosives and binders that benefit from economy as well as safety and effectiveness; picrylamino-triazole (PATO) is an excellent material example of these characteristics.

Technical Outcomes

This project demonstrated PATO formulations have good safety and performance characteristics. If challenges involving morphology can be overcome, then PATO would be an attractive alternative to Triaminotrinitrobenzene (TATB) as the result of rapid synthesis, good safety, detonability, and energy density. Due to the modest response of PATO to both high heat and flame, the success achieved in SDT testing strongly implies that this material will succeed in full IHE qualification testing.

Publications

Leonard, P., P. R. Bowden, M. Shorty, and M. M. Schmitt.
Synthesis and Evaluation of 3-Picrylamino-1,2,4-Triazole (PATO) Formulations. To appear in *Propellants, Explosives, Pyrotechnics*. (LA-UR-17-29104 DOI: 10.1002/prep.201800144)

Watt, G. L. Examination of the Formulation and Suitability of CL-20/HMX Cocrystal. Unpublished report. (LA-UR-17-31317)

In Situ Quantification and Characterization of Phase Evolution during Metal Additive Manufacturing

John Carpenter
20170641ER

Project Description

Using a Los Alamos built experimental rig, additive manufacturing will be conducted in a high energy beamline with the x-rays providing diffraction data that will help us understand how the metal is cooling and solidifying. The time and length scales we will be achieving experimentally are significant improvements over earlier experiments and will exploit the cutting edge available in detectors and diagnostics to achieve these improvements. The data obtained will both motivate and inform microstructural evolution models which do not currently exist because of the dearth of experimental data at the correct time and length scales. With these models in hand, we could potentially exploit the additive manufacturing process to create materials with microstructures that exhibit enhanced properties and performance. In addition, this information is critical for understanding the science behind using additive manufacturing as a repair or refurbishment technology for components important to programmatic missions within the NNSA.

and Components, ASTM International. (Atlanta, Georgia, United States, 2017-11-13 - 2017-11-13). (LA-UR-17-28223)

Technical Outcomes

The goal was to obtain quantitative phase fractions (diffraction) and phase morphology on the mesoscale (SAXS) with 0.01 second resolution during solidification and cooling following deposition in relevant additive manufacturing processes for a stainless steel and a titanium alloy using an innovative in situ set-up within APS. This project achieved this goal and acquired data points every 0.005 seconds while providing detail for solid/liquid phase fraction as well as solid phase fraction evolutions.

Publications

Brown, D. W., J. S. Carpenter, B. Clausen, J. C. Cooley, M. A. M. Bourke, A. S. Losko, and P. Kenesei. Time Evolution of Phases Stresses During Additive Manufacture of 304L Stainless Steel. Presented at *Symposium on Fatigue and Fracture of Additive Manufactured Materials*

Light-Driven Nonlinear Phenomena in Weyl and Dirac Semimetals

Rohit Prasankumar
20180146ER

Project Description

Three-dimensional topological materials, known as Dirac and Weyl semimetals, have attracted much attention recently due to the fascinating phenomena they exhibit, as well as their potential for applications in quantum computing, information, and sensing. We have recently used light to probe novel effects in these materials, such as strong coupling between Weyl fermions (electrons in these materials) and lattice vibrations. However, intense, ultrashort light pulses have arguably more potential for studying these materials; theoretical predictions have shown that second harmonic generation, in which intense light pulses interact with a material to generate light at twice the frequency (e.g., red light turns into blue light), can exhibit signatures of new quantum phenomena intrinsic to these systems. Here, we will use second harmonic generation to probe various quantum effects predicted to occur in Weyl semimetals, which give insight into their unique properties and could enable them to be optimized for future applications. Furthermore, intense light pulses can potentially be used to control these effects, enabling applications in ultrafast switching and information. These studies thus have great potential for extending our understanding of topological materials, directly impacting Department of Energy interests in quantum materials and computation beyond Moore's law.

Technical Outcomes

This work has shown that nonlinear optical techniques are a powerful tool for shedding new light on the properties of Weyl semimetals. We have revealed a new transient photoinduced phase using time-resolved second harmonic generation and also used THz emission to detect the circular photogalvanic effect in TaAs and NbAs, demonstrating that ultrashort optical pulses can both drive and probe novel phenomena in these systems.

Engineered Functionality and Structural Hierarchy in Additively Manufactured Materials

Matthew Lee
20180588ER

Project Description

This project addresses the current national security challenge of developing new advanced manufacturing methods for non-SNM (special nuclear material) nuclear explosive package components, including functional plastics and ceramics with controlled physical and chemical properties. The goals of the research include (1) demonstrating control over the mechanical properties of 3-D printed plastics and foam materials using a model-driven approach where theory and experiment are coupled within a robust feedback loop, and (2) interlacing desired functionalities such as electrical/thermal conductivity or neutron reflectivity into 3-D printed composite objects. A successful project would create a new materials development paradigm for the nuclear weapons complex and enable the production of new materials that simply did not exist before now, together ensuring the future reliability and security of the enduring stockpile. In addition, this work will be directly translatable to other research areas pertinent to the DOE, including materials for novel energy technology (e.g. catalysis, supercapacitors, high performance batteries), sensing and surveillance, and waste heat recovery.

Technical Outcomes

Through stereolithography 3-D printing, this project demonstrated moderate control over the mechanical properties of printed materials and began to develop a deterministic model. Simultaneously, we interlaced desired functionalities such as conductivity, magnetism, and selective reactivity into 3-D printed composite objects, which will be directly translatable to other research areas pertinent to the DOE.

Solution Processible Laser Diodes Based on Engineered Quantum Dots with Suppressed Auger Recombination

Victor Klimov
20180654ER

Project Description

Since the invention of epitaxially-grown semiconductor laser diodes, these devices have become ubiquitous in our daily life and can be found in applications ranging from barcode readers to optical communication and eye surgery. Chemically synthesized quantum dots (QDs) can potentially enable a new class of highly flexible laser diodes processible from solutions without complications associated with vacuum-based epitaxial techniques. Despite a considerable progress over the past years, colloidal-QD lasing, however, is still at the laboratory stage, and an important challenge - realization of lasing with electrical injection - is still unresolved. The progress in this field has been hindered by fast nonradiative Auger recombination of gain-active multi-carrier species. In this project, we propose to combine recent advances in "Auger-decay-engineered" QDs with novel architectures for high-current-density light emitting diodes for demonstrating for the first time a lasing regime in solution-processed electroluminescent structures. The success of the proposed work will open exciting opportunities for realizing new types of low-threshold lasing devices that can be fabricated from solution using a variety of substrates and optical cavity designs for applications ranging from fiber optics and large-scale lasing arrays to laser lighting and lab-on-a-chip sensing technologies.

Technical Outcomes

This project demonstrated for the first time optical gain in colloidal quantum dots (QDs) excited by electrical current. Two key advances leading to this demonstration are the new generation of compositionally graded QDs with suppressed "parasitic" Auger recombination and a special "current-focusing" device architecture that allows for obtaining ultrahigh current densities. These studies bring us considerably closer to the important goal of practical realization of solution-processible laser diodes.

Park, Y. S., K. Wu, H. J. Yun, V. I. Klimov, and J. Lim. Droop-Free Colloidal Quantum Dot Light-Emitting Diodes. To appear in *Nano Letters*. (10) 6645-6653. (LA-UR-18-28788 DOI: 10.1021/acs.nanolett.8b03457)

Publications

Spin-Orbit Materials for Quantum Information

Filip Ronning
20180656ER

Project Description

We now have a good understanding of quantum mechanics and how it describes the world around us. We've used this knowledge to improve our daily lives—computers, portable electronics, cell phones, etc. We have only just begun to explore a completely new paradigm: controlling quantum mechanics in novel ways, called the “2nd Quantum Revolution”, to solve looming societal problems such as a global energy crisis, and to protect our Nation from threats or foreign influence. Entirely new quantum information technologies that harness the unique collective effects of quantum mechanics and collective novel states of matter hold exceptional promise for energy-efficient quantum computing to help solve the imminent failure of Moore's Law, quantum cryptography and algorithms to bolster our national security, and quantum photonics and spintronics for unparalleled optical sensors or communication. This work will provide a foundation for future development.

Technical Outcomes

This project demonstrated that the size of the anomalous Hall effect could be tuned with uniaxial strain and doping in the antiferromagnetic manganese tin material, Mn_3Sn . We also performed detailed measurements of the spin wave spectrum on the skyrmion lattice material manganese silicide. Both results will help us understand how anomalous transport properties arise in novel spin-orbit coupled quantum materials.

Artificial Intelligence for Materials Design

Turab Lookman
20180660ER

Project Description

A large fraction of activity and resources in materials genome work in the US and elsewhere have been focused on generating large databases in a high throughput manner using electronic structure codes. The rationale behind this paradigm is to “down select” promising compounds, in contrast to the AI approach which involves an active learning loop starting from an initial data set, typically from experiments. However, little work exists in determining the value and quality of these databases (e.g. materialsproject.com, OQMD or AFLOWLIB). Why should an experimentalist go to such a database to select a possible compound for synthesis if there have been virtually no comparisons of predictions from such databases (that contain output from T=0 codes) of “promising” compounds with desired properties to those from experimental data? Here it is proposed to undertake such a study for a given materials class, namely, the prediction of new stable, perovskite compounds not synthesized previously. These materials have important applications in energy storage and harvesting.

Technical Outcomes

The key finding is that major differences exist in the predictions of compounds from data bases, such as the Open Quantum Mechanical Database (OQMD) we utilized, compared to using Artificial Intelligence (AI) based on experimental data. The agreement is only to the 60% level. However, interestingly, both approaches predict the formability of the same 87 new compounds (including actinides and Lanthanides). Therefore, these represent the most promising compounds for future experimental synthesis.

Publications

Gubernatis, J. E., and T. Lookman. Use of Machine Learning in Materials Design and Discovery: Examples from the Present and Suggestions for the Future.. Submitted to *Physical Review M*. (LA-UR-18-29277)

Watching Nucleation Dynamics of Complex Electronic and Magnetic Phases in Space and Time

Constantine Sinnis
20180661ER

Project Description

The research vision brings together two ultrafast optical techniques for the first time to image in time and space the evolution of electronic and magnetic phases in materials. The resultant techniques are broadly applicable to a wide range of material classes and device architectures and will allow the measurement of spatially dependent order parameters, on length scales spanning 10s of nanometers to many microns, and their temporal dynamics on timescales ranging from femtoseconds to milliseconds.

Technical Outcomes

This project achieved initiation and development of magnetic imaging experiments using the high harmonic generation scheme based in the LUMOS at TA-35. Initiated and completed a measurement of chiral ultrafast currents in Weyl semimetal materials. Analyzed data and wrote two papers base on work from Groningen, which include a LANL affiliation. Supported the writing of PhD theses of two of my students. Applied, unsuccessfully, for beamtime at LCLS. Applied, successfully, for a CINT user proposal.

Publications

Chang, C. L., R. I. Tobey, S. Mieszczak, M. Zelent, V. Besse, U. Martens, R. Tamming, J. Janusonis, P. Graczyk, M. Munzenberg, and J. Klos. An on-demand magnonic crystal induced by an optical interference pattern. Submitted to *Physical Review Applied*. (LA-UR-18-25297)

Chang, C. L., R. Tamming, T. Broomhall, J. Janusonis, P. Fry, R. I. Tobey, and T. Hayward. Selective Excitation of Localized Spin Wave Modes by Optically Pumped Surface Acoustic Waves. Submitted to *Physical Review Applied*. (LA-UR-18-26529)

X-ray Bragg Coherent Diffraction Imaging from Complex Oxide Nanostructures

Constantine Sinnis
20180665ER

Project Description

This project explores the feasibility of creating oxide based nanocapacitors that could be later integrated into or could replace the conductive channels in complementary metal–oxide–semiconductor (CMOS)-based devices. We will focus on perovskites and multiferroics nanostructures, where formation of complex topologies and configurations of electric and magnetic polarization can accommodate stress release. To map the order parameters such as strain, the morphology and evolution of the electronic, optical and transport properties in nanocapacitors, will be probed using X-ray Bragg coherent diffraction imaging (BCDI) and neutron scattering probes. During this project, the design of a periodic array of nanocapacitors will not only help improve CMOS technology but could also advance quantum computation and storage technologies if the vortex phase in each individual nanostructure can be controlled to achieve quantum coherence.

Technical Outcomes

This project used coherent X-ray sources to develop lensless Bragg Coherent Diffractive Imaging (BCDI) techniques for correlated electron materials. The goal was to understand the structure property relationship in complex oxide nanostructure materials under the application of an external electric field. The result of this project provides phase retrieval algorithms for highly strained materials under external fields and understanding of emergent topological phases in complex oxides.

Accelerated Microstructure Reconstruction from High-Energy X-ray Diffraction Data Collected at Light Sources

Reeju Pokharel
20180677ER

Project Description

DOE/NNSA missions heavily rely on the use of advanced light sources for material science studies. High energy diffraction microscopy (HEDM) is a novel non-destructive imaging technique at the mesoscale (microns) for 3Dimensional samples that provides both crystallographic orientations at ~ 0.01 deg resolution and grain-averaged strain data. Because it is non-destructive, HEDM allows the study of the evolution of polycrystalline materials and their response to external stresses. The work is extremely important for material science in general and for DOE/NNSA missions which rely on an accurate ability to simulate and predict materials behavior at the mesoscale, under extreme conditions. One of the main limitations of HEDM is that the reconstruction process is extremely computationally intensive, requiring millions of central processing unit (CPU) hours. The goal of this project is to significantly accelerate the 3Dimensional HEDM reconstruction process at rates which could allow for real time feedback during experiments. This task is currently not possible even with dedicated 1024 core computers on which the current brute force reconstruction techniques take dozens of hours.

diffraction using convolution neural nets. Submitted to *Acta Materialia*. (LA-UR-18-28515)

Technical Outcomes

A convolutional neural network framework was developed which could use large amounts of easily available simulation data to learn how to map diffraction images to crystal orientations. Several of the initial layers of these networks were then re-tuned utilizing small amounts of experimental data and were then able to accurately and quickly (3000x speed increase over state-of-the-art methods) reconstruct crystal orientations from diffraction images.

Publications

Shen, Y. F., R. Pokharel, A. Kumar, T. J. Nizolek, and T. Lookman.
Real time orientation indexing for electron backscatter

In-situ Measurements of Strain at X-ray Light Sources within Irradiated Microstructures

Richard Sandberg
20180683ER

Project Description

Understanding how radiation damages materials and ultimately leads to their failure is crucial to many areas including nuclear energy, infrastructure lifetimes, and the nuclear weapons stockpile stewardship. In order to be able to design better materials, for say automobiles and bridges, we must understand what limits their lifetime. Radiation damage is one potential precursor for materials damage that can lead to failure of the materials. Our proposed technique will develop the tools necessary to first image at near atomic resolution the effects of radiation damage that will then lead to the understanding necessary to design better materials.

Technical Outcomes

This project performed two groundbreaking experiments with x-rays at the Advanced Photon Source: 1) nanometer scale strain imaging in a metal foil while being pulled and 2) imaging of radiation damage in copper nanocrystals. The work developed a tool that enables understanding of where and why metals begin to fail under extreme conditions. Developing this nanometer strain imaging of metals is a first step to designing materials that can tolerate increasingly harsh environments.

Publications

Sandberg, R. L., S. J. Fensin, R. Pokharel, M. J. Cherukara, J. K. S. Baldwin, T. S. O'Leary, W. Cha, E. Maxey, R. J. Harder, and J. Maser. Three-dimensional X-ray diffraction imaging of dislocations in polycrystalline metals under tensile loading. 2018. *Nature Communications*. (1) 3776. (LA-UR-18-28692 DOI: 10.1038/s41467-018-06166-5)

Multi-branch X-ray Split and Delay

Dinh Nguyen
20180684ER

Project Description

A single-shot/single-target platform, proposed here, will yield time-resolved data with higher resolution (at least four-fold or better) and therefore gather more accurate kinetics information and stereoscopic imaging, from which vastly improved material models and predictive capabilities will follow. This project directly addresses the call for new experimental tools to elucidate mesoscale materials phenomena and achieves the technical functional requirements to probe shocked samples at sub-ns intervals.

Technical Outcomes

This project successfully built, tested and benchmarked the first hard X-ray (11.5-keV) split-and-delay optics with a static, sub-nanosecond delay suitable for high-resolution shock physics studies. This unique X-ray diagnostic can follow the passage of a compressive wave through a single target and detect changes in the material properties with unparalleled temporal and spatial resolution. The new multi-branch X-ray split-and-delay technique will enable the next generation of dynamic compression kinetics experiments on X-ray FELs.

In-situ Studies of Hydriding and Transport of Hydrogen through Plutonium Dioxide

Erik Watkins
20180708ER

Project Description

This work will have immediate impact on our understanding of hydriding and hydrogen transport through plutonium oxide, which is of great interest to its aging and waste storage. The work will also have a direct impact on polymer assisted deposition of thin films and other surface science studies that are currently being done on such films.

Technical Outcomes

The research objective is the in-situ study of the role that interfaces and defects play in hydriding and hydrogen transport in actinide oxides, particularly PuO₂. A better understanding of these mechanisms is needed to predict the behavior during aging and storage of plutonium waste^{1,2}. Designing and commissioning of an UHV sample chamber that will allow to study hydrogen diffusion through PuO₂ under a range of pressures and temperatures is an important part of this project.

Elucidating the Unexpected High Temperature Strength of Additively Manufactured Ferritic/Martensitic Steels

Stuart Maloy
20180726ER

Project Description

Grade 91 steels (Gr 91) are used broadly in the nuclear energy and fossil energy applications because of their strength at elevated temperatures, corrosion resistance, adequate ductility and toughness. Our recent results show that Gr 91 samples produced using laser-powder bed additive manufacturing (AM) possess improved strength at room temperature and elevated temperatures up to 600 C. The proposed research will determine the microstructural features responsible for these improved properties, and the evolution and high temperature stability of the features. The expected outcomes from this project include a fundamental understanding of the microstructure/mechanical property relationships in AM Gr 91 alloys over the range of applicable operating temperatures. These advances could lead to improved material capabilities for advanced nuclear energy plants, recuperator and heat exchanger components for numerous energy applications (including fossil energy), or for repairing cracks where similar steels are presently being used.

Technical Outcomes

Excellent progress was made at understanding and quantifying the stability of as-deposited additively manufactured grade 91. Minor changes were observed in the microstructure after 600 and 700C treatments. The effects of heat treatment up to 700C on the mechanical properties resulted in increased in yield stress at room temperature with only small reduction in ductility. New materials were produced with the same microstructure by a different company using the same manufacturing parameters.

Informatics Based Design of Low-dimensional Materials

Alejandro Lopez-Bezanilla
20180736ER

Project Description

Although the Materials Genome initiative, issued by the White House Office of Science and Technology Policy in 2011, catalyzed interest in accelerated materials discovery, very little has been done in the class of materials belonging to the actinide and lanthanide subclass. This research is part of the Lab's effort to expand the discovery of a class of new materials that, entailing important technical and safety issues for their treatment, are ideally suited for Los Alamos activities. This proposal is in line with work supported by the Lab's Nu-clear Deterrence and Energy Security mission areas and the Information, Science, and Technology and Materials for the Future science pillars. Exploring the physics and chemistry of actinide materials has been a priority of Los Alamos National Lab since its founding 75 years ago. Through the exploration of actinide/lanthanide materials, Los Alamos pursues the discovery science and engineering required to establish design principles, synthesis pathways, and manufacturing processes for advanced and new materials to intentionally control functionality relevant to the Lab's national security mission

Lopez-Bezanilla, A. Interplay between p- and d- orbitals yields multiple Dirac states in one- and two-dimensional CrB₄. To appear in *2D Materials*. (3) 35041. (LA-UR-18-28578 DOI: 10.1088/2053-1583/aac9f9)

Technical Outcomes

Theoretical evidence of the existence of Dirac fermions in a uranium compound was provided. The interaction in a honeycomb lattice of uranium f-orbitals with a delocalized network of p-orbitals from boron atoms allows UB₄ to exhibit Dirac cones. The contribution of f-orbitals to their formation is determined beyond the theoretical approximation used. The origin of the itinerant electronic states of atomic-thick layers is ascribed to the interplay between f- and p-orbitals of the different atoms.

Publications

Lopez-Bezanilla, A. Parameter transferability, self-doping, and metallicity in LaNiO₃ /LaMnO₃ superlattices. Submitted to *Physical Review B*. (LA-UR-18-28837)

Phase Transformation in Magnesium at Ultra-high-pressure

Nitin Daphalapurkar
20180738ER

Project Description

Physics and engineering models are crucial for science-based stockpile stewardship. Materials models in DOE shock codes, with application to nuclear stockpile stewardship, are increasingly required to be predictive under ultra-high-pressure environments. An approach to improve the predictive ability is to incorporate mechanisms of deformation at micrometer and smaller length scales. This project develops fundamental understanding on the physics of phase transformation at the atomistic scale in response to shock loading in magnesium metal.

Technical Outcomes

The project enabled identification and understanding of key constitutive response at the atomistic length scale. Accomplishments of this project were: (1) demonstrated the feasibility of simulating the thermodynamically well-characterized HCP to BCC phase transition using a realistically accurate intermolecular potential for pure magnesium; (2) characterized the kinetics of phase boundary using molecular dynamics simulations; (3) investigated the critical pressure for phase transformation in presence of a shear stress.

Publications

Knutsen, A., J. Glaister, Y. C. Lu, N. P. Daphalapurkar, J. Prince, P. Bayly, D. Pham, J. Butman, and K. Ramesh. A 3D Computational Head Model Under Dynamic Head Rotation and Head Extension Validated Using Live Human Brain Data, Including the Falx and the Tentorium. *Annals of Biomedical Engineering*. (LA-UR-19-20972 DOI: 10.1007/s10439-019-02226-z)

Understanding the Magnetic Properties of Heavy Fermion Materials

Shizeng Lin
20170539ECR

Project Description

Heavy fermion materials have generated much excitement due to their exotic properties and potential for novel functionalities. This work directly addresses the Grand Challenge in Materials, which underpins all three Laboratory mission areas. The goal of this project is to understand the magnetic properties of the heavy fermion materials. Specifically, we will develop theories to describe the magnetic properties in these prototypical quantum materials.

Publications

- He, M., G. Li, Z. Zhu, Y. Zhang, L. Peng, R. Li, J. Li, H. Wei, T. Zhao, X. G. Zhang, S. Wang, S. Lin, L. Gu, G. Yu, J. Cai, and B. G. Shen. Evolution of topological skyrmions across the spin reorientation transition in Pt/Co/Ta multilayers. 2018. *Physical Review B*. (17) 174419. (LA-UR-18-24332 DOI: 10.1103/PhysRevB.97.174419)
- Kim, T., C. C. Chien, and S. Lin. Re-entrant Fulde-Ferrell-Larkin-Ovchinnikov State in Small-Sized Superconductors. Submitted to *Physical Review B*. (LA-UR-18-30667)
- Lin, S. Annual reports for IC projects. Unpublished report. (LA-UR-18-21212)
- Lin, S., J. Zhu, and A. B. Saxena. Kelvin modes of a skyrmion line in chiral magnets and the associated magnon transport. Submitted to *Physical Review B*. (LA-UR-19-20239)
- Lin, S., S. M. Thomas, and P. Ferrari Silveira Rosa. Design principles for skyrmions in f-electron materials. Unpublished report. (LA-UR-19-21423)
- Lin, S., and Y. Su. Pairing symmetry and spontaneous vortex-antivortex lattice in superconducting twisted-bilayer graphene: Bogoliubov-de Gennes approach. 2018. *Physical Review X*. (19) 195101. (LA-UR-18-26090 DOI: 10.1103/PhysRevB.98.195101)
- Lin, S., and Y. Su. Nontrivial topology and localization in the double exchange model with possible applications to perovskite manganites. 2018. *Phys. Rev. Lett.* (23) 235116. (LA-UR-18-29965 DOI: 10.1103/PhysRevB.98.235116)

High Resolution Laser Velocimetry and Ranging for Materials Research

Patrick Younk
20170541ECR

Project Description

With this project, we are developing new technology that will significantly increase the resolution of our laser systems that measure velocity and position in dynamic experiments. This new technology will enhance our capability to perform dynamic experiments relevant to stockpile stewardship and possibly other national security challenges.

New Nanomaterials with Confined Oxide/Metal Interfaces for Flexible Electrodes

Aiping Chen
20170610ECR

Project Description

Flexible electronics have a huge impact on many applications, from health care to wearable devices. The goal of this project is the design and synthesis of new electrodes with high optical transmission, electrical conductivity, and mechanical stress for the future electronics. This directly addresses the laboratory's grand challenge in materials science. This research not only advances the fundamental understanding of oxide/metal deformation mechanisms, it further provides a unique approach to integrate enhanced mechanical performance and functional properties for applications in future flexible electronics. This research will enable the flexible sensors and functional devices for wearable applications from daily life to the battlefield.

Publications

- Chen, A., Q. Su, H. Han, E. Enriquez, and Q. Jia. Metal Oxide Nanocomposites: A Perspective from Strain, Defect, and Interface. To appear in *Advanced Materials*. 1803241. (LA-UR-18-28283 DOI: 10.1002/adma.201803241)
- Li, M., Y. Wang, A. Chen, A. Naidu, B. S. Napier, W. Li, C. L. Rodriguez, S. A. Crooker, and F. G. Omenetto. Flexible magnetic composites for light-controlled actuation and interfaces. 2018. *Proceedings of the National Academy of Sciences*. (32) 8119-8124. (LA-UR-18-28365 DOI: 10.1073/pnas.1805832115)
- Wang, Q., A. Chen, E. Guo, M. A. Roldan, M. Varela, Q. Jia, and M. Fitzsimmons. Upper limit for the effect of elastic bending stress on the saturation magnetization of. 2018. *Physical Review B*. (1) 014437. (LA-UR-18-28583 DOI: 10.1103/PhysRevB.97.014437)
- Zhang, Y., L. Shen, M. Liu, X. Li, X. Lu, L. Lu, C. Ma, A. Chen, C. Huang, L. Chen, and C. L. Jia. Flexible Quasi-Two-Dimensional CoFe₂O₄ Epitaxial Thin Films for Continuous Strain Tuning of Magnetic Properties. Submitted to *ACS Nano*. (LA-UR-18-28697)

Excited State Dynamics for Spin Systems

Tammie Nelson
20180552ECR

Project Description

This project will use and develop nonadiabatic excited state molecular dynamics, a software package acknowledged by NNSA for open source, to provide novel computational capabilities critical for understanding light-induced dynamics in many technologically relevant materials. The developed capabilities will have extremely broad applications relevant to the current and future Laboratory/DOE missions, particularly benefitting the primary goal of the Materials for the Future focus area and in the future modeling of materials important for the Laboratory core mission, such as explosives. The project will develop a new computational capability that can be applied to advance modeling of photostability and photodegradation, and spin-crossover induced sensitivity changes in new classes of explosive materials. The high level goals of the project are to develop a modeling capability to describe the spin dynamics in realistic materials and to apply the capability for the prediction, control and design of specific material properties.

2018. *Nature Communications*. (1) 2316. (LA-UR-17-30143 DOI: 10.1038/s41467-018-04694-8)

Nelson, T. R., S. Tretiak, Y. Zhang, and L. A. Lystrom. Site-Specific Photodecomposition in Conjugated Energetic Materials. To appear in *The Journal of Physical Chemistry A*. (29) 6055-6061. (LA-UR-18-24161 DOI: 10.1021/acs.jpca.8b04381)

Sifain, A. E., B. J. Gifford, L. A. Lystrom, D. W. Gao, T. R. Nelson, and S. Tretiak. NEXMD Modeling of Photoisomerization Dynamics of 4-Styrylquinoline. Submitted to *Journal of Physical Chemistry A*. (LA-UR-18-28405)

Publications

Nelson, T. R. Excited State Dynamics for Spin Systems. Unpublished report. (LA-UR-18-25372)

Nelson, T. R., S. Fernandez Alberti, A. Roitberg, and S. Tretiak. Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. 2017. *The Journal of Physical Chemistry Letters*. (13) 3020-3031. (LA-UR-17-23765 DOI: 10.1021/acs.jpcllett.7b00790)

Nelson, T. R., S. Tretiak, D. O. Alvarez, S. Fernandez-Alberti, and J. M. Lupton. Let Digons be Bygones: The Fate of Excitons in Curved pi-systems. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-18-29242)

Nelson, T. R., S. Tretiak, D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. Jalindo, V. Kleiman, S. Fernandez-Alberti, and A. Roitberg. Coherent exciton-vibrational dynamics and energy transfer in conjugated organics.

Hybrid Density Functional Theory

Travis Sjostrom
20180613ECR

Project Description

This proposal is primarily motivated by a pressing need to understand and predict the basic properties of matter in the so-called warm dense matter regime. Under these extreme conditions materials properties are often difficult to measure and manipulate in well-controlled experiments and a reliable theoretical support is needed. These properties, such as the equation of state and transport properties, are critical for modeling in astrophysics, inertial confinement fusion, and weapons physics, making the ability to simulate and predict materials properties of particular importance. Our approach does not lead to the prohibitive computational scaling cost of the conventional numerical implementations, and is amenable to temperatures and pressures that are presently inaccessible by current approaches. Los Alamos has a prime interest in the materials properties of warm dense matter in terms of application to various programs. This will be the first ab initio method to bridge ambient to plasma conditions and will significantly enhance the theoretical characterization of high-energy density materials and matter in extreme conditions.

Probing Quantum Fluctuations via Thermal Expansion Measurements under Pressure

Priscila Ferrari Silveira Rosa
20180618ECR

Project Description

This project will investigate quantum fluctuations by the development of thermal expansion measurements under pressure. This theme directly addresses the Laboratory's vision of Materials for the Future by providing the science required to discover, understand and ultimately control complex and collective forms of matter. As outlined in the DOE/BES Basic Research Needs report, quantum matter specifically is the next frontier for realizing this vision and has exceptional potential to revolutionize energy relevant technologies. Not only addressing a fundamental problem of immediate scientific importance that underlies an ability to anticipate new quantum states, this project also develops a new capability of thermal expansion measurements under extreme conditions that will enable understanding and control of new materials and new physics that may emerge in the future.

Publications

Ferrari Silveira Rosa, P., S. M. Thomas, F. F. Balakirev, E. D. Bauer, J. D. Thompson, R. Fernandes, M. Jaime, and F. Ronning. Enhanced hybridization sets the stage for electronic nematicity in CeRhIn5. Submitted to *Physical Review Letters*. (LA-UR-18-30371)

Overdriven Shock and Initiation Effects on Detonator-Scale Energetic Materials

Kathryn Brown
20180633ECR

Project Description

One of the missions of Los Alamos National Laboratory is the development of new primary detonators for our nuclear stockpile. Research and development of new detonators is costly and time-consuming, and relevant physics data, including velocity and shock wave propagation, on the detonator scale is currently unavailable to the scientists that model old and new detonators. This project seeks to develop a rapid throughput detonator test bed by using a laser-driven configuration rather than an electrically-driven configuration. The use of high-speed imaging diagnostics will characterize explosive material that has been overdriven to detonation.

Publications

Brown, K. E., K. J. Ramos, and S. D. Mcgrane. Considerations for Ultrafast Spectroscopy on Shocked Explosives: Preliminary Investigations into using the Explosive as Impactor. Submitted to *Proceedings of the 2018 International Detonation Symposium*. (LA-UR-18-29489)

Brown, K. E., K. J. Ramos, and S. D. Mcgrane. Considerations for Ultrafast Spectroscopy on Shocked Explosives: Preliminary Investigations into using the Explosive as Impactor. Presented at *16th International Detonation Symposium*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-15). (LA-UR-18-25798)

Brunell, A. Internship After Action Review (AAR). Unpublished report. (LA-UR-18-26605)

Brunell, A. Internship Review Essay. Unpublished report. (LA-UR-18-26606)

Formation, Stability, and Chemistry of Tetravalent Actinide Nanocrystals

Ping Yang
20160604ECR

Project Description

This project directly addresses a widely known scientific problem of understanding the fundamental bonding interactions involved with 5f-electrons in order to master the chemistry and physics of actinides and actinide-bearing materials. The long-term goal of this project is to build the knowledge foundation of structures, energetics, and chemical and physical characteristics of tetravalent actinide nanocrystals as a function of particle size, composition, and surface ligands, using a novel high-performance computational framework. Understanding, predicting, and controlling their formation and chemical reactivity is crucial to improve the efficiency of the nuclear fuel cycle, long-term management of nuclear waste, and assessment of contaminated sites.

to PCCP. *Physical Chemistry Chemical Physics*. (LA-UR-17-31042)

Technical Outcomes

This project has built knowledge foundation of structures, energetics, and chemical and physical characteristics of tetravalent actinide NCs using a novel high-performance computational framework. The team has searched global minima of the nanocrystalline cores of ThO₂, identified the structural-stability relations, as well as understood the interfacial chemistry between NCs and surface ligands that control the morphology of NCs. The knowledge gained will provide guiding principles for controlling the formation and stability of actinide oxide NCs.

Publications

- Aguirre Castiblanco, N. F., J. C. A. O. Jung, and P. Yang. First-Principle Study of Structure and Stability of Thorium Dioxide Nanoclusters, Th_nO_{2n} (n = 1 – 8). Submitted to *ACS Nano*. (LA-UR-18-29967)
- Wang, G., E. R. Batista, and P. Yang. Nature of excess electrons on reduced AnO₂ (111) surfaces (An = Th, U, Pu): From delocalization to localization. Submitted to *Journal of the American Chemical Society*. (LA-UR-18-29910)
- Wang, G., E. R. Batista, and P. Yang. Ligand induced shape transformation of thorium dioxide nanocrystals. Submitted

Microstructural Characterization of Shock-Recovered Explosives for Mesoscale Model Development

John Yeager
20160619ECR

Project Description

We will controllably damage high explosives without detonation, using radiography during the damage event, and recover them afterwards for characterization. This data will be used to improve models that describe damage and detonation of explosives. Relevant fields will be impacted in several ways: 1) soft recovery (i.e. without further damaging the sample) would be a new capability for Los Alamos; 2) this type of mesoscale model has been difficult to validate using real data for high explosives; and 3) long-standing questions about the damage to initiation process will be addressed. Successful execution of this program will provide fundamental understanding of high explosive materials in the form of data and models that inform thermomechanical codes, particularly for abnormal events such as fragment impact or low-pressure shock.

Technical Outcomes

This project demonstrated a comprehensive new capability for in-situ measurements of real explosive materials during small-scale deformation and coupled to mesoscale simulations. We used in-situ microCT (computed tomography) during quasistatic compression and tension to precisely study PBX (plastic-bonded explosive) damage, while employing a recovery system for dynamically tested samples. Our new mesoscale model used these novel experimental measurements to optimize constituent behavior of PBX systems, in particular high explosive HE-binder delamination.

Publications

Manner, V. W., J. D. Yeager, B. M. Patterson, N. L. Cordes, B. C. Tappan, D. J. Walters, D. J. Luscher, and K. C. Henderson. Damaging HMX/binder formulations: In-situ compression imaging using X-ray micro computed tomography. Submitted to *Propellants Explosives Pyrotechnics*. (LA-UR-16-29590)

Manner, V. W., J. D. Yeager, B. M. Patterson, N. L. Cordes, D. J. Walters, J. A. Stull, D. J. Luscher, K. C. Henderson,

B. C. Tappan, and A. M. Schmalzer. In Situ Imaging during Compression of Plastic Bonded Explosives for Damage Modeling. 2017. *Materials*. (6) 638. (LA-UR-17-23838 DOI: 10.3390/ma10060638)

Walters, D. J., D. J. Luscher, J. D. Yeager, and B. M. Patterson. Investigating Deformation and Mesoscale Void Creation in HMX Based Composites Using Tomography Based Grain Scale FEM. Submitted to *20th Biennial APS Conference on Shock Compression of Condensed Matter (SCCM17)* by AIP Publishing. (LA-UR-17-27813)

Walters, D. J., D. J. Luscher, J. D. Yeager, and B. M. Patterson. Cohesive finite element modeling of the delamination of HTPB binder and HMX crystals under tensile loading. 2018. *International Journal of Mechanical Sciences*. 151-162. (LA-UR-17-27403 DOI: 10.1016/j.ijmecsci.2018.02.048)

Walters, D. J., D. J. Luscher, and J. D. Yeager. Volume Mesh Generation from Real and Artificial Microstructural Geometries. Submitted to *MethodsX*. (LA-UR-18-29478)

Yeager, J. D., V. W. Manner, J. A. Stull, D. J. Walters, A. M. Schmalzer, D. J. Luscher, and B. M. Patterson. Importance of Microstructural Features in Mechanical Response of Cast-Cured HMX Formulations. Submitted to *AIP Conference Proceedings*. (LA-UR-17-27947)

On the Origin of Colossal Ion Conductivity

Edward Kober
20160655PRD2

Project Description

This work focuses on understanding how mechanical strain and chemical diffusion are coupled and how layering materials can lead to changes in diffusion properties. This understanding will allow for tailored materials for solid oxide fuel cell membranes. An analytical dipole theory based model will be developed for stress mediated oxygen diffusion, including diffusion through epitaxial layers. Application of these models will yield highly tuned oxide materials structures with improved oxygen conductivity ideal for solid-oxide fuel cell membranes.

Publications

- Francis, M. F. Fluctuations of Kinetically Constrained States from Multinomial Probability Theory. Submitted to *Physical Review Letters*. (LA-UR-18-24746)
- Francis, M. F. Continuum Microkinetic Rate Theory of Lattice Systems: Formalization, Current Limitations, and a Possible Basis for Continuum Rate Theory. 2018. *The Journal of Physical Chemistry A*. (37) 7267-7275. (LA-UR-17-29795 DOI: 10.1021/acs.jpca.8b06238)
- Francis, M. F. A new strain engineering approach reveals defects may take on multiple morphologies. Submitted to *Nature Nanotechnology*. (LA-UR-17-21109)
- Francis, M. F., E. F. Holby, and A. W. Richards. A first principles evaluation of the structure, stiffness, and low index traction curves of UO_2 , UC, UO_3 , and U_2O_3 . Submitted to *Journal of Nuclear Materials*. (LA-UR-19-21867)

Radiation Effects and Plasma Interactions in Tungsten Based Materials

Osman El Atwani

20160674PRD3

Project Description

The proposed research will develop a fundamental understanding of radiation effects and plasma material interactions in tungsten-based materials, which applies to the development of improved materials for fusion and spallation applications. This work will lay a foundation for understanding materials in fusion conditions and will ultimately lead to the design of new materials. Los Alamos already has existing expertise in materials at irradiation extremes, focusing mostly on fission environments. The proposed research will strengthen these existing capabilities and also further extend the Laboratory's capabilities in fusion materials research.

Publications

- El Atwani, O., C. Taylor, J. Frishkoff, W. Harlow, E. V. Esquivel, S. A. Maloy, and M. Taheri. Thermal desorption spectroscopy of high fluence irradiated ultrafine and nanocrystalline tungsten: helium trapping and desorption correlated with morphology. 2018. *Nuclear Fusion*. (1) 016020. (LA-UR-17-24924 DOI: 10.1088/1741-4326/aa86cf)
- El Atwani, O., E. Aydogan, E. V. Esquivel, M. Efe, Y. Wang, and S. A. Maloy. Detailed Transmission Electron Microscopy Study on Dislocation Loop Rafting in Tungsten. Submitted to *Acta Materialia*. (LA-UR-17-27884)
- El Atwani, O., E. Martinez Saez, E. V. Esquivel, M. Efe, C. Taylor, Y. Wang, B. P. Uberuaga, and S. A. Maloy. Does sink efficiency unequivocally characterize how grain boundaries impact radiation damage?. Submitted to *Nature Communication*. (LA-UR-18-26334)
- El Atwani, O., J. G. Gigax, M. R. Chancey, J. K. S. Baldwin, and S. A. Maloy. Nanomechanical Properties of Pristine and Heavy Ion Irradiation Nanocrystalline Tungsten. Submitted to *Scripta Materialia*. (LA-UR-18-31796)
- El Atwani, O., J. Hinks, G. Greaves, J. P. Allain, and S. A. Maloy. Grain size threshold for enhanced irradiation resistance in nanocrystalline and ultrafine tungsten. 2017. *Materials Research Letters*. 1-7. (LA-UR-16-28940 DOI: 10.1080/21663831.2017.1292326)
- El Atwani, O., J. Nathaniel, A. Leff, B. Muntifering, J. K. S. Baldwin, K. Hattar, and M. Taheri. The role of grain size in He bubble formation: Implications for swelling resistance. 2017. *Journal of Nuclear Materials*. 236-244. (LA-UR-17-31194 DOI: 10.1016/j.jnucmat.2016.12.003)
- El Atwani, O., J. Nathaniel, A. Leff, J. K. S. Baldwin, K. Hattar, and M. Taheri. Evidence of a temperature transition for denuded zone formation in nanocrystalline Fe under He irradiation. 2016. *Materials Research Letters*. 1-6. (LA-UR-17-31234 DOI: 10.1080/21663831.2016.1243591)
- El Atwani, O., J. Nathaniel, A. Leff, K. Hattar, and M. Taheri. Direct Observation of Sink-Dependent Defect Evolution in Nanocrystalline Iron under Irradiation. 2017. *Scientific Reports*. (1) 1836. (LA-UR-17-30505 DOI: 10.1038/s41598-017-01744-x)
- El Atwani, O., N. Li, M. Li, A. Devaraj, M. M. Schneider, D. Sobieraj, J. Wrobel, D. Nguyen-Manh, S. A. Maloy, and E. Martinez Saez. Tungsten-based High Entropy Alloy with Outstanding Radiation Resistance for Extreme Environments. Submitted to *Nature Materials*. (LA-UR-18-27481)
- Barr, C., O. El Atwani, D. Kaoumi, and K. Hattar. Interplay between Grain Boundaries and Radiation Damage. Submitted to *Journal of the Minerals, Metals and Materials Society (JOM)*. (LA-UR-18-30654)
- Cunningham, W. S., O. El Atwani, B. P. Uberuaga, J. Trelewicz, M. Li, E. V. Esquivel, and S. A. Maloy. In-situ irradiation tolerance investigation of high strength ultrafine tungsten-titanium carbide alloy. To appear in *Acta Materialia*. 547-559. (LA-UR-18-27540 DOI: 10.1016/j.actamat.2018.10.038)
- Efe, M., E. Aydogan, Y. Wang, S. A. Maloy, O. El Atwani, and E. V. Esquivel. Loop and void damage during heavy ion irradiation on nanocrystalline and coarse grained tungsten: Microstructure, effect of dpa rate, temperature, and grain size. 2018. *Acta Materialia*. 206-219. (LA-UR-17-31237 DOI: 10.1016/j.actamat.2018.02.035)
- Esquivel, E. V., M. Li, E. Aydogan, E. Martinez Saez, O. El Atwani, B. P. Uberuaga, S. A. Maloy, and J. K. S. Baldwin. Unprecedented irradiation resistance of nanocrystalline tungsten with equiaxed nanocrystalline grains to dislocation loop accumulation. 2019. *Acta*

Materialia. 118-128. (LA-UR-18-26832 DOI: 10.1016/j.actamat.2018.11.024)

Nathaniel II, J. E., A. C. Lang, O. El Atwani, P. K. Suri, J. K. S. Baldwin, M. A. Kirk, Y. Wang, and M. L. Taheri. Toward High-Throughput Defect Density Quantification: A Comparison of Techniques for Irradiated Samples. Submitted to *Ultramicroscopy*. (LA-UR-19-21178)

Trelewicz, J. R., S. A. Maloy, M. Efe, C. N. Taylor, O. El Atwani, J. Gentile, and W. S. Cunningham. Softening due to Grain Boundary Cavity Formation and its Competition with Hardening in Helium Implanted Nanocrystalline Tungsten. 2018. *Scientific Reports*. (1) 2897. (LA-UR-17-26895 DOI: 10.1038/s41598-018-20990-1)

Extrinsic Manipulation of Quantum Emitter Properties through Assembly and Surface Chemistry

Jennifer Hollingsworth
20160680PRD4

Project Description

Semiconducting nanomaterials, like quantum dots (QDs) and single-walled carbon nanotubes (SWCNTs), can be induced to emit light under photoexcitation. Structural size and symmetry factors have long been used as intrinsic parameters to manipulate photoluminescence in these materials systems. More recently, external factors have been established as alternative routes to fine-tune, optimize and even fundamentally alter emission in QDs and SWCNTs. The objective is to explore new advances in external manipulation of fundamental optical processes in these nano-emitters. In the case of QDs, the focus will be on plasmonic and electromagnetic field-mediated processes, while for SWCNTs, the strategy entails advancing chemical techniques for introducing quantum defect states. The former will be achieved by employing advanced QDs and novel plasmonic nanoparticles to create quantum dot/plasmonic nanoparticle assemblies and arrays of assemblies that take advantage of short and long-range field enhancement of emission properties. The latter will entail controlling the photoluminescence of covalently-introduced defect states by introducing new types of molecular dopants toward controlling defect-state location on the nanotube, further narrowing of emission bands, and inducing coupled emissions. Taken together, the new nano-emitter properties achieved will enable applications from quantum information science to efficient ultra-bright light emission.

Publications

Owuor, P. S., O. K. Park, C. F. Woellner, A. S. Jalilov, S. Susarla, J. Joyner, S. Ozden, L. Duy, R. V. Salvatierra, R. Vajtai, J. M. Tour, J. Lou, D. S. Galva, C. S. Tiwary, and P. M. Ajayan. Lightweight Hexagonal Boron Nitride Foam for CO₂ Absorption. Submitted to *ACS Nano*. (LA-UR-18-26004)

- Owuor, P. S., T. Tsafack, H. Y. Hwang, O. K. Park, S. Ozden, S. Bhowmick, S. A. S. Amanulla, R. Vajtai, J. Lou, C. S. Tiwary, and P. M. Ajayan. Role of Atomic Layer Functionalization in Building Scalable Bottom-Up Assembly of Ultra-Low Density Multifunctional Three-Dimensional Nanostructures. Submitted to *ACS Nano*. (LA-UR-18-26024)
- Ozden, S., I. G. Macwan, P. S. Owuor, S. Kosolwattana, P. A. S. Autreto, R. Vajtai, C. S. Tiwary, A. Mohite, P. K. Patra, and P. M. Ajayan. Bacteria as Bio-Template for 3D Carbon Nanotube Architectures. 2017. *Scientific Reports*. (1) 9855. (LA-UR-17-21459 DOI: 10.1038/s41598-017-09692-2)
- Ozden, S., R. Koizumi, A. Samanat, A. P. P. Alves, A. Mishra, G. Ye, G. G. Silva, R. Vajtai, A. K. Singh, C. S. Tiwary, and P. M. Ajayan. Origami-Inspired 3D Interconnected Molybdenum Carbide Nanoflakes. 2018. *Advanced Materials Interfaces*. (6) 1701113. (LA-UR-17-27486 DOI: 10.1002/admi.201701113)
- Ozden, S., T. Tsafack, P. S. Owuor, A. S. Jalilov, Y. Li, R. Vajtai, C. S. Tiwary, J. Lou, J. M. Tour, A. Mohite, and P. M. Ajayan. Chemically interconnected light-weight 3D-carbon nanotube solid network. 2017. *Carbon*. 142-149. (LA-UR-17-21894 DOI: 10.1016/j.carbon.2017.03.086)
- Vinod, S., C. S. Tiwary, A. Samanta, S. Ozden, T. N. Narayanan, R. Vajtai, V. Agarwal, A. K. Singh, G. John, and P. M. Ajayan. Graphene Oxide Epoxy (GO-xy): GO as Epoxy Adhesive by Interfacial Reaction of Functionalities. Submitted to *Advanced Materials Interfaces*. (LA-UR-18-25996)

Novel Topological Orders in Strongly-Correlated Systems

Jianxin Zhu

20170664PRD1

Project Description

Topology is a branch of mathematics that studies properties that only change incrementally, in integer steps, rather than continuously. For example, for a topologist, the only difference between the three foods --- a cinnamon bun, a bagel, and a pretzel --- is the number of holes in them, rather than their taste. The same idea (characterizing the topology number) can be used to explain phase changes in matter, albeit not familiar ones such as a liquid freezing to a solid or sublimating to gas. The postdoc fellow's work is centered on topological phases of quantum matter. It is aimed to search for novel electronic and spin states that are of huge technological impact. For example, topological insulators block the flow of electrons in their interiors while simultaneously conducting electricity across their surfaces. This unique property could make these quantum materials useful for ferreting out new types of fundamental particles, and for forming circuitry within quantum computers. Scientists are already discussing and in some cases making other even more exotic materials, topological superconductors and topological metals that each hold vast potential for new applications in computation and electronics.

Publications

Fu, B., W. Zhu, Z. F. Wang, Q. Shi, J. L. Yang, Q. X. Li, and Z.

Zhang. Multi-scattering induced power-law self-energy correction in disordered graphene. Submitted to *Phys. Rev. B*. (LA-UR-18-20329)

- Gong, S., W. Zhu, J. Zhu, D. Sheng, and K. Yang. Global phase diagram and quantum spin liquids in a spin-1/2 triangular antiferromagnet. 2017. *Physical Review B*. (7) 075116. (LA-UR-17-23332 DOI: 10.1103/PhysRevB.96.075116)
- Huang, Z., J. Zhu, A. V. Balatsky, W. Zhu, and D. P. Arovas. Invariance of Topological Indices Under Hilbert Space Truncation. 2018. *Physical Review Letters*. (1) 016403. (LA-UR-17-24060 DOI: 10.1103/PhysRevLett.120.016403)
- Ren, Y. F., W. Zhu, T. S. Zeng, D. N. Sheng, and Z. Qiao. Spontaneous Quantum Anomalous Hall Phase Stabilized via Extended Hubbard Interactions on a Kagome Lattice. Submitted to *Phys. Rev. B*. (LA-UR-18-25287)
- Wang, L., W. Zhu, F. Li, D. K. Ki, A. F. Morpurgo, N. Chepiga, F. Mila, L. Li, D. Mandrus, O. S. Ovchinnikova, and I. Martin. Controlling the Topological Sector of Magnetic Solitons in Exfoliated Cr₁/3NbS₂ Crystals. 2017. *Physical Review Letters*. (25) 257203. (LA-UR-17-22951 DOI: 10.1103/PhysRevLett.118.257203)
- Wang, Z., W. Zhu, O. Starykh, A. E. Feiguin, A. V. Chubukov, and C. Batista. Chiral liquid phase of simple quantum magnets. 2017. *Physical Review B*. (18) 184409. (LA-UR-17-22905 DOI: 10.1103/PhysRevB.96.184409)
- Zeng, T. S., W. Zhu, and D. N. Sheng. Two-component quantum Hall effects in topological flat bands. 2017. *Physical Review B*. (12) 125134. (LA-UR-17-20075 DOI: 10.1103/PhysRevB.95.125134)
- Zhang, S., W. Zhu, and C. Batista. Pairing from strong repulsion in triangular lattice Hubbard model. 2018. *Physical Review B*. (14) 140507. (LA-UR-17-28927 DOI: 10.1103/PhysRevB.97.140507)
- Zhu, W., A. A. Chacon Salazar, and J. Zhu. Ultrafast Laser Driven Many-Body Dynamics and Kondo Coherence Collapse. Submitted to *Nature Photonics*. (LA-UR-18-31170)
- Zhu, W., Z. Huang, and Y. C. He. Reconstructing Entanglement Hamiltonian via Entanglement Eigenstates. Submitted to *Phys. Rev. B*. (LA-UR-18-25481)
- Zhu, W., and D. N. Sheng. Disorder-driven transition and intermediate phase in the $\nu = 5/2$ fractional quantum Hall effect. Submitted to *Phys. Rev. B*. (LA-UR-18-28368)
- Zhu, W., and J. Zhu. Local quantum criticality of a one-dimensional Kondo insulator model. 2018. *Physical Review B*. (24) 245119. (LA-UR-18-20364 DOI: 10.1103/PhysRevB.97.245119)

A Gruneisen Approach to Quantum Criticality

Priscila Ferrari Silveira Rosa
20170667PRD1

Project Description

An important aspect of the DOE mission is the discovery and manipulation of new quantum states of matter that could lead to entirely new energy relevant technologies. This project will develop a new capability of thermal expansion measurements under extreme conditions that will enable understanding and control of quantum phase transitions and the quantum states that emerge from them.

Publications

Ferrari Silveira Rosa, P., S. M. Thomas, F. F. Balakirev, J. B. Betts, S. Seo, E. D. Bauer, J. D. Thompson, and M. Jaime. An FBG Optical Approach to Thermal Expansion Measurements under Hydrostatic Pressure. Submitted to *Sensors*. (LA-UR-18-30370)

Toward Controlled Synthesis of Actinide Oxide Nanocrystals: A Theoretical Perspective

Enrique Batista
20170670PRD1

Project Description

The long-term goal of this project is to build the knowledge foundation of structures, energetics, and chemical and physical characteristics of tetravalent actinide nanocrystals as a function of particle size, composition, and surface ligands, using a novel high-performance computational framework. Understanding, predicting, and controlling their formation and chemical reactivity is crucial to improve the efficiency of the nuclear fuel cycle, long-term management of nuclear waste, and assessment of contaminated sites.

Publications

Wang, G., E. R. Batista, and P. Yang. Nature of excess electrons on reduced AnO₂ (111) surfaces (An = Th, U, Pu): From delocalization to localization. Submitted to *Journal of the American Chemical Society*. (LA-UR-18-29910)

Wang, G., E. R. Batista, and P. Yang. Ligand induced shape transformation of thorium dioxide nanocrystals. Submitted to *PCCP. Physical Chemistry Chemical Physics*. (LA-UR-17-31042)

Wang, G., P. Yang, N. A. Moody, and E. R. Batista. Overcoming the quantum efficiency-lifetime tradeoff of photocathodes by coating with atomically thin two-dimensional nanomaterials. 2018. *npj 2D Materials and Applications*. (1) 17. (LA-UR-17-26824 DOI: 10.1038/s41699-018-0062-6)

Valley Dynamics and Coherence in Atomically-Thin Semiconductors

Scott Crooker
20170672PRD2

Project Description

The goal of this project is to study a new class of recently discovered semiconductors that are only a single atomic layer thick. These "two-dimensional" semiconductors hold great promise for future applications in ultra-light-weight and low-power electronics.

Joint Mapping of Charge and Spin Degrees of Freedom in Intermediate Valence Materials

Filip Ronning
20170674PRD2

Project Description

In normal metals, the electrons that conduct electricity do not interact with each other and can be described like the atoms in a gas. However, our recent work and the work of others shows that in functional materials such as plutonium the electrons interact strongly, and more importantly that these strong electronic correlations are crucial for understanding functional material properties. Strong electronic correlations are challenging to measure quantitatively, but in this project, we will establish methods that will allow making significant progress in imaging electronic correlations.

Modeling of Two-Dimensional Materials and Hybrid Perovskite Optoelectronic Devices

Sergei Tretiak
20170686PRD3

Project Description

This project involves theoretical modeling of novel layered and three-dimensional materials such as hybrid perovskites. These are promising materials for applications in the area of green energy technologies, such as photovoltaics and water splitting, as well as gamma- and x-ray detector devices pertinent to the core DOE/NNSA missions. Insights gained in this theoretical research will help guiding materials design and fabrication efforts towards applications.

Publications

- Li, W., J. Tang, L. Zhou, A. V. Akimov, and O. V. Prezhdo. Spin-Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. 2018. *ACS Energy Letters*. (9) 2159-2166. (LA-UR-18-26702 DOI: 10.1021/acsenergylett.8b01226)
- Sun, Y., Z. Huang, Z. Zhou, J. Wu, L. Zhou, Y. Cheng, J. Liu, C. Zhu, M. Yu, P. Yu, W. Zhu, Y. Liu, J. Zhou, B. Liu, H. Xie, Y. Cao, H. Li, X. Wang, K. Liu, X. Wang, J. Wang, L. Wang, and W. Huang. Band Structure Engineering of Interfacial Semiconductors Based on Atomically Thin Lead Iodide Crystals. Submitted to *Advanced Materials*. (LA-UR-18-31375)
- Zhang, J., J. zhang, L. Zhou, C. Cheng, J. Liu, S. Tretiak, J. Lischner, F. Giustino, and S. Meng. Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. 2018. *Angewandte Chemie International Edition*. (17) 4585-4589. (LA-UR-18-20121 DOI: 10.1002/anie.201800087)
- Zhou, L., A. J. Neukirch, D. J. Vogel, D. S. Kilin, L. Pedesseau, M. A. Carignano, A. D. Mohite, J. Even, C. Katan, and S. Tretiak. Density of States Broadening in CH₃NH₃PbI₃ Hybrid Perovskites Understood from ab Initio Molecular Dynamics Simulations. 2018. *ACS Energy Letters*. (4) 787-793. (LA-UR-18-20635 DOI: 10.1021/acsenergylett.8b00166)

Engineering Deoxyribonucleic Acid (DNA) Protected Silver Nanoclusters via Doping and Alloying

Peter Goodwin
20170688PRD3

Project Description

Developing stable and bright taggants for commerce, wellness detection and national security is a grand challenge. Nanoclusters are collections of a few atoms of metal, where even one extra atom can drastically change the fluorescent properties. We will develop precisely tuned clusters that have defined fluorescence, as a result of the atom tuning. Once successful, these clusters can be used to better detect biothreat agents and tag commodities important in threat reduction.

Publications

Chakraborty, S., J. Martinez, M. E. Phipps, J. H. Werner, and Y. Chen. DNA Templated Metal Nanoclusters: From Emergent Properties to Unique Applications. To appear in *Accounts of Chemical Research*. (11) 2756-2763. (LA-UR-18-25907 DOI: 10.1021/acs.accounts.8b00366)

Accelerated Discovery of New Nanocomposites for Energy Applications

Turab Lookman
20170691PRD4

Project Description

Accelerated discovery of promising materials to achieve U.S. DOE's goal of developing advanced water splitting materials with enhanced performance and durability for hydrogen generation.

Publications

Han, H. Sb-Doped SnO₂ Nanorods Underlayer Effect to the γ -Fe₂O₃ Nanorods Sheathed with TiO₂ for Enhanced Photoelectrochemical Water Splitting. 2018. *Small*. (19) 1703860. (LA-UR-18-21360 DOI: 10.1002/smll.201703860)

Han, H. Highly Ordered N-Doped Carbon Dots Photosensitizer on Metal-Organic Framework-decorated ZnO Nanotubes for Improved Photoelectrochemical Water Splitting. Submitted to *Nature Catalysis*. (LA-UR-19-20825)

Excited State Dynamics for Photochemistry and Light-Matter Interactions

Tammie Nelson
20170695PRD4

Project Description

This project will use and develop nonadiabatic excited state molecular dynamics, a software package acknowledged by NNSA for open source, to provide novel computational capabilities critical for understanding light-induced dynamics in many technologically relevant materials. The developed capabilities will have extremely broad applications relevant to the current and future Los Alamos National Laboratory/DOE missions, particularly benefitting the primary goal of the Materials for the Future focus area and in the future modeling of materials important for Los Alamos National Laboratory core mission, such as explosives. The project will develop a new computational capability that can be applied to advance modeling of photostability and optical initiation in high explosives involving bond breaking pathways. The high level goals of the project are to develop a modeling capability to describe the light-induced bond breaking reactions in realistic materials and to apply the capability for the prediction, control and design of specific material properties. In addition, our advance will set the stage for the future abilities to model spin and charge dynamics in electronic materials, transition-metal complexes, as well as general photocatalysis phenomena.

Zhang, Y., T. R. Nelson, S. Tretiak, H. Guo, C. Yam, and G. C. Schatz. Plasmonic Hot-Carrier-Mediated Solar Energy Conversion and Tunable Photochemical Reactions. Presented at *The 10th International Conference on Metamaterials, Photonic Crystals and Plasmonics*. (Lisbon, Portugal, 2019-07-22 - 2019-07-26). (LA-UR-19-21628)

Zhang, Y., T. R. Nelson, S. Tretiak, H. Guo, and G. C. Schatz. Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. To appear in *ACS Nano*. (8) 8415-8422. (LA-UR-18-24121 DOI: 10.1021/acsnano.8b03830)

Publications

Nelson, T. R. Excited State Dynamics for Photochemistry and Light-Matter Interactions. Unpublished report. (LA-UR-18-25439)

Nelson, T. R., S. Tretiak, Y. Zhang, and L. A. Lystrom. Site-Specific Photodecomposition in Conjugated Energetic Materials. To appear in *The Journal of Physical Chemistry A*. (29) 6055-6061. (LA-UR-18-24161 DOI: 10.1021/acs.jpca.8b04381)

Zhang, Y. Plasmonic Hot-Carrier-Mediated Solar Energy Conversion and Tunable Photochemical Reactions. Presented at *The 10th International Conference on Metamaterials, Photonic Crystals and Plasmonics*. (Lisbon, Portugal, 2019-07-22 - 2019-07-26). (LA-UR-19-20076)

Soft Matter-Directed Photonic Materials by Data-Driven Design

Stacy Copp

20180701PRD1

Project Description

Materials discovery lies at the heart of countless national security challenges because materials are ubiquitous across technologies. Scientists and engineers develop materials to sense nuclear weapons, detect biological pathogens and prevent pandemics, provide more energy-secure light sources, or withstand extreme conditions on a missile head or space shuttle. Traditionally, materials science has relied on an “informed guessing” strategy, combining intuition and known science to sift through the many ingredients and process steps that can go into a material system. This process is inherently slow and inefficient. We seek to dramatically expedite materials discovery by combining new advances in high-throughput data collection with data science, such as machine learning. We will use experimental observations to “train” machine learning classifiers to predict the components that will assemble a material of choice, focusing first on a model system: polymer-directed assembly of photonic nanoparticles for control over photon emission. While our study focuses on one material system of interest, the implications of our research are wide-reaching across all areas of science and technology, creating a roadmap for materials design of any kind. By increasing the efficiency of materials discovery, we will accelerate innovation while reducing cost and make the US a more secure society.

Swasey, S. M., S. M. Copp, H. C. Nicholson, A. Gorovitz, P. Bogdanov, and E. G. Gwinn. High throughput near infrared screening discovers DNA-templated silver clusters with peak fluorescence beyond 950 nm. *Nanoscale*. (LA-UR-18-29958 DOI: 10.1039/C8NR05781H)

Publications

Copp, S. M., A. Gorovits, S. M. Swasey, S. Gudibandi, P. Bogdanov, and E. G. Gwinn. Fluorescence Color by Data-Driven Design of Genomic Silver Clusters. Submitted to *ACS Nano*. (LA-UR-18-29957)

Copp, S. M., C. J. Hanson, J. A. Hollingsworth, and G. A. Montano. Directing assembly of semiconductor colloidal quantum dots with short-chain amphiphilic block copolymers. Presented at *American Physical Society March Meeting*. (Los Angeles, California, United States, 2018-03-05 - 2018-03-09). (LA-UR-18-30336)

A Multi-scale Approach to Modeling the Competitive Adsorption of Different Species on Molten Salt Reactor (MSR) Structural Components and Their Role in Corrosion Initiation

Blas Uberuaga
20180707PRD1

Project Description

This work addresses challenges in energy security and nuclear energy systems. It will examine the fundamental mechanisms of corrosion in molten salt reactors, a reactor concept that is attractive due to efficiency, safety, stability, and economics. New insight into the fundamental drivers of corrosion will aid in advancing this concept for practical use. Upon completion, this project will generate a fundamental understanding of those mechanisms that dictate corrosion at the salt/metal interface and thus suggest new avenues for mitigating corrosion. This work complements other activities in Los Alamos National Laboratory's nuclear energy portfolio. The Laboratory has extensive simulation efforts on light water reactors, but little on molten salt reactors. This will enhance the Laboratory's capabilities in nuclear energy modeling and simulation.

Samin, A. J. A review of radiation-induced demagnetization of permanent magnets. Submitted to *Journal of Nuclear Materials*. (LA-UR-18-28395)

Samin, A. J., B. P. Uberuaga, A. D. R. Andersson, and E. F. Holby. A first-principles localized cluster expansion study of the kinetics of hydrogen diffusion in homogeneous and heterogeneous Fe-Cr alloys. Submitted to *Physical Review B*. (LA-UR-19-21216)

Samin, A. J., and C. D. Taylor. A combined density functional theory and Monte Carlo investigation of the competitive adsorption of atomic oxygen and chlorine to the Ni (111) surface. Submitted to *Journal of the Electrochemical Society*. (LA-UR-18-28387)

Publications

R. Andersson, A. D., B. P. Uberuaga, E. F. Holby, and A. J. Samin. On the role of electro-migration in the evolution of radiation damage in nanostructured ionic materials. To appear in *Electrochemistry Communications*. 47-52. (LA-UR-18-25848 DOI: 10.1016/j.elecom.2018.09.010)

Atomic Layer Deposition of Templated Electrode Structures for Electrochemical Devices

Jacob Spendelow
20180711PRD2

Project Description

Energy security, including the limited availability of domestic energy resources and the need to replace fossil fuels with clean energy alternatives, is a major national challenge. Electrochemical energy storage and conversion technologies, including batteries and fuel cells, could enable a faster transition to clean energy sources such as solar and wind, and could help reduce our national dependence on imported petroleum for transportation. Current batteries and fuel cells are limited by unsatisfactory electrode performance, causing decreased efficiency, slow charging, and poor lifetime. The proposed project will yield new electrode structures with enhanced performance and durability, enabling batteries and fuel cells to have higher power, increased robustness, and longer lifetimes. By accelerating the deployment of batteries and fuel cells, the project will enable a more rapid transition to a new clean energy economy.

Exploration of New Topological States of Matter in Strongly Correlated Materials and in Ultra-high Magnetic Fields

Neil Harrison
20180713PRD2

Project Description

The use of the world-unique 100 Tesla (T) capability at the Los Alamos National High Magnetic Field Laboratory (NHMFL) and f-electron materials to search for novel topological phases will open up a new field of research on topology in strongly correlated matter. Topology is seen as a promising route for the development of new electronics and quantum computation, and it is therefore in the national interest to develop the highest quality materials. It is anticipated that several entirely new regimes of physics will emerge in very strong magnetic fields. This project will help establish Los Alamos as a world-leader in topology at extremely high magnetic field and in topological materials with strong electronic correlations.

Publications

Boschini, F., D. Bugini, M. Zonno, M. Michiardi, R. P. Day, E. Razzoli, B. Zwartsenberg, E. H. da Silva Neto, S. dal Conte, S. K. Kushwaha, R. J. Cava, S. Zhdanovich, A. K. Mills, G. Levy, E. Carpene, C. Dallera, C. Giannetti, D. J. Jones, G. Cerullo, and A. Damascelli. Role of matrix elements in the time-resolved photoemission signal. Submitted to *Physical Review B*. (LA-UR-18-30021)

Understanding and Controlling Ultrafast Exciton Dynamics in Group-VII Transition Metal Dichalcogenides

Rohit Prasankumar
20180718PRD2

Project Description

Group-VII transition metal dichalcogenides (TMDs) have attracted attention for their potential to impact a variety of applications, such as quantum information and computing. In fact, they represent one of the most promising avenues for going beyond the functionality of conventional materials like silicon, due to the ability to control their unique nanoscale optical and electronic properties by simply modifying their thickness and combining different TMD layers into heterostructures. However, to date their properties remain relatively unexplored. Here, we will provide new insight into their properties by using ultrashort pulses of light to drive them out of equilibrium and dynamically track their relaxation back to equilibrium, with immediate impact on applications in, e.g., optical and electronic switching. Our research is well aligned with the Los Alamos' materials strategy in the focus area of Materials for the Future. Furthermore, Department of Energy-Basic Energy Sciences(DOE-BES) is heavily invested in this field, with recent reports on "Quantum Materials" and "Harnessing coherence in light and matter" that are directly addressed here. Our studies also connect to the Beyond Moore's Law Big Idea through the "Fundamental Materials Science" and "Devices and CMOS Technology" thrusts.

Development of an Innovative Mechanical Testing System and Techniques for Characterizing Irradiated Advanced Cladding Concepts and Novel Materials

Nan Li

20180744PRD3

Project Description

The goal of this project is to develop a novel in situ mechanical testing devices to perform analysis on specimen volumes on the microscale and approaching the macroscale. The device (commercially unavailable) will integrate high temperature and high strain rate capabilities to probe the mechanical response under extreme conditions. Macroscale mechanical testing of neutron irradiated materials has been used extensively to understand mechanical property (tensile, ductility, creep, hardness) changes after irradiation. Such testing is critical to the continued safe operation of the nuclear reactor as dramatic changes in mechanical properties (i.e. embrittlement) may result in fuel cladding failure and undesired radioactivity release. Thus, the development of mechanical testing techniques on the mesoscale enables one to obtain data from small volumes (e.g. produced by ion irradiation) and samples with larger (bulk) volumes irradiated by neutrons to obtain data that is essential to further validate mechanical testing of ion irradiated alloys and advance materials development for next generation nuclear reactors such as those being developed in DOE's Nuclear Energy Programs.

Publications

- Gigax, J. G., H. T. Vo, Q. Mcculloch, M. R. Chancey, Y. Wang, S. A. Maloy, N. Li, and P. Hosemann. Micropillar compression response of femtosecond laser-cut single crystal Cu and proton irradiated Cu. Submitted to *Scripta Materialia*. (LA-UR-19-21957)
- Gigax, J. G., J. K. S. Baldwin, C. J. Sheehan, S. A. Maloy, and N. Li. Microscale shear specimens for evaluating the shear deformation in single crystal and nanocrystalline Cu and at Cu/Si interfaces. Submitted to *Journal of Materials Research*. (LA-UR-19-21222)

Ferromagnetism and Spin Fluctuations in the Atomically-Thin Limit

Scott Crooker
20180747PRD3

Project Description

Two-dimensional (2D), atomically-thin materials are poised to revolutionize electronics and opto-electronics technologies. The most well-known example is graphene, discovered in 2004, which is a single atomic layer of carbon atoms: graphene exhibits remarkable electronic properties such as high electrical conductivity and also remarkable mechanical properties such as high strength. More recently, other 2D materials have been discovered that exhibit additional technologically useful properties, such as semiconducting behavior (which allows for light-emitting and light-detection capabilities) and also magnetism (which allows for information storage and processing). This project is focused on exploring an entirely new route towards achieving magnetism in a new class of 2D materials based on the semiconductor gallium selenide (GaSe). Recent theory indicates that magnetic behavior can be induced in GaSe by electrical means. Electrically-controllable magnetism is a longstanding 'holy grail' in the broad field of semiconductor electronics, with immediate technological relevance in the areas of data storage and information processing (ie, computing).

Dynamic Strength and Phase Transition Kinetics in Geophysical Materials

Arianna Gleason Holbrook
20150707PRD2

Project Description

The project will use a brilliant x-ray laser to examine how geophysical materials change the positions and lattice structure of their atoms in response to shock compression. The resulting information will advance the current level of understanding about how these materials behave in geophysical events, such as asteroid impacts and the dynamics of the earth's molten iron core. Understanding the behavior of matter during extreme shocks is directly relevant to the nuclear weapons program.

Technical Outcomes

The most critical outcomes of the project are direct measurements of strength, elasticity, plasticity and the kinetics of phase transformations on several common materials: SiO₂, H₂O and Fe with implications in geophysics, planetary science, materials sciences, as well as fundamental physics and chemistry. Mesoscale materials properties measurements at high strain rate are needed for accurate and predictive modeling.

Publications

- Armstrong, M., H. Radousky, R. Austin, J. Belof, E. Stavrou, S. Brown, J. Crowhurst, A. E. Gleason Holbrook, E. Granados, P. Grivickas, N. Holtgrewe, H. J. Lee, T. Li, S. Lobanov, J. McKeown, B. Nagler, I. Nam, A. Nelson, V. Prakapenka, C. Prescher, J. Roehling, N. Teslich, P. Walter, J. Zaug, and A. Goncharov. Experimental observation of fundamental mechanisms of compression-induced phase transformations using ultrafast time-resolved x-ray diffraction. Submitted to *Physical Review B*. (LA-UR-17-28672)
- Briggs, R., M. Gorman, A. Coleman, R. McWilliams, E. McBride, D. McGonegle, J. Wark, L. Peacock, S. Rothman, S. Macleod, C. A. Bolme, A. Gleason, G. Collins, J. Eggert, D. Fratanduono, R. Smith, E. Galtier, E. Granados, H. J. Lee, B. Nagler, I. Nam, Z. Xing, and M. McMahon. Ultrafast X-Ray Diffraction Studies of the Phase Transitions and Equation of State of Scandium Shock Compressed to 82 GPa. 2017. *Physical Review Letters*. (2) 025501. (LA-UR-17-24602 DOI: 10.1103/PhysRevLett.118.025501)

- Brown, S., A. Hashim, A. Gleason, E. Galtier, I. Nam, Z. Xing, A. Fry, A. Mackinnon, B. Nagler, E. Granados, and H. J. Lee. Shock drive capabilities of a 30-Joule laser at the matter in extreme conditions hutch of the Linac Coherent Light Source. 2017. *Review of Scientific Instruments*. (10) 105113. (LA-UR-17-24632 DOI: 10.1063/1.4997756)
- Dresselhaus-Cooper, L., J. Gorfain, C. Key, B. Ofori-Okai, S. Ali, D. Martynowych, A. Gleason, S. Kooi, and K. Nelson. Development of single-shot multi-frame imaging of cylindrical shock wave for deeper understanding of a multi-layered target geometry. Submitted to *Physical Review Applied*. (LA-UR-17-26391)
- Gleason, A., C. A. Bolme, E. Galtier, H. J. Lee, E. Granados, D. Dolan, C. Seagle, T. Ao, S. Ali, A. Lazicki, D. Swift, P. Celliers, and W. Mao. Compression Freezing Kinetics of Water to Ice VII. 2017. *Physical Review Letters*. (2) 025701. (LA-UR-17-22076 DOI: 10.1103/PhysRevLett.119.025701)
- Gleason, A., C. A. Bolme, H. J. Lee, B. Nagler, E. Galtier, D. Milathianaki, J. Hawreliak, R. Kraus, J. Eggert, D. Fratanduono, G. Collins, R. L. Sandberg, W. Yang, and W. Mao. Ultrafast visualization of crystallization and grain growth in shock-compressed SiO₂. 2015. *Nature Communications*. 8191. (LA-UR-15-25589 DOI: 10.1038/ncomms9191)
- Gleason, A., C. A. Bolme, H. J. Lee, B. Nagler, E. Galtier, R. Kraus, R. L. Sandberg, W. Yang, F. Langenhorst, and W. Mao. Time-resolved diffraction of shock-released SiO₂ and diaplectic glass formation. 2017. *Nature Communications*. (1) 1481. (LA-UR-17-23638 DOI: 10.1038/s41467-017-01791-y)
- Glenzer, S., L. Fletcher, E. Galtier, B. Nagler, R. Alonso-Mori, B. Barbrel, S. Brown, D. Chapman, Z. Chen, C. Curry, F. Fiuza, E. Gamboa, M. Gauthier, D. Gericke, A. Gleason, S. Goede, E. Granados, P. Heimann, J. Kim, D. Kraus, M. MacDonald, A. Mackinnon, R. Mishra, A. Rivasio, C. Roedel, P. Sperling, S. Schumaker, Y. Tsui, J. Vorberger, U. Zaustrau, A. Fry, W. White, J. Hastings, and H. J. Lee. Matter under extreme conditions experiments at the Linac Coherent Light Source. 2016. *Journal of Physics B: Atomic, Molecular and Optical Physics*. (9) 092001. (LA-UR-17-24600 DOI: 10.1088/0953-4075/49/9/092001)
- Gleason Holbrook, A. E. Dynamic Strength and Phase Transition Kinetics in Geophysical Materials. Unpublished report. (LA-UR-18-21293)

- Gleason Holbrook, A. E., D. Rittman, C. A. Bolme, E. Galtier, H. J. Lee, E. Granados, S. Ali, A. Lazicki, D. Swift, P. Celliers, B. Militzer, and W. Mao. Dynamic compression of water to pressures of ice giant interiors. Submitted to *Proceedings of the National Academy of Sciences*. (LA-UR-17-28193)
- Pardini, T., J. Alameda, A. Aquila, S. Boutet, T. Decker, A. E. Gleason Holbrook, S. Guillet, P. Hamilton, M. Hayes, R. Hill, J. Koglin, B. Kozioziemski, J. Robinson, K. Sokolowski-Tinten, R. Soufli, and S. Hau-Riege. Delayed Onset of Nonthermal Melting in Single-Crystal Silicon Pumped with Hard X Rays. 2018. *Physical Review Letters*. (26) 265701. (LA-UR-17-29806 DOI: 10.1103/PhysRevLett.120.265701)
- Shahar, A., E. Schauble, R. Caracas, A. Gleason, M. Reagan, Y. Xiao, J. Shu, and W. Mao. A Pressure Effect on Iron Isotope Partitioning in Iron Alloys. Submitted to *Science*. (LA-UR-16-20905)

Macroporous/Nanoporous Hierarchical Carbon Structure (MNHCS) for High-Performance Energy Storage Devices

Jeffrey Pietryga
20150760PRD4

Project Description

This project aims to develop next-generation, carbon-based porous materials for high performance energy storage devices such as lithium ion batteries and supercapacitors. We expect to achieve synthesis of 3D reduced nanoporous graphene oxides and fullerene-based composites that offer several unique properties: i) an interconnected electrolyte-filled macroporous network that enables increased contact surfaces between the 3D network and electrolytic solution, and rapid ion transport, ii) short ion and electron transport lengths, iii) a high electrode specific surface area and (iv) high electron conductivity in the electrode assembly. This method will be extended to the synthesis of a variety of 3D conjugated systems that will render the formation of conducting macroporous/nanoporous structures, ideally suited for the fabrication of highly efficient supercapacitors and lithium ion batteries. Success in this project will have widespread impact on the development of high performance energy storage technologies.

Nano Energy. 327-335. (LA-UR-17-21496 DOI: 10.1016/j.nanoen.2017.08.033)

Technical Outcomes

Advanced carbon materials, including functionalized C60 and 3D silicon/graphene oxides, were developed to fabricate high-performance lithium ion batteries (LIBs). The functionalized C60s showed much better capacity with great cycling stability than graphite, a commercial material. The silicon based LIBs, with 3D graphene oxide as a binder, showed much better stability than that with Polyvinylidene fluoride as binder, a commercial binder. Developing new 3D carbon materials with functionalization would be promising for developing high performance LIBs.

Publications

Shan, C., H. J. Yen, K. Wu, Q. Lin, X. Guo, H. Zhang, G. Wu, H. L. Wang, and D. Wu. Functionalized fullerenes for highly efficient lithium ion storage: Structure-property-performance correlation with energy implications. 2017.

Investigating Complex Superconducting Phases via Field-Rotating Transport and Thermodynamic Measurements

Roman Movshovich
20150762PRD4

Project Description

The project will conduct thermal conductivity and specific measurements in a high magnetic field (14 Tesla) and a very low temperature (down to 20 milliKelvins) to probe the nature of unconventional superconducting states. This project will address the issue of unconventional superconductivity, by directly measuring the symmetry of the superconducting order parameter in a number of compounds. Some states that will be explored represent unique states of matter. This research is therefore of great interest to the mission of the basic understanding of materials.

Technical Outcomes

The project developed a unique capability to measure thermal conductivity in a rotating magnetic field up to 14 Tesla, in a dilution refrigerator capable of reaching temperatures down to 20 mK. He investigated the superconducting state of CeCoIn₅, observing triply intertwined orders in a high field low temperature superconducting (HFSC) phase: d-wave superconductivity, magnetic spin density wave (SDW), and superconducting p-wave pair density wave. Numerous resonance-like features in thermal conductivity were observed in lower fields.

Theory of Spin and Valley Dynamics in 2D Dirac Semiconductors

Nikolai Sinitsyn
20160648PRD2

Project Description

This project will focus on achieving control of spin and valley magnetic moments of electrons in the new class of atomically thin semiconductor materials known as “Dirac semiconductors.” This emerging family of semiconductors is very similar in structure to graphene but superior. The new 2D materials have an optical gap that makes them similar to commercial semiconductor, but being atomically thin and very stable, they will outperform all currently used semiconductors in energy efficiency, solar cells, and quantum information applications. Dirac semiconductors have the potential to replace commercial semiconductors for energy-efficient electronics and solar cell applications.

Technical Outcomes

The main result of the project was the solution of the model of quantum annealing model. This model shed light one of the fundamental problems - thermalization in closed quantum interacting models, such as nanostructure made of Dirac semiconductors. Several other results were obtained on spin noise spectroscopy of 2-Dimensional (atomically thin) magnetic cobalt films.

Plasmonics-Transformed Quantum Emitters Through Theory-Guided Synthesis

Jennifer Hollingsworth
20160653PRD2

Project Description

We will transform quantum emitters through plasmonics to be ideal single- and entangled-photon-pair sources. The new semiconducting-metallic nanostructures will have unique properties that cannot be obtained in either type of material alone. The work will provide new fundamental understanding for the design of controlled plasmon-photon interactions across scale, which will underpin the advancement of quantum dots as gain media for cavity-enhanced lasers. Such advanced light emitters are needed for next-gen communications and computing (light-enabled or even all-optical networks).

Technical Outcomes

This basic science research resulted in novel functional optical/plasmonic building-blocks for nanomaterials integration, and new strategies for achieving "useful" integration, i.e., yielding complex, emergent and multifunctional materials.

Publications

- Hanson, C. J., N. F. Hartmann, A. Singh, X. Ma, W. J. DeBenedetti, J. L. Casson, J. K. Grey, Y. J. Chabal, A. V. Malko, M. Sykora, A. Piryatinski, H. Htoon, and J. A. Hollingsworth. Giant PbSe/CdSe/CdSe Quantum Dots: Crystal-Structure-Defined Ultrastable Near-Infrared Photoluminescence from Single Nanocrystals. 2017. *Journal of the American Chemical Society*. (32) 11081-11088. (LA-UR-18-21088 DOI: 10.1021/jacs.7b03705)
- Hu, Z., A. Singh, S. V. Goupalov, J. A. Hollingsworth, and H. Htoon. Influence of Morphology on Blinking Mechanisms and Excitonic Fine Structure of Single Colloidal Nanoplatelets. To appear in *Nanoscale*. (LA-UR-18-28802 DOI: 10.1039/C8NR06234J)
- Orfield, N. J., S. Majumder, J. R. McBride, F. C. Koh, A. Singh, S. J. Bouquin, J. L. Casson, A. Johnson, L. Sun, X. Li, C. K. Shih, S. J. Rosenthal, J. A. Hollingsworth, and H. Htoon. Photophysics of Thermally-Assisted Photobleaching in "Giant" Quantum Dots Revealed in Single Nanocrystals. To appear in *ACS Nano*.

(5) 4206-4217. (LA-UR-18-28798 DOI: 10.1021/acsnano.7b07450)

Peer, A., Z. Hu, A. Singh, J. A. Hollingsworth, R. Biswas, and H. Htoon. Photoluminescence Enhancement of CuInS₂ Quantum Dots in Solution Coupled to Plasmonic Gold Nanocup Array. 2017. *Small*. (33) 1700660. (LA-UR-17-25520 DOI: 10.1002/smll.201700660)

Deoxyribonucleic Acid (DNA) Mediated Photonic Superstructures for Enhanced Artificial Photosynthesis

Sergei Ivanov
20160675PRD3

Project Description

This research project directly addresses energy needs of the future, which is a critical national security challenge. A goal within this challenge is to enhance the efficiency of capture and utilization of light (photonic) energy for materials applications, such as improving efficiency in photovoltaics and solid-state lighting. This project seeks to develop molecular-scaled materials, based upon Deoxyribonucleic Acid (DNA) and polymers, which exhibit dynamic photonic properties and can be incorporated to existing photonic platforms for enhanced efficiency through dynamic regulation. Hybrid constructs consisting of DNA-polymer assemblies will be synthesized for this study. The polymer component induces material stability and device integration in a stimuli-responsive matrix, as well as serves as a home for photonic chromophores and the DNA allows for creation of clusters of metal ions that result in tunable light response. Coupled together, these constructs have the potential of exhibiting a wide breadth of tunable photonic response not typically observed in photonic materials. Coupling to existing platforms could result in new classes of tunable, efficient photonic materials for a range of applications.

copolymers. Presented at *American Physical Society March Meeting*. (Los Angeles, California, United States, 2018-03-05 - 2018-03-09). (LA-UR-18-30336)

Technical Outcomes

This project developed methods to direct assembly of light-active nanoparticles and chromophores using amphiphilic block copolymers. Specifically, we have developed a dual-chromophore system where a pH-tuned changes in polymer morphology control resonant energy transfer between chromophores. We have also realized encapsulation of core/shell CdSe/CdS “giant” quantum dots inside block copolymer nanostructures, which may allow for further integration of these photonic materials in applications.

Publications

Copp, S. M., C. J. Hanson, J. A. Hollingsworth, and G. A. Montano. Directing assembly of semiconductor colloidal quantum dots with short-chain amphiphilic block

Understanding Non-Collinear Magnets: From Crystal Structure to Magnetic Function

Eric Bauer
20160679PRD4

Project Description

The project proposes to discover new, unusual non-collinear/non-coplanar magnets to understand how structure controls magnetic functionality. These magnets are promising candidates for future memory storage devices or as sensors. The discovery and understanding of novel topological and unconventional superconducting states is at the forefront of condensed matter research. Finding a new superconducting helimagnet, a novel spin structure, a large Hall effect, or other unusual temperature dependent of the physical properties in a non-collinear magnet would be a significant advance because it would uncover the mechanism required to generate these novel states of matter. This project will provide insight into unusual spin structures, which could be used as the basis for future electronics applications.

Technical Outcomes

The work synthesized single crystals of manganese-tin (Mn_3Sn) and characterized this material by means of electrical resistivity and Hall effect. It was found that a very large Hall effect exists, which is comparable to that of ferromagnetic materials, in the antiferromagnetic state at room temperature of Mn_3Sn . Because this material has a very small net magnetization in the antiferromagnetic state, it is superior to many ferromagnets for use as a magnetic switch or for a sensor.

Publications

Sung, N., F. Ronning, J. D. Thompson, and E. D. Bauer. Magnetic phase dependence of the anomalous Hall effect in Mn Sn single crystals. 2018. *Applied Physics Letters*. (13) 132406. (LA-UR-17-31089 DOI: 10.1063/1.5021133)



Nuclear and Particle Futures

Dark Matter Search with a Neutrino Experiment

Richard Van De Water
20160037DR

Project Description

The project will significantly improve the search for sub-Giga Electron Volt (GeV) Dark Matter with the Short Baseline Neutrino Detector (SBND) at Fermilab by building a powerful photon detection system, and developing new theoretical models of the Dark Sector physics. Final state charged particles that interact in the SBND liquid argon time projection chamber produce recoil electrons, which in turn produce scintillation light that can be detected by the photon detection system (PDS). The PDS reconstructs the neutrino or dark matter event position and time from the scintillation light. The timing of the scintillation light is approximately one nanosecond, which enables the PDS to significantly reduce backgrounds and expand the physics scope of SBND by enabling a search for sub-GeV dark matter. The development of liquid argon scintillation light detection capability at Los Alamos could lead to applications in nuclear nonproliferation such as enhanced neutron and gamma-ray portal detection.

Technical Outcomes

The physics capabilities of the SBND program has been greatly improved by designing and constructing a comprehensive photon detection system (PDS) for the near detector, reducing the sterile neutrino run time from five to three years and allowing an expansive and novel search for sub-GeV dark matter. As well, the LDRD project developed a consistent theoretical framework of neutrino-nucleus cross sections which are required to understand backgrounds and improve the dark matter search.

Publications

- Gupta, R., T. Bhattacharya, B. Yoon, Y. C. Jang, and H. W. Lin. Contribution of the quarks to the proton spin from $2+1+1$ -flavor lattice QCD. Submitted to *Physical Review Letters*. (LA-UR-18-25337)
- Gupta, R., V. Cirigliano, Y. C. Jang, T. Bhattacharya, B. Yoon, and H. W. Lin. Flavor diagonal tensor charges of the nucleon from $(2+1)$ -flavor lattice QCD. To appear in *Physical*

Review D. (9) 091501. (LA-UR-18-28007 DOI: 10.1103/PhysRevD.98.091501)

Jang, Y. C., R. Gupta, T. Bhattacharya, B. Yoon, and H. W. Lin. Nucleon Vector and Axial-Vector Form Factors. Presented at *34th annual International Symposium on Lattice Field Theory 24-30 July 2016 University of Southampton, UK*. (Southampton, United Kingdom, 2016-07-24 - 2016-07-30). (LA-UR-17-21346)

Ma, L., S. M. Shalgar, and H. Duan. Matter parametric neutrino flavor transformation through Rabi resonance. Submitted to *Physical Review D*. (LA-UR-18-25879)

Shalgar, S. M. Multi-angle calculation of the matter-neutrino resonance near an accretion disk. To appear in *Journal of Cosmology and Astroparticle Physics*. (02) 10-10. (LA-UR-17-26195 DOI: 10.1088/1475-7516/2018/02/010)

Rapid Response to Future Threats (U)

Charles Nakhleh
20160664DR

Project Description

This project addresses weapons design challenges for the 21st century by laying the groundwork that enables weapons designers to respond quickly and efficiently to mission needs. At its end, this project will supply the first version of a set of tools that will enable a designer to quickly and efficiently execute design iteration calculation with modern design codes. The project will also provide the calculational modeling for developing a non-traditional weapons physics package outside the design space of the existing stockpile.

Minnesota, United States, 2016-10-06 - 2016-10-07). (LA-UR-16-29501)

Publications

Boyd, Z. M., and J. R. Wendelberger. An Integrated Approach to Parameter Learning in Infinite-Dimensional Space. Unpublished report. (LA-UR-17-28326)

Boyd, Z. M., and J. R. Wendelberger. An Integrated Approach to Parameter Learning in Infinite-Dimensional Space. Unpublished report. (LA-UR-17-28326)

Tappan, B. C., L. G. Hill, J. P. Lichthardt, P. R. Bowden, D. L. McDonald, M. Shorty, and V. W. Manner. Diameter Effect Observations in Pressed HMX-Aluminum Explosive Formulations. Presented at *International Symposium on Detonation*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-15). (LA-UR-18-26010)

Tappan, B. C., P. R. Bowden, V. W. Manner, J. A. Leiding, and M. S. Jakulewicz. Evaluation of the Deuterium Isotope Effect in the Detonation of Aluminum Containing Explosives. 2018. *Propellants, Explosives, Pyrotechnics*. (1) 62-68. (LA-UR-17-27057 DOI: 10.1002/prop.201700197)

Tappan, B. C., P. R. Bowden, V. W. Manner, S. F. Son, J. P. Lichthardt, and D. L. McDonald. Exploring the effects of reactive additives in explosives: In search of higher efficiency with various energetic combinations. Presented at *New Trends in Research of Energetic Materials*. (Pardubice, Czech Republic, 2018-04-16 - 2018-04-20). (LA-UR-18-22268)

Wendelberger, J. R. Understanding Today's Complex World. Presented at *2016 Fall Technical Conference*. (Minneapolis,

New Science and Technology for a Tabletop Accelerator

Evgenya Simakov
20170006DR

Project Description

The project will deliver a stand-alone laser powered compact accelerator that produces mega-electron-volt electron beams with femtosecond bunch lengths. Dielectric laser accelerator (DLA) technology has been identified as one of the most promising advanced accelerator approaches by both the accelerator community and the Office of Science/High Energy Physics (HEP) directorate, and is arguably the best match for compact light sources and accelerators for medical therapy and national security. Compact accelerators are desired by a number of national security applications, including war-fighter support (weaponized Free-Electron Lasers) and active interrogation (electron accelerators as compact front ends for muon active interrogation sources or to generate bremsstrahlung radiation). With increased efficiency and decreased weight provided by DLA technology, Free-Electron Lasers (FELs) might become fieldable on airborne platforms. This work also positions Los Alamos at the forefront of advanced high current cathode development for multi-megawatt accelerators for applications such as environmental remediation (e.g., cleaning up toxic chemical spills), and accelerator-driven fission power.

Publications

Andrews, H. L. Current Experimental Work with Diamond Field-Emitter Array Cathodes. Presented at *38th International Free Electron Laser Conference*. (Santa Fe, New Mexico, United States, 2017-08-20 - 2017-08-25). (LA-UR-17-27451)

Andrews, H. L., J. W. I. Lewellen, E. I. Simakov, K. Nichols, D. Shchegolkov, R. L. Fleming, D. Kim, and B. K. Choi. An Investigation of Electron Beam Divergence from a Single DFEA Emitter Tip. Presented at *IPAC '18*. (Vancouver, Canada, 2018-04-29 - 2018-04-29). (LA-UR-18-23694)

Fleming, R. L. A Simple Variable Focus Lens For Field-Emitter Cathodes. Presented at *Advanced Accelerators Conference*.

(breckenridge, Colorado, United States, 2018-08-20 - 2018-08-20). (LA-UR-18-29143)

Fleming, R. L., H. L. Andrews, K. A. Bishofberger, D. Kim, J. W. I. Lewellen, K. Nichols, D. Shchegolkov, and E. I. Simakov. A SIMPLE VARIABLE FOCUS LENS FOR FIELD-EMITTER CATHODES. Presented at *International Particle Accelerator Conference*. (Vancouver, Canada, 2018-04-29 - 2018-05-04). (LA-UR-18-23565)

Huang, C., H. L. Andrews, R. C. Baker, R. L. Fleming, D. Kim, T. J. T. Kwan, A. Piryatinski, V. Pavlenko, and E. I. Simakov. Modeling of diamond field emitter arrays for a compact source of high brightness electron beams. Submitted to *Journal of Applied Physics*. (LA-UR-18-31776)

Huang, C., H. L. Andrews, T. J. T. Kwan, J. W. I. Lewellen, D. C. Nguyen, K. Nichols, V. Pavlenko, A. Piryatinski, D. Shchegolkov, E. I. Simakov, B. K. Choi, and R. L. Fleming. Modeling of Diamond Field-Emitter-Arrays for high brightness photocathode applications. Presented at *38th International Free-Electron Laser Conference*. (Santa Fe, New Mexico, United States, 2017-08-21 - 2017-08-25). (LA-UR-17-27297)

I. Lewellen, J. W., H. L. Andrews, R. L. Fleming, K. Nichols, and E. I. Simakov. An Electrostatic Fixed-Slit Emittance Measurement System. Presented at *9th International Particle Accelerator Conference*. (vancouver, Canada, 2018-04-29 - 2018-04-29). (LA-UR-18-23362)

Pavlenko, V., D. Kim, H. L. Andrews, C. Huang, T. J. T. Kwan, A. Piryatinski, R. L. Fleming, R. J. Aragonz, and E. I. Simakov. Field Assisted Photoemission from Nanocrystalline Diamond and Diamond Field Emitter Arrays. Presented at *18th Advanced Accelerator Concepts Workshop (AAC 2018)*. (Breckenridge, Colorado, United States, 2018-08-12 - 2018-08-17). (LA-UR-18-29732)

Pilania, G., E. Weis, E. M. Walker, R. D. Gilbertson, R. E. Muenchausen, and E. I. Simakov. Computational screening of organic polymer dielectrics for novel accelerator technologies. 2018. *Scientific Reports*. (1) 9258. (LA-UR-18-20571 DOI: 10.1038/s41598-018-27572-1)

Piryatinski, A., C. Huang, and T. J. T. Kwan. Model for electron transport and emission from semiconductor nanotip. Submitted to *Journal of Applied Physics*. (LA-UR-19-20009)

- Piryatinski, A., C. Huang, and T. J. T. Kwan. Model for electron transport and emission from semiconductor nanotip. Submitted to *Journal of Applied Physics*. (LA-UR-19-20009)
- Simakov, E. I., D. Kim, H. L. Andrews, and B. K. Choi. Fabrication of Micron-Scale Diamond Field Emitter Arrays for Dielectric Laser Accelerators. Presented at *18th Advanced Accelerator Concepts Workshop (AAC 2018)*. (Breckenridge, Colorado, United States, 2018-08-13 - 2018-08-13). (LA-UR-18-29662)
- Simakov, E. I., H. L. Andrews, D. Kim, V. Pavlenko, D. Black, and K. Leedle. Observations of the femtosecond-laser-induced emission from diamond field emitter tips. Submitted to *Physical Review Letters*. (LA-UR-18-30551)
- Simakov, E. I., H. L. Andrews, R. L. Fleming, D. Kim, J. W. I. Lewellen, K. Nichols, V. Pavlenko, and D. Y. Shchegolkov. Study of the Beam Divergence in Diamond Field Emitter Array Cathodes. Presented at *18th Advanced Accelerator Concepts Workshop (AAC 2018)*. (Breckenridge, Colorado, United States, 2018-08-13 - 2018-08-13). (LA-UR-18-29664)
- Simakov, E. I., N. Yampolsky, and K. Wootton. Preface: 18th Advanced Accelerator Concepts Workshop (AAC 2018). Presented at *Advanced Accelerator Concepts Workshop*. (Breckenridge, Colorado, United States, 2018-08-12 - 2018-08-12). (LA-UR-18-31629)
- Simakov, E. I., R. D. Gilbertson, M. J. Herman, E. Weis, D. Shchegolkov, G. Pilania, E. M. Walker, R. England, and K. Wootton. POSSIBILITIES FOR FABRICATING POLYMER DIELECTRIC LASER ACCELERATOR STRUCTURES WITH ADDITIVE MANUFACTURING. Presented at *International Particle Accelerator Conference*. (Vancouver, Canada, 2018-04-30 - 2018-04-30). (LA-UR-18-23527)
- Walker, E. M., R. D. Gilbertson, E. I. Simakov, G. Pilania, and R. E. Muenchausen. High-Dielectric 3-D Printable Materials for Laser Accelerators. Submitted to *IEEE Conference Proceedings*. (LA-UR-18-29310)

Probing Quark-Gluon Plasma with Bottom Quark Jets at sPHENIX

Ming Liu

20170073DR

Project Description

The goal of this project is to address important physics questions in Quark-Gluon-Plasma (QGP) physics using a new silicon tracker that will be added to the sPHENIX experiment at the Relativistic Heavy Ion Collider at the Brookhaven National Lab. Measurements of modification of heavy quark production in high energy heavy ion collisions at RHIC will help us to understand various quark energy loss mechanisms, including radiative and collisional energy loss inside the QGP. This project will make it possible to address key aspects of heavy quark physics at the next generation heavy ion detector, sPHENIX.

Publications

Kang, D., C. Lee, and V. P. Vaidya. A fast and accurate method for perturbative resummation of transverse momentum-dependent observables. 2018. *Journal of High Energy Physics*. (4) 149. (LA-UR-17-27820 DOI: 10.1007/JHEP04(2018)149)

Lee, C., V. P. Vaidya, and D. Kang. Semi-analytic method for resummation of TMD cross sections. Submitted to *Advances in High Energy Physics*. (LA-UR-18-31095)

Li, A., H. Li, I. Moulton, and H. X. Zhu. The Transverse Energy-Energy Correlator in the Back-to-Back Limit. Submitted to *Physical Review Letters*. (LA-UR-19-20914)

Li, H., and I. M. Vitev. Jet splitting functions in the vacuum and in a QCD medium. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-20679)

Li, H., and I. M. Vitev. Inclusive heavy flavor jet production with semi-inclusive jet functions: from proton to heavy-ion collisions. Submitted to *Journal of High Energy Physics*. (LA-UR-19-20952)

Vaidya, V. P., and Y. Makris. Transverse momentum spectra at threshold for groomed heavy quark jets. Submitted to *JHEP, Physics Web arXiv*. (LA-UR-18-26754)

Vitev, I. M. Vector-boson-tagged jet production in heavy ion collisions at energies available at the CERN Large

Hadron Collider. 2017. *Physical Review C*. (1) 014912. (LA-UR-17-21900 DOI: 10.1103/PhysRevC.96.014912)

Vitev, I. M. Future physics opportunities for high-density QCD at the LHC with heavy-ion and proton beam. Unpublished report. (LA-UR-19-22345)

Vitev, I. M. A complete set of in-medium splitting functions to any order in opacity. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-19-22343)

Vitev, I. M., and H. Li. Inverting the mass hierarchy of jet quenching effects with prompt - jet substructure. To appear in *Journal of Physics: Conference Series*. 12020. (LA-UR-18-20402 DOI: 10.1088/1742-6596/1070/1/012020)

Vitev, I. M., and R. Sharma. Collisional and thermal dissociation of J/ψ and $\psi(2S)$ states at the LHC. 2018. *Physics Letters B*. 384-391. (LA-UR-18-20593 DOI: 10.1016/j.physletb.2018.01.038)

Understanding Ejecta, Transport, Break-up and Conversion Processes (U)

William Buttler
20170082DR

Project Description

The scientific understanding essential for stockpile stewardship encompasses a broad range of phenomena that require a concerted effort in theoretical and experimental physics. The phenomena occurring at high density and very short micro-second time scales require sophisticated, frontier, experimental techniques and new theoretical methods. These are joined in this project for one of the unresolved issues in the physics of what occurs when a shockwave impacts a metal-gas interface susceptible to chemical reaction, in this case hydriding at a cerium-hydrogen gas interface. The detailed understanding of the state, composition, size and velocity of hydride material particulates (ejecta) produced that this project will provide will result in essential understanding and predictive models for these important phenomena for the first time.

Lone, A. Llobet Megias, R. Manzanares, J. I. Martinez, D. W. Schmidt, D. G. Sheppard, G. D. Stevens, W. D. Turley, and L. R. Veaser. Ejecta Transport, Breakup and Conversion. *Journal of Dynamic Behavior of Materials*. (LA-UR-16-28075 DOI: 10.1007/s40870-017-0114-6)

Hammerberg, J. E. (U) A model for the initial stage of ejecta breakup. Presented at *NECDC2018*. (Los Alamos, New Mexico, United States, 2018-10-15 - 2018-10-19). (LA-UR-19-20821)

Shivprasad, A. P., J. R. Wermer, T. A. Saleh, J. T. White, E. P. Luther, and V. R. Dasari. DEVELOPMENT OF SINTERED YTTRIUM DIHYDRIDE COMPACTS FOR NUCLEAR REACTOR MODERATOR APPLICATIONS. Presented at *Nuclear and Emerging Technologies for Space*. (Richland, Washington, United States, 2019-02-25 - 2019-02-25). (LA-UR-18-29796)

Publications

Bjorgaard, J. A., D. G. Sheppard, and J. E. Hammerberg. Density functional theory study of cerium deuterides. Submitted to *AIP Conference Proceedings*. (LA-UR-17-27804)

Bjorgaard, J. A., and D. G. Sheppard. Material properties of metal hydrides from ab initio calculations. Unpublished report. (LA-UR-17-27863)

Buttler, W. T., J. D. Schwarzkopf, R. K. Schulze, J. C. Cooley, J. E. Hammerberg, J. E. Barefield, J. J. I. Goett, M. Grover, B. M. La Lone, R. Manzanares, J. I. Martinez, D. W. Schmidt, G. D. Stevens, W. D. Turley, J. A. Bjorgaard, J. J. Charonko, A. T. Nelson, M. M. Schauer, D. G. Sheppard, R. J. Valencia, J. R. Wermer, and J. G. Mance. (U) Ejecta transport, breakup and conversion 2.0. Submitted to *NEDPC Proceedings*. (LA-UR-18-21663)

Buttler, W. T., R. J. R. Williams, and F. M. Najjar. Foreword to the Special Issue on Ejecta. 2017. *Journal of Dynamic Behavior of Materials*. (2) 151-155. (LA-UR-17-23785 DOI: 10.1007/s40870-017-0120-8)

Buttler, W. T., S. K. Lamoreaux, R. K. Schulze, J. D. Schwarzkopf, J. C. Cooley, M. Grover, J. E. Hammerberg, B. M. La

Deepening Los Alamos National Laboratory's Neutrino Legacy

Steven Elliott
20180038DR

Project Description

This project will develop and maintain several important capabilities for the Laboratory. These include isotope identification skills defined by both experimental and analytical techniques; the development of radiation detection skills and the analysis of arrays of radiation detectors; the development of radio-pure materials; and the theoretical and large-scale computational analysis of phenomena in hadronic physics and in complex nuclei and novel double beta decay physics. This proposal paves the way and reduces risk for the Department of Energy's plan for a 1000-kg project and enhances Los Alamos' reputation as a scientific leader. This program has had a large impact on recruitment at the laboratory. Of the 15 completed post-docs from the last decade on the Weak Interactions team, 5 are now staff scientists at LANL and 5 are faculty at Universities. The remaining are working in industry or other laboratories. Past Theory postdocs at the lab are employed within the laboratory, as faculty at universities, or continue as postdocs at universities or laboratories.

Publications

Elliott, S. R., P. Chu, B. White, K. R. Rielage, R. Massarczyk, and X. B. Zhu. A Search for Neutrinoless Double-Beta Decay in ^{76}Ge with 26 kg-yr of Exposure from the Majorana Demonstrator. Submitted to *Physical Review C*. (LA-UR-19-20700)

Elliott, S. R., P. Chu, R. Massarczyk, K. R. Rielage, B. White, and X. B. Zhu. Search for Tri-Nucleon Decay in the MAJORANA DEMONSTRATOR. Submitted to *Physical Review D*. (LA-UR-18-31257)

Elliott, S. R., P. Chu, R. Massarczyk, K. R. Rielage, X. B. Zhu, and B. White. Multi-site event discrimination for the Majorana Demonstrator. Submitted to *Physical Review C*. (LA-UR-19-20305)

Elliott, S. R., and F. Avignone. The Search for Double Beta Decay with Germanium Detectors: Past, Present and Future. Submitted to *Frontiers in Physics*. (LA-UR-18-30325)

Nuclear and Particle Futures

Directed Research
Continuing Project

Quantifying Effects of Magnetic Fields for Inertial Confinement Fusion (ICF)/High-Energy-Density (HED) Plasmas with Instabilities and Turbulence (U)

Kirk Flippo
20180040DR

Project Description

This project helps address energy security and stockpile stewardship challenges by helping to understand and quantify the roles of self-generated magnetic fields in Inertial Confinement Fusion (ICF) implosions like those at the National Ignition Facility (NIF).

Publications

Li, H. Signatures of Alfvén-mode and Slow-mode Waves and Non-Propagating Structures in 3D Compressive MHD Turbulence. Submitted to *Astrophysical Journal*. (LA-UR-18-30429)

Rasmus, A. M. Shock driven discrete vortex growth on oblique interfaces. Unpublished report. (LA-UR-18-26572)

Nuclear and Particle Futures

Directed Research
Continuing Project

A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility

Mark Schmitt
20180051DR

Project Description

We will investigate key aspects of achieving ignition using direct laser drive of a triple shell implosion system. The achievement of fusion in the laboratory is a grand challenge problem whose solution would be recognized worldwide and advance research in both fusion energy and weapons science. If successful, a completely new venue for experiments to understand and explore the conditions of ignition in the laboratory would be born.

Publications

- Betti, R., E. M. Campbell, P. McKenty, K. Molvig, and M. J. Schmitt. Stable and confined burn in a Revolver ignition capsule. 2018. *Physics of Plasmas*. (8) 82708. (LA-UR-18-23353 DOI: 10.1063/1.5037224)
- Scheiner, B. S., and M. J. Schmitt. The role of incidence angle in the laser ablation of ICF targets. Submitted to *Physics of Plasmas*. (LA-UR-18-24731)
- Schmitt, M. J., and B. S. Scheiner. The role of incidence angle in the laser ablation of a planar target. 2019. *Physics of Plasmas*. (2) 024502. (LA-UR-18-29321 DOI: 10.1063/1.5085122)

Cosmic Positrons from Pulsar Winds and Dark Matter

Brenda Dingus
20160007DR

Project Description

Satellite observations reveal a puzzling excess of cosmic positrons, the anti-matter partner of electrons. We will use observations of high energy gamma rays and theoretical models to constrain positrons from astrophysical sources and from dark matter. While the existence of dark matter is well known, the nature of the particles that comprise dark matter is not. With this project, we will increase our understanding of the possible properties of dark matter. Also, the existence of high energy emission from pulsars is well known; however, the physical mechanisms by which the particles are accelerated is not. With this project, we will detect higher energies from pulsars and compare these observations with new theoretical models. Finally, we will use radiation transport simulations to predict the locally-measured, cosmic positrons from both dark matter and pulsars. These investigations will increase the Laboratory's capabilities in information science and technology as well as remote sensing of radiation and other experimental techniques relevant to studies of our nuclear stockpile.

Technical Outcomes

This project made observations with the High Altitude Water Cherenkov (HAWC) observatory that have ruled out the prior best explanation of the origin of the locally measured excess of positrons. We have also found new sources of TeV gamma rays and have made theoretical predictions of how positrons are accelerated in these sources and travel to Earth. Dark matter models have been constrained by the TeV gamma-ray observations and alternative theoretical models have been investigated.

Publications

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Pushing the Precision Frontier at the Upgraded Los Alamos National Laboratory Ultra-cold Neutron Facility

Takeyasu Ito
20180085DR

Project Description

We will develop an experiment to study a small separation of the positive and negative charges inside the neutron and the theory to interpret the results, to solve the mystery of why this universe has so much more matter than antimatter. This project will advance the nation's experimental capability to detect small signals and computational capability to solve complex problems using supercomputers. Both of these will have a wide variety of applications in many areas, including science, industry, and national security. In addition, this project will help attract new young talent to the Los Alamos National Laboratory's weapon complex.

Technical Outcomes

This project focused on initial studies to reduce the risk of further R&D in this area. Our achievements are: (1) detailed characterization of a commercially available atomic magnetometer, (2) ultracold neutron transport study through the new ultracold neutron beamline, (3) development of a design for non-magnetic 200kV high-voltage feedthrough, and (4) procurement of a ultracold neutron switcher, and (5) technology development needed to compute neutron electric dipole moment signal from time-reversal violating gluonic operators.

Publications

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Search for Low Mass Dark Photons in High Energy Proton-Nucleus (p+A) Collisions at Fermilab

Ming Liu
20160081ER

Project Description

A new detector and theory will be developed in this project to identify the signal of dimuons from dark photon decays at Fermilab. Dark photons are a candidate for dark matter that is needed to account for the key properties of the observed Universe. We propose to carry out a new direct search for dark photons by colliding the 120 Giga Electron Volt (GeV) proton beam from the Fermilab Main Injector with the 5 meter (m) thick iron beam dump at the E906 experiment. With the world highest integrated luminosity, we could directly create and detect dark photons in the so called visible decay mode. A new dedicated trigger detector will be developed in this project to identify dimuon events from dark photon decays. The development of new fast high-resolution tracking detectors and trigger systems would benefit global security and the production of materials at the mesoscale.

Technical Outcomes

This project established a new dark sector physics search program with a new dark photon trigger in the SeaQuest experiment, utilizing the 120GeV proton beam from the Fermilab. The new detectors were successfully installed and commissioned in 2017, and have shown high tracking efficiency over 95%, exceeding the design goal of 90%. Full physics data will be taken parasitically with the E1039 experiment in 2019-2021 to produce world best measurements of dark photon search.

Publications

Liu, M. X. Prospects of direct search for dark photon and dark Higgs in SeaQuest/E1067 experiment at the Fermilab main injector. 2017. *Modern Physics Letters A*. (10) 1730008. (LA-UR-17-23021 DOI: 10.1142/S0217732317300087)

The Cosmogenic Origins of Iron-60

Aaron Couture
20160173ER

Project Description

In this project, we will perform measurements taking advantage of beams of iron-59 to study the nuclear physics needed to provide robust reaction rate predictions and incorporate them into hydrodynamic models of the supernova progenitor. The successful completion of this project will deliver, for the first time, experimentally based iron-60 yield and uncertainties from a core-collapse supernova. It will provide first studies of turbulence-based asymmetries in that yield. In the process of answering this over-arching question, it will answer additional questions about anomalous low-lying strength in the photon-strength function of iron isotopes, including answering questions about the multipolarity of that strength. This project will test and implement techniques to provide reliable neutron capture cross sections in regions where they cannot be measured directly, a critical step towards developing a fully predictive theoretical framework for nuclear reaction cross-sections in intermediate and heavy nuclei.

Technical Outcomes

Capture measurements on ^{57}Fe , ^{61}Ni , and ^{56}Fe were completed at LANSCE. Intensities were lower than predicted for $d(^{59}\text{Fe}, ^{60}\text{Fe})p$ at Argonne due to accelerator issues. A path to study this at TAMU was developed, and design simulation was completed for future experimental implementation. Nuclear theory work providing a correlation of M1 strength to nuclear deformation was developed and implemented in the CoH code. Sensitivity studies were performed for massive stars to study the ^{60}Fe ejected.

Publications

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Shining Light on the Dense Gluon Structure of Large Nuclei

Ivan Vitev
20160183ER

Project Description

This project will perform the first global extraction of a new class of 3D gluon densities in heavy nuclei, make them available to the wider community, and establish conclusively if a quantum coherent scattering regime has been reached in proton-nucleus reactions. Nucleons (protons and neutrons) are not fundamental building blocks of matter, but are in turn made up of quarks and gluons. Quantum Chromodynamics (QCD), the underlying theory of strong interactions, describes how quarks and gluons determine the properties of nucleons and nuclei. The overarching goal of this project is to develop theoretical and computational tools to unambiguously identify and accurately characterize such novel quantum coherent scattering regime of QCD at the Relativistic Heavy Ion Collider and the Large Hadron Collider. This work will enhance national scientific capabilities needed to address DOE milestones set by the Nuclear Science Advisory committee.

Technical Outcomes

This project developed a broadly-applicable theoretical framework to handle the problem of multiple scattering between an external probe and nuclear matter in the full range of kinematic relevance: from a dilute to a dense gluon system. We applied this formalism to understand virtual photon production, jet production, as well as spin-dependent quark and gluon distributions in large nuclei, providing essential theoretical constraints on the three-dimensional gluon densities in nucleons and nuclei.

Publications

Kang, Z., F. Ringer, and I. Vitev. Effective field theory approach to open heavy flavor production in heavy-ion collisions. Submitted to *JOURNAL OF HIGH ENERGY PHYSICS*. (LA-UR-18-29561)

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Martinez, M., M. D. Sievert, and D. E. Wertepny. Multiparticle Production at Mid-Rapidity in the Color-Glass Condensate. Submitted to *Journal of High Energy Physics (JHEP)*. (LA-UR-18-27839)

Martinez, M., M. D. Sievert, and D. Wertepny. Toward initial conditions of conserved charges. Part I. Spatial correlations of quarks and antiquarks. 2018. *Journal of High Energy Physics*. (7) 3. (LA-UR-18-20595 DOI: 10.1007/JHEP07(2018)003)

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A Rigorous Multiscale Method to Couple Kinetic and Fluid Models

Xianzhu Tang
20160361ER

Project Description

This project will develop a rigorous multiscale method that couples kinetic (microscopic) model at internal boundary layers to a global continuum (macroscopic) model elsewhere for superior computational efficiency and global physics fidelity. This project will produce a physically sound and mathematically rigorous multiscale scheme that couples a non-perturbative kinetic model at internal boundary layers (IBL) to a perturbative fluid model away from the IBLs. We will demonstrate the fidelity and efficiency of the multiscale scheme in two prototypical applications of importance to space weather, inertial confinement fusion, and magnetic confinement fusion. DOE has identified these problems as key mission challenges in national security and energy security. Our innovation is also of a fundamental nature in the context of kinetic transport theory and multiscale modeling.

Technical Outcomes

The development and deployment of the proposed rigorous coupling scheme allowed this project to perform first-in-kind simulations that showed how hydrodynamic mix in an inertial confinement fusion target can both aggravate and mitigate the kinetic modification of fusion reactivity. The aggravation comes from the well-known Knudsen-layer reactivity reduction due to decrease in fuel pocket size. The mitigation effect is due to the so-called diffusive tunneling mechanism caused by the reduction of the inert pusher layer width.

Publications

Guo, Z., T. M. Elder, X. Tang, and C. J. McDevitt. Diffusive tunneling in an isobaric but non-isothermal fuel-pusher mixture. 2019. *Physics of Plasmas*. (1) 012711. (LA-UR-18-27564 DOI: 10.1063/1.5057444)

McDevitt, C. J., X. Tang, and Z. Guo. Yield reduction via the Knudsen layer effect in a mixture of fuel and pusher material. To appear in *Plasma Physics and Controlled Fusion*. (LA-UR-17-23111 DOI: 10.1088/1361-6587/aeee5a)

McDevitt, C. J., X. Tang, and Z. Guo. Fast ion transport at a gas-metal interface. 2017. *Physics of Plasmas*. (11) 112702. (LA-UR-17-25628 DOI: 10.1063/1.4998462)

Tang, X., T. M. Elder, C. J. McDevitt, and Z. Guo. Diffusive tunneling of Gamow fuel ions in a mixture of fusion fuel and inert pusher. Submitted to *Europhysics Letters*. (LA-UR-18-27583)

Bridging Knowledge Gaps in Simulations of Inertial Confinement Fusion (ICF) Implosions

Andrei Simakov
20160458ER

Project Description

Standard numerical simulation tools for Inertial Confinement Fusion miss some important physics and are thus not predictive. We will use our new code to identify which missing physics is important and assess how to include it into the standard codes. We hope to achieve four major goals: (i) to perform detailed kinetic studies of several individual physical mechanisms not included in hydrodynamic codes and assess their importance; (ii) to carry out several integrated kinetic simulations of realistic implosions of gas-filled OMEGA capsules and, by comparing with hydrodynamic simulations, assess which kinetic mechanisms play important roles under realistic circumstances; (iii) this should allow us to start charting applicability boundaries for hydrodynamic simulations of gas-filled capsule implosions; (iv) once the importance of a kinetic mechanism is established, we will explore possible approaches for incorporating the missing physics into hydrodynamic codes.

Technical Outcomes

This project successfully (i) performed kinetic simulations of OMEGA ICF capsule implosions; (ii) demonstrated that accounting for shock-driven mix at material interfaces and capsule-fuel ion stratification, and plasma-ion viscosity is crucial for the implosions simulations; (iii) demonstrated that hydrodynamics fails to accurately describe strong plasma shocks with Mach numbers above 3, which are essential for ICF; (iv) helped xRAGE developers with testing the new multi-ion-hydro capability, aiming at incorporating the missing physics, against kinetic simulations.

Publications

Keenan, B., A. N. Simakov, L. Chacon, and W. Taitano. Deciphering the kinetic structure of multi-ion plasma shocks. 2017. *Physical Review E*. (5) 053203. (LA-UR-17-25337 DOI: 10.1103/PhysRevE.96.053203)

Keenan, B., A. N. Simakov, W. Taitano, and L. Chacon. Ion species stratification within strong shocks in two-ion plasmas. 2018. *Physics of Plasmas*. (3) 32103. (LA-UR-17-31485 DOI: 10.1063/1.5020156)

Simakov, A. N., B. Keenan, W. Taitano, and L. Chacon. Plasma ion stratification by weak planar shocks. 2017. *Physics of Plasmas*. (9) 092702. (LA-UR-17-25524 DOI: 10.1063/1.4995427)

Taitano, W., A. N. Simakov, L. Chacon, and B. Keenan. Shock-Driven Kinetic Fuel-Species Separation and Yield Degradation in Inertial-Confinement-Fusion Implosions. Submitted to *Physics of Plasmas*. (LA-UR-17-31453)

Taitano, W., A. N. Simakov, L. Chacon, and B. Keenan. Yield degradation in inertial-confinement-fusion implosions due to shock-driven kinetic fuel-species stratification and viscous heating. 2018. *Physics of Plasmas*. (5) 56310. (LA-UR-18-20952 DOI: 10.1063/1.5024402)

Taitano, W., L. Chacon, A. N. Simakov, and S. E. Anderson. A conservative phase-space moving-grid strategy for a 1D-2V Vlasov-Fokker-Planck Equation. Submitted to *Journal of Computational Physics*. (LA-UR-19-22284)

Taitano, W., L. Chacon, and A. N. Simakov. An adaptive, implicit, conservative, 1D-2V multi-species Vlasov-Fokker-Planck multi-scale solver in planar geometry. 2018. *Journal of Computational Physics*. 173-205. (LA-UR-17-26086 DOI: 10.1016/j.jcp.2018.03.007)

Kinetic Modeling of Next-Generation High-Energy High-Intensity Laser-Ion Accelerators as an Enabling Capability

Lin Yin
20160472ER

Project Description

This project will apply a best-in-class vector particle-in-cell (VPIC) kinetic modeling capability on Los Alamos supercomputing platforms to guide a comprehensive, theoretical study of nonlinear, relativistic, laser-plasma interaction physics. Laser-driven ion accelerators enable important applications in high energy density science, matter in the extremes, and diagnostic science at the Laboratory. Such short pulse lasers continue to be a vital development path for advanced diagnostics of materials, and our work will help define more clearly the design requirements of facilities like MaRIE. The culmination of this work will be an advanced, validated design capability for developing ion sources of relevance to Los Alamos science campaigns.

Technical Outcomes

The most critical, lasting outcome of this project is the resolution of a long-standing controversy in the field of next-generation laser-ion accelerators as well as documentation of simulation best practices for reliable kinetic modeling of these accelerators. This project has been highly successful, garnering several invited talks and high-profile papers, and has further established Los Alamos as world leaders in this field.

Publications

Jansen, O., T. Wang, D. J. Stark, E. d'Humieres, T. Toncian, and A. Arefiev. Leveraging extreme laser-driven magnetic fields for gamma-ray generation and pair production. 2018. *Plasma Physics and Controlled Fusion*. (5) 54006. (LA-UR-18-21518 DOI: 10.1088/1361-6587/aab222)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom, and R. F. Bird. A detailed examination of laser-ion acceleration mechanisms in the relativistic transparency regime using tracers. To appear in *Physics of Plasmas*. (4) 43114. (LA-UR-18-21781 DOI: 10.1063/1.5028129)

Stark, D. J., L. Yin, B. J. Albright, and F. Guo. Effects of dimensionality on kinetic simulations of laser-ion acceleration in the transparency regime.

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Stark, D. J., L. Yin, and B. J. Albright. Harnessing the relativistic Buneman instability for laser-ion acceleration in the transparency regime. To appear in *Physics of Plasmas*. (6) 62107. (LA-UR-18-21829 DOI: 10.1063/1.5028128)

Lepton Number Violation: Connecting the Tera Electron Volt (TeV) Scale to Nuclei

Vincenzo Cirigliano
20170290ER

Project Description

Neutrinoless double beta decay is a rare nuclear process whose observation would prove that neutrinos, the most elusive elementary particles, coincide with their own antiparticles. This could happen only if at a fundamental level the "matter number" is not conserved in nature. The observation of such a process would therefore have deep implications on our understanding of the matter-antimatter asymmetry in the universe. In the Nuclear Science Advisory Committee's 2015 Long Range Plan, the US Nuclear Physics community identified "the timely development and deployment of a US-led ton-scale neutrinoless double beta decay experiment" as the highest priority for new projects across all the subfields of nuclear physics. By developing a broader theoretical framework for the interpretation of neutrinoless double beta decay searches, our project will strengthen the case for such a high-profile DOE endeavor.

Publications

- Alioli, S., E. Mereghetti, W. G. Dekens, V. Cirigliano, and J. de Vries. Right-handed charged currents in the era of the Large Hadron Collider. 2017. *Journal of High Energy Physics*. (5) 86. (LA-UR-17-21898 DOI: 10.1007/JHEP05(2017)086)
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Exploring the Multi-scale Physics that Regulates Black Hole Accretion

Joseph Smidt
20170317ER

Project Description

This project aims to provide the first definitive simulations showing how black holes with over a billion solar masses formed in the early universe. These calculations will require next-generation radiation-hydrodynamics simulations at many lengths scales. Understanding radiation hydrodynamics and radiation-matter coupling are primary science objectives of the Department of Energy (DOE). Black holes provide radiation feedback to matter on energy scales that range from a few eV to several keV. These radiation-hydrodynamical simulations will utilize multigroup radiation transport methods to analyze these feedback effects on matter that builds the underlying science of interest to the DOE. The effects of this multigroup radiation transport and matter coupling will be documented in our publications. The observational signatures published by this work will be directly used by NASA surveys such as JWST to classify supermassive black holes, as well as surveys that collaborate with NASA efforts such as ALMA. Probing black holes is one of NASA's main science goals and objectives. How the billion solar mass supermassive black holes formed in the early universe is one of the outstanding questions in cosmology. By detailing comprehensively how such black holes formed, this work will have a major impact on the cosmology and astrophysics communities.

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Black, W. K. Primordial Origins of Supermassive Black Holes. Unpublished report. (LA-UR-18-26505)

Johnson, J. L., and A. Aykotalp. Extreme Population III Starbursts and Direct Collapse Black Holes Stimulated by High Redshift Quasars. Submitted to *Monthly Notices of the Royal Astronomical Society.* (LA-UR-18-31390)

Smidt, J. M., J. L. Johnson, H. Li, and D. Whalen. HOW SUPERMASSIVE BLACK HOLES FORM BY $Z \sim 7$. Submitted to *The Astrophysical Journal.* (LA-UR-16-28026)

Waters, T. R. Magnetothermal disc winds in X-ray binaries: poloidal magnetic fields suppress thermal winds. To appear in *Monthly Notices of the Royal Astronomical Society.* (LA-UR-18-25178 DOI: 10.1093/mnras/sty2398)

Publications

Aykotalp, A., K. Barrow, and J. Wise. X-RAY INDUCED STELLAR POPULATION IN DCBH HOST GALAXIES. Submitted to *ApJL.* (LA-UR-17-31075)

S. Barrow, K. S., A. Aykotalp, and J. H. Wise. Photometry and Spectrometry of a Direct-Collapse Black Hole Scenario. Submitted to *Nature.* (LA-UR-17-30611)

S. Barrow, K. S., J. H. Wise, A. Aykotalp, B. W. OShea, M. L. Norman, and H. Xu. First light – II. Emission line extinction, population III stars, and X-ray binaries. 2018. *Monthly*

Realization of a Laboratory Turbulent Magnetic Dynamo: A Gateway to New Laboratory Astrophysics and Inertial Confinement Fusion Experiments

Kirk Flippo
20170367ER

Project Description

When plasmas flow they create electric and magnetic fields, and as it turns out, these processes essentially magnetize the entire universe; turbulent magnetic dynamo in particular is poorly understood. Recently it has been suggested that these fields can also have a larger impact on the flow of plasmas on the small scale, like in an Inertial Confinement Fusion (ICF) capsule, than previously had been thought. This could lead to degradation in ICF yields. This project will help us understand how easily and how strongly these fields are created under similar conditions using a turbulent plasma plume design. Studying how these dynamos can saturate is an important step in understanding how important these fields can be to the dynamics of an ICF implosion.

Publications

Li, S., A. S. Liao, H. Li, K. A. Flippo, A. M. Rasmus, D. H. Barnak, C. Y. Fiedler Kawaguchi, K. V. Kelso, C. C. Kuranz, C. Li, S. R. Klein, and J. Levesque. Design of a New Turbulent Dynamo Experiment on the OMEGA-EP. Submitted to *Physics of Plasmas*. (LA-UR-18-30966)

Rasmus, A. M. Shock driven discrete vortex growth on oblique interfaces. Unpublished report. (LA-UR-18-26572)

Quantum Effects on Cosmological Observables: Probing Physics Beyond the Standard Model

Mark Paris
20170430ER

Project Description

The Laboratory's mission to maintain the safety and reliability of the nuclear stockpile requires detailed numerical computations that describe how weapons function. In particular, ever-more precise and complete descriptions of the nuclear reactions, which our proposal will constrain to high accuracy, are required. This project will use new, precision data obtained from astronomy and cosmology from some of the largest observables length scales to constrain the microscopic physics relevant for nuclear reactions, which are also important for understanding the function of nuclear weapons.

Publications

Coriano, C., E. Mottola, and M. M. Maglio. TTT in CFT: Trace Identities and the Conformal Anomaly Effective Action. Submitted to *Journal of High Energy Physics*. (LA-UR-17-22382)

Giorgi, E. E. An alternative theory looks at black holes $\text{as surfaces, not holes}$. Unpublished report. (LA-UR-17-21316)

Grohs, E. B., M. W. Paris, G. M. Fuller, and C. T. Kishimoto. Lepton asymmetry, neutrino spectral distortions, and big bang nucleosynthesis. 2017. *Physical Review D*. (6) 063503. (LA-UR-16-29176 DOI: 10.1103/PhysRevD.95.063503)

Ma, L., S. M. Shalgar, and H. Duan. Matter parametric neutrino flavor transformation through Rabi resonance. Submitted to *Physical Review D*. (LA-UR-18-25879)

Mottola, E. Decay of the de Sitter Vacuum. Submitted to *Physical Review D*. (LA-UR-17-28548)

Paris, M. W. Institutional Computing: Final Report Quantum Effects on Cosmology: Probing Physics Beyond the Standard Model with Big Bang Nucleosynthesis. Unpublished report. (LA-UR-18-21137)

Paris, M. W. Institutional Computing: Annual Report, Quantum Effects on Cosmology: Precision Probes of Nuclear

and Particle Physics with Big Bang Nucleosynthesis. Unpublished report. (LA-UR-19-21816)

Paris, M. W., V. Cirigliano, and S. M. Shalgar. Collective neutrino oscillations with the halo effect in single-angle approximation. Submitted to *Journal of Cosmology and Astroparticle Physics*. (LA-UR-19-20928)

Shalgar, S. M. Collective neutrino oscillations with the halo effect in single-angle approximation. Submitted to *Journal of cosmology and astroparticle physics*. (LA-UR-18-25562)

Shalgar, S. M. Multi-angle calculation of the matter-neutrino resonance near an accretion disk. To appear in *Journal of Cosmology and Astroparticle Physics*. (02) 10-10. (LA-UR-17-26195 DOI: 10.1088/1475-7516/2018/02/010)

Shalgar, S. M., V. Cirigliano, and M. W. Paris. Effect of collisions on neutrino flavor inhomogeneity in a dense neutrino gas. 2017. *Physics Letters B*. (LA-UR-17-24744 DOI: 10.1016/j.physletb.2017.09.039)

Nuclear and Particle Futures

Exploratory Research
Continuing Project

Beat-Wave Magnetization of a Dense Plasma

Scott Hsu
20170457ER

Project Description

The beat-wave magnetization problem studied in this project could enable a new lower-cost pathway to fusion energy, synergistic with the approaches being studied as part of the ARPA-E ALPHA program in developing lower-cost approaches to fusion energy.

Publications

Hsu, S. C., and S. Langendorf. Magnetized Plasma Target for Plasma-Jet-Driven Magneto-Inertial Fusion. To appear in *Journal of Fusion Energy*. (LA-UR-18-21935 DOI: 10.1007/s10894-018-0168-z)

Enabling Electron Excitations in the Modeling of Warm Dense Matter

Jerome Daligault
20170490ER

Project Description

The issues we address affect national energy and security missions at Los Alamos, which require high-fidelity computer simulations that rely on accurate plasma properties over a wide range of physical conditions, and in particular of warm dense matter (WDM) conditions that occur during the implosion phase of inertial confinement fusion capsules and in nuclear explosions. By its intermediate nature, the WDM regime does not fall neatly within the parameter space typical of either ordinary condensed-matter physics or plasma physics, and the standard simplifying approximations of these fields no longer apply. As a consequence, our theoretical understanding of this extreme state of matter relies mostly on advanced computer simulations. The new computational tools we are developing in this project will open the door to simulations of non-equilibrium processes in WDM. This will greatly advance our ability to compute self-consistently a large number of physical properties of WDM. In particular, programmatically relevant processes include the energy exchange rates between electrons and ions, and the stopping power of charged projectiles.

Daligault, J. O., and D. V. Mozyrsky. Nonadiabatic quantum molecular dynamics with detailed balance. To appear in *Physical Review B*. (20) 205120. (LA-UR-17-26600 DOI: 10.1103/PhysRevB.98.205120)

Daligault, J. O., and S. Baalrud. Transport regimes spanning magnetization-coupling phase space. 2017. *Physical Review E*. (4) 043202. (LA-UR-17-25086 DOI: 10.1103/PhysRevE.96.043202)

Publications

Baalrud, S. D., and J. O. Daligault. Mean Force Plasma Kinetic Theory: a Convergent Kinetic Theory for Weakly and Strongly Coupled Plasmas. Submitted to *Physics of Plasmas*. (LA-UR-19-22330)

Daligault, J. O. Constrained-Search Variational Formulation of Time-Dependent Density Functional Theory. Submitted to *Physical Review A*. (LA-UR-18-26666)

Daligault, J. O. Universal character of atomic motions at the liquid-solid transition. Submitted to *Physical Review Letters*. (LA-UR-18-27895)

Daligault, J. O. Crossover from Classical to Fermi Liquid Behavior in Dense Plasmas. 2017. *Physical Review Letters*. (4) 045002. (LA-UR-17-22894 DOI: 10.1103/PhysRevLett.119.045002)

Nuclear and Particle Futures

Exploratory Research
Continuing Project

MEXRAY- (ME)chanical XRAY

Scott Watson
20180037ER

Project Description

This project will enable lightweight, field-portable, x-ray units for use in nuclear counter-terrorism environs. In addition, this project will enable x-ray movies suitable for use with a wide variety of explosive testing for Stockpile Stewardship programs.

Publications

Winch, N. M., S. A. Watson, E. B. Sorensen, and D. Platts.
MEchanical X_RAY (MEXRAY) Generator for Megavolt Radiography. Presented at *IEEE Nuclear Science Symposium and Medical Imaging Conference*. (Sydney, Australia, 2018-11-10 - 2018-11-10). (LA-UR-18-31645)

Nuclear and Particle Futures

Exploratory Research
Continuing Project

Nonlinear Dynamics of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams

Lin Yin
20180074ER

Project Description

Achieving inertial fusion ignition in the Laboratory has broad national security implications for understanding the challenging physics inside nuclear weapons. Laser-plasma instabilities (LPI) hamper the ability to compress laser-driven inertial fusion capsules to ignition conditions by decreasing the amount of laser energy that can be used for compression. This project seeks to apply best-in-class modeling capability to understand and mitigate LPI. If successful, the work may enable the design of inertial fusion experiments with higher yield and improved applicability to outstanding weapons science issues.

Publications

Yin, L., B. J. Albright, D. J. Stark, R. F. Bird, W. D. Nystrom, and K. J. Bowers. Nonlinear electron and ion dynamics in the saturation of crossed-beam energy transfer. Submitted to *Physical Review Letters*. (LA-UR-19-22181)

Production of Shaped Electron Bunches with Diamond Field Emitter Array Cathodes

Evgenya Simakov
20180078ER

Project Description

This project has the potential to advance the diamond field emitter array (DFEA) cathode technology and make it suitable for a number of national security applications that require high current, high power electron beams. This includes compact accelerators for warfighter support (e.g. small weaponized free-electron lasers), active interrogation, environmental remediation, and multi-MW X-ray sources. DFEAs present the most natural means of producing very high current electron bunches: they produce electron beams from the tips of diamond pyramids that can be fabricated and arranged in customized arbitrary patterns to suit the particular application, they generate a very stable and robust electron beam, and they produce the extremely high current densities that are necessary for obtaining multi-nano-Coulomb bunches.

Publications

Nichols, K., E. I. Simakov, D. Shchegolkov, and H. L. Andrews.
MODELING OF DIAMOND FIELD EMITTER ARRAYS FOR
SHAPED ELECTRON BEAM PRODUCTION. Presented at *IPAC*
18. (Vancouver, Canada, 2018-04-29 - 2018-05-04). (LA-
UR-18-23590)

Search for Axion-mediated Interactions with a Spin-exchange Relaxation-free (SERF) Magnetometer

Young Jin Kim
20180129ER

Project Description

This project will improve the experimental limits of certain axion-mediated spin-dependent interactions over existing experiments, setting new experimental limits on the interaction range below 1 cm. The experimental results will have a profound impact on nuclear physics, astrophysics, and cosmology, and place Los Alamos in the leading position for precision testing of fundamental symmetries and axion searches. This project relies on Los Alamos' expertise in magnetic field sensing to develop new capabilities in fundamental physics and the search for axions. This research will expand the applications of spin-exchange relaxation-free (SERF) magnetometers beyond biophysics.

Publications

- Chu, P., L. D. Duffy, Y. J. Kim, and I. M. Savukov. Sensitivity of proposed search for axion-induced magnetic field using optically pumped magnetometers. 2018. *Physical Review D*. (7) 072011. (LA-UR-18-20811 DOI: 10.1103/PhysRevD.97.072011)
- Chu, P., Y. J. Kim, and I. M. Savukov. Search for an axion-induced oscillating electric dipole moment for electrons using atomic magnetometers. Unpublished report. (LA-UR-18-28540)
- Kim, Y. J., P. Chu, I. M. Savukov, and S. G. Newman. New limit on an exotic parity-odd spin- and velocity-dependent interaction using an optically polarized vapor. Submitted to *Nature Communications*. (LA-UR-19-20817)
- Kim, Y. J., P. Chu, and I. M. Savukov. Experimental Constraint on an Exotic Spin- and Velocity-Dependent Interaction in the Sub-meV Range of Axion Mass with a Spin-Exchange Relaxation-Free Magnetometer. 2018. *Physical Review Letters*. (9) 091802. (LA-UR-18-22161 DOI: 10.1103/PhysRevLett.121.091802)

Missing Physics behind X-ray Emission from High-Energy-Density Plasmas

Grigory Kagan
20180197ER

Project Description

Inertial confinement fusion (ICF) is the one of the most promising concepts for practical fusion energy. Its central idea is imploding a spherical capsule with the deuterium-tritium (DT) fuel, which is achieved by ablating its outer layers with high power lasers. In the successful scenario the resulting DT plasma is sufficiently hot and dense to attain and sustain the thermo-nuclear burn. While such scenarios are routinely seen in radiation-hydrodynamics (rad-hydro) simulations, their realization in experiments has failed. In the ignition scale experiments the main figure quantifying the implosion performance, the fusion yield, is found much lower than predicted. The key piece of information needed to understand the reasons and cure for this problem is the temperature of the burning plasma. Our project will develop a crucial model which will allow such a temperature diagnostics.

Publications

Kagan, G., O. Landen, D. Svyatsky, H. Sio, N. Kabadi, R. Simpson, M. Gatu Johnson, J. Frenje, R. Petrasso, R. Shah, T. R. Joshi, P. Hakel, T. Weber, H. Rinderknecht, D. Thorn, M. Schneider, D. Bradley, and J. Kilkenny. Inference of the electron temperature in inertial confinement fusion implosions from the hard X-ray spectral continuum. To appear in *Contributions to Plasma Physics*. (LA-UR-17-28158 DOI: 10.1002/ctpp.201800078)

Sio, H., J. A. Frenje, A. Y. Le, S. Atzeni, T. J. T. Kwan, M. Gatu Johnson, G. Kagan, C. Stoeckl, C. K. Li, C. E. Parker, C. J. Forrest, V. Glebov, N. V. Kabadi, A. Bose, H. G. Rinderknecht, P. Amendt, D. T. Casey, R. Mancini, W. Taitano, B. Keenan, A. N. Simakov, L. Chacon, S. P. Regan, T. C. Sangster, E. M. Campbell, F. H. Seguin, and R. D. Petrasso. Observations of multiple nuclear reaction histories and fuel-ion species dynamics in Inertial Confinement Fusion implosions. Submitted to *Physical Review Letters*. (LA-UR-18-30435)

Nuclear and Particle Futures

Exploratory Research
Continuing Project

Properties of Medium Nuclei from First Principles

Stefano Gandolfi
20180210ER

Project Description

This work will enable new algorithms for large scale supercomputing simulations of nuclei and nuclear reactions. Ultimately this work will be valuable for a better description of nuclei and reactions.

Publications

Roggero, A., and J. A. Carlson. Linear Response on a Quantum Computer. Submitted to *Physical Review Letters*. (LA-UR-18-22120)

Tews, I., J. Margueron, and S. Reddy. Confronting gravitational-wave observations with modern nuclear physics constraints. Submitted to *European Physical Journal A. Hadrons and Nuclei*. (LA-UR-19-20198)

Nuclear and Particle Futures

Exploratory Research
Continuing Project

Pinning Down the Neutrino-proton Process Importance in Heavy Element Production via Reaction Studies on Radioactive Nickel-56

Hye Young Lee
20180228ER

Project Description

The entire project effort, from radioactive sample production at the Isotope Production Facility to performing neutron-induced reactions at Los Alamos Neutron Science Center, can be only performed at the Los Alamos National Lab in the US. The project results will extend to the study of nuclear reactions on radioactive samples, directly related to the NNSA missions, including Rad Chem detector analysis, device diagnostics, etc. Through this project we will improve our understanding of nuclear reaction mechanisms for mission relevance.

Publications

- Lee, H. Y. LDRD Data Sheet for "Pinning Down the nu-p Process Importance in Heavy Element Production via Reaction Studies on Radioactive Ni-56 at LANSCE". Unpublished report. (LA-UR-18-25488)
- Lee, H. Y. Pinning Down the nu-p Process Importance in Heavy Element Production via Reaction Studies on Radioactive ^{56}Ni at LANSCE. Unpublished report. (LA-UR-17-30772)

Nuclear and Particle Futures

Exploratory Research
Continuing Project

Ultra-Diffuse Galaxies, Tidal Streams and Dwarf Galaxies: The Low-Surface Brightness Frontier

W Vestrand
20180257ER

Project Description

Detecting low surface brightness features is a long standing challenge for optical imagers that are conducting national security missions. The new imaging technology and image software that we are developing will dramatically improve the ability to detect low surface brightness features that would otherwise have gone undetected. Successful development of technology has the potential to favorably impact our capability to conduct the DOE/NNSA treaty monitoring mission. Additionally, it is likely to have important application to difficult remote sensing problems like the detection of plumes and chemical release clouds.

Disrupting Actinide Aqueous Processing: Additively Manufacturing High-Speed Counter-Current Chromatography Devices

Alexandria Marchi
20180602ER

Project Description

Advancing engineering design and manufacturing will produce more efficient processes affecting the way Los Alamos National Laboratory handles aqueous nuclear materials. For example, current Americium (Am) recovery from spent nuclear fuels involves multi-step processes including repetitive solvent separation lines to achieve sufficient purification. This complicated processing line accomplishes the separation of only one element from the nuclear fuel pool. HSCCC has shown the efficient elemental separation of rare earth elements. Thus, this individual technique, coupled with in-house manufacturing via additive manufacturing of chemical- and radiation-tolerant materials, could reduce the multi-step mono-elemental separation technique to the purification of multi-elements from a soup of radionuclides in a single step process.

Translational Cold Cathode Designs for Mission-Specific Applications

Nathan Moody
20180655ER

Project Description

Present and future x-ray light sources for both Los Alamos National Laboratory and the DOE complex require a robust, long-lived, high-brightness electron source that provides an ultra-low transverse emittance beam with bunch charge on the order of 1 nanocoulomb (nC), while other applications can benefit from photo-gated high-current emission with much less emphasis on reduced emittance. By supporting a first-principles understanding of the physics and chemistry governing emittance, quantum efficiency, and lifetime, the data obtained in this project provides upgrade and design options for a given X-ray Free-Electron Laser (XFEL). Specific advances include the option to switch from metal cathodes to higher performance semiconductor cathodes, yielding up to a 50% reduction in emittance. This reduces risk and increases flexibility throughout the design or upgrade path of a user facility. Additionally, evolving machine architectures requires a versatile electron source capability which this project supports.

Demonstration of Electron Beam Generation with a Novel Solid-State Amplifier Driven Accelerator for Space Deployment Applications

Dinh Nguyen
20170521ER

Project Description

Novel low-voltage-transistor-driven electron accelerators are needed for miniature, lightweight particle accelerators, which could enable cutting-edge tools for space science, environmental remediation, and homeland security missions. By eliminating high-power, high-voltage tube-based radio frequency (RF) sources, the new accelerators will be less expensive, require less supporting infrastructure, and be safer to maintain and operate. The goal of this effort is to demonstrate the ability of a new class of RF amplifier chips, high-electron-mobility transistors (HEMTs), to successfully power a particle accelerator. Specifically, the research team has delivered an energy boost to electrons emitted from a commercial electron beam source, using an RF accelerator cavity driven by a single HEMT chip. Over a distance of approximately 6 millimeters (mm), electrons in the beam had been given a 15-kilovolt (kV) increase in energy. This demonstration of energy gain in RF cavities individually driven by low-voltage transistors advances the readiness level of compact, lightweight RF accelerator technology, and demonstrates the promise of this technology to revolutionize the design, engineering and utilization of particle accelerators.

Technical Outcomes

In FY18, this project extended the HEMT-driven accelerator concept from one cavity to ten cavities by designing and fabricating ten high-efficiency C-band cavities, completing an all-HEMT preamp/amplifier system, installing the new accelerator prototype cavities in a new accelerator test-stand with an energy spectrometer, and demonstrating energy modulations in one of these cavities under high-power RF from the all-HEMT RF system. We also evaluated the radiation hardness of 20 high-power GaN HEMT at the LBNL 88" Cyclotron.

Publications

Buechler, C. E., J. W. I. Lewellen, M. A. Holloway, G. E. Dale, D. E. Patrick, D. C. Nguyen, V. Dolgashev, J. M. Lauenstein,

E. Jongewaard, J. Neilson, and S. Tantawi. Linac Design Elements for Spaceborne Accelerators. Presented at *9th International Particle Accelerator Conference*. (Vancouver, Canada, 2018-04-29 - 2018-04-29). (LA-UR-18-23359)

Patrick, D. E., J. Neilson, V. Dolgashev, E. Jongewaard, E. Nanni, A. Sy, S. Tantawi, C. E. Buechler, D. C. Nguyen, R. L. Fleming, G. E. Dale, J. W. I. Lewellen, and M. A. Holloway. The Path to Compact Efficient Solid-state Transistor-driven Accelerators. Presented at *9th International Particle Accelerator Conference, IPAC'18*. (Vancouver, Canada, 2018-04-29 - 2018-05-04). (LA-UR-18-23591)

Wakefield Study for Superconducting Accelerator Cavities

Bruce Carlsten
20170628ER

Project Description

What is known as "long-range wakefields" can degrade electron beam quality when there are bursts of closely spaced electron bunches, especially for beams in superconducting accelerators. This has the potential to impact future accelerators needed for national security and discovery science missions, such as the X-ray free-electron laser proposed for MaRIE, as well as future Department of Energy Office of Science accelerators for Basic Energy Science light sources or High Energy Physics energy frontier research. The consequence could be some limitation in the pulse structure of the burst or, alternatively, indicate a different accelerator architecture such as short-pulse, normal-conducting accelerators. This is a fundamental accelerator research question with urgency to answer.

Technical Outcomes

This project successfully measured the long-range wakefields in TESLA superconducting accelerators structures which are used in many current and planned accelerators. While the longitudinal wakefields appear manageable, the transverse wakefields appear to be strong enough to be a limiting factor in the design of future accelerators and may lead to a reduction in the number of bunches in each burst or, alternatively, require more complicated and costly beam transport through the accelerator.

Publications

Lumpkin, A., B. E. Carlsten, K. A. Bishofberger, R. Thurman-Keup, D. Edstrom, J. Ruan, O. Napoly, N. Eddy, and P. Prieto. Submacropulse electron-beam dynamics correlated with higher-order modes in Tesla-type superconducting rf cavities. 2018. *Physical Review Accelerators and Beams*. (6) 064401. (LA-UR-18-22639 DOI: 10.1103/PhysRevAccelBeams.21.064401)

Adaptive Feedback for Automatic Phase Space Tuning of Electron Beams in Advanced X-ray Free-Electron Lasers

Alexander Scheinker
20170630ER

Project Description

Collaboration with Stanford Linear Accelerator Center and testing algorithms at Linac Coherent Light Source increases the Laboratory's core capability of advanced accelerator and controls algorithm development. By improving the performance of the light source, Los Alamos will see a direct benefit to our on-going weapons related experiments there. As the algorithms are, by design, model-independent and applicable to a wide range of complex systems, they will be of interest to other laboratories and industry that rely on accelerators. This work has the potential to improve the performance of existing particle accelerators and enable performance goals of future light sources such as the European X-ray Free Electron Laser and Matter and Radiation Interaction in Extremes.

Technical Outcomes

This project developed tools to take in synchronized accelerator and beam data from the Linac Coherent Light Source (LCLS) free electron laser (FEL). Data was used to perform simulation studies to develop automatic feedback and optimization tools for the LCLS. Simulations demonstrated an ability to automatically tune the electron beam and were published in conference proceedings. An experiment was also performed at LCLS in which we automatically tuned the longitudinal phase space of the electron beam.

Publications

Scheinker, A., and D. Bohler. Adaptive Feedback for Automatic Phase-space Tuning of Electron Beams in Advanced XFELs. Presented at *International Free-Electron Laser Conference FEL 2017*. (Santa Fe, New Mexico, United States, 2017-08-21 - 2017-08-21). (LA-UR-17-27505)

Neutrino Energy Spectroscopy of Electron-Capture Decay for Neutrino Mass

Michael Rabin
20180014ER

Project Description

The purpose of this project is to address the biggest open question in the field of direct neutrino mass measurement by electron capture decay: Can we know the spectral shape well enough for a sensitive neutrino mass measurement? Neutrino energy spectroscopy of electron capture decay is under intense development for determining the neutrino kinematic mass, a key goal of the U.S. Long Range Plan for Nuclear Science and of the worldwide physics community. This is an exciting endeavor, with multiple groups worldwide (including ours) measuring spectra, calculating higher-fidelity theoretical predictions of the spectral shape, and developing enabling technologies for a full-scale experiment to measure neutrino kinematic mass. Our research goal is to develop an experimentally-validated theoretical framework to understand the systematic error limits of neutrino energy spectroscopy of electron capture decay in a future full-scale experiment.

Technical Outcomes

This was a one-year, Reserve Study project. Though the general approach emphasizes multi-isotope cross-validation, this project focused only on ^{193}Pt . The main results are: the first experimental and theoretical calorimetric electron capture spectra of ^{193}Pt ; improved experimental data (2X in quality, 3X in quantity), recasting of the theoretical calculations in terms of four key decision categories; and concrete predictions of spectral features linked to the four key decisions in near-term experimental reach.

Enabling Physics-based Design of Next-generation Photocathode Guns: An Integrated First-principle Approach

Chengkun Huang
20180670ER

Project Description

DOE recognizes the need of next generation photocathode guns in meeting the requirements of high brightness electron/X-ray sources to support multiple DOE mission areas and to enable frontier material science research. Additionally, Los Alamos National Laboratory also identified low-emittance high-brightness injector technology as a high priority area for the future hard X-ray Free Electron Laser (XFEL) facility. Semiconductor materials with low band-gap and high quantum efficiency are the preferred candidates for these photocathodes with the potential of an order of magnitude increase in performance over the state-of-the-art metallic photocathodes. We aim to enable such advance with physics-based understanding and predictive design capability of next generation semiconductor photocathode guns. Specifically, a unique photocathode gun modeling capability will be developed by integrating the first-principle cathode emission model and the accurate gun electromagnetic model.

Technical Outcomes

This project has resulted in a physics-based and integrated modeling capability for next generation semiconductor photocathode guns. This unique capability can be used to validate and compare simplified/ad-hoc emission models currently used in accelerator design and provide detail design capability for gun performance optimization.

Hybrid Cryogenic Accelerators

Frank Krawczyk
20180671ER

Project Description

Many national security challenges, ranging from stockpile stewardship to border protection and special nuclear material detection, can be addressed with particle accelerators. However, the limitations inherent in existing accelerator designs often force the application to adapt to the needs of the accelerator, rather than the other way around. This is due to the limited, and disconnected, performance trade space offered by low-duty-factor accelerators operating at room temperature on the one hand, and high-duty-factor superconducting accelerators operating near absolute zero on the other hand. We propose development of a hybrid ceramic-copper accelerator structure that expands the performance tradespace to encompass more efficient operation at longer duty factors (compared to room-temperature accelerators), with simplified refrigeration and tuning systems (compared to superconducting accelerators). The eventual goal is development of a type of accelerator that can fill mission-critical needs in a smaller footprint, at lower cost, and with fewer compromises than possible with existing designs.

Technical Outcomes

This project successfully quantified generic advantages of the introduction of dielectrics into traditional RF-resonator structures in a practical configuration. Increased efficiency was demonstrated in simulated structure optimization, and compatibility of dielectrics with cryogenic operation was experimentally demonstrated. A generic material study explained the quality of already used dielectrics, like alumina and indicated preferred properties that can be exploited to design other more beneficial dielectrics or ceramics.

Time-varying Free Electron Laser (FEL) Control

Alexander Scheinker
20180688ER

Project Description

DOE/NNSA missions increasingly rely on particle accelerators, especially free electron lasers, for conducting research and experiments. With increasing complexity, more stringent beam requirements, and a wider user base, there are extreme challenges in quickly tuning between various user-required setups. The algorithms developed as part of this work will be directly applicable to the Linac Coherent Light Source at Stanford and are applicable to particle accelerators in general including many DOE/SC facilities. The tools created here could be modified for implementation in other facilities to speed up tuning and optimize beam quality. A facility such as the Matter-Radiation Interactions in Extremes (MaRIE) free electron laser, with its incredible flexibility and desire to enable extremely closely spaced electron bunches, will face even greater tuning, control, and optimization difficulties than existing accelerators and would greatly benefit from the types of algorithms being developed in this work. Nuclear weapons and reliability of the nuclear stockpile work being done at the Los Alamos Neutron Science Center (LANSCE) could benefit from the algorithms developed in this work being applied to speed up the tuning of and optimize the performance of the LANSCE linear accelerator.

Technical Outcomes

This project developed an adaptive machine learning approach for automatic longitudinal (energy vs time) phase space control of particle accelerator beams. The algorithm combines a neural network for coarse global tuning and model-independent adaptive feedback to locally zoom in on and track uncertain time-varying optimal component settings. We demonstrated the technique at Stanford's Linac Coherent Light Source Free Electron Laser, automatically tuning the accelerator to achieve a desired 2D phase space distribution of the electron beam.

Publications

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Numerical Modeling in Support of Experimental Formation of Novel Thermal-pressure-dominated Magnetized Plasmas

Scott Hsu
20180720ER

Project Description

This project will advance the fundamental understanding of plasma physics, an important scientific discipline underlying DOE/NNSA's mission in stockpile stewardship without nuclear testing. It also has the potential to advance an innovative fusion concept, based on the compression of a thermal-pressure-dominated magnetized plasma to fusion conditions, that could enable a lower-cost development path toward economical fusion energy.

Technical Outcomes

This project established a new capability to perform state-of-the-art supercomputer simulations (using the FLASH code) to support the design and analysis of planned experiments to form novel, thermal-pressure-dominated, magnetized plasmas, which offer a unique platform for (1) discovery-science plasma experiments and (2) a candidate plasma target for a proposed innovative fusion-energy concept. We have obtained initial computer-simulation results that provide the basis for further simulations to guide upcoming experiments.

Innovative Methods for Very Large-Scale Simulations of Richtmyer-Meshkov instability (RMI) Sheet Breakup in Gases

James Hammerberg
20180721ER

Project Description

The project addresses the challenge of understanding the physical processes underlying the creation of ejecta from shocked interfaces. The information gained in this project will lead to new models for ejecta creation and transport that are useful for new computational models in support of stockpile stewardship. The techniques developed in this project will increase the computational size fidelity of atomistic simulations of these phenomena by a factor of ten and are at the forefront of advanced scientific computing supporting important mission goals of Los Alamos National Laboratory. The new models developed from this work will enhance the reliability of advanced scientific computer codes for predicting materials phenomena at rates and pressures important for these missions in national security.

Technical Outcomes

This project formulated new boundary conditions for the study of shock and release phenomena in the microscopic simulation of ejecta production. Such simulations provide detailed physics information necessary to construct macroscopic models of ejecta source, transport and breakup important to Los Alamos National Laboratory's mission. A new boundary condition has been identified and implemented in a NonEquilibrium Molecular Dynamics (NEMD) simulation code showing very promising results that will provide essential information for model development.

Assessment of Pulsed-Power-Driven Inertial Confinement Fusion (ICF) for Extremely High Thermonuclear Yield (U)

Richard Olson
20180729ER

Project Description

With the cessation of nuclear testing and the creation of the Stockpile Stewardship Program (SSP), an Inertial Confinement Fusion (ICF) facility having a thermonuclear yield of >200 MJ is ultimately required to further our understanding of weapons effects, reliability, survivability, and safety of our nuclear weapons. One of the options that should be considered (but is currently not being pursued by the NNSA ICF program) is Magnetic Indirect Drive (MID). Successful completion of the proposed work will help to establish whether high thermonuclear yields are feasible on a future pulsed power facility using the MID option.

Technical Outcomes

Achieving a 200 MJ thermonuclear yield with a Magnetic Indirect Drive (MID) Inertial Confinement Fusion (ICF) concept requires a future pulsed power driver capable of generating peak X-ray power of about 1000 TW with a total X-ray energy in excess of 10 MJ. Research indicates achieving the yield is feasible. Existing measurement and power flow capabilities at the Sandia Z facility are adequate to perform meaningful MID scaling and validation experiments within the next few years.

Laser-driven High-collimated Neutron Pulse Source for High Precision Radiography and Global Security Applications

Andrea Favalli
20180732ER

Project Description

Compact bright collimated neutron sources have several applications. Within the global security mission, such sources enable the assay of special nuclear materials for accountancy—including the special challenge of quantitatively assaying highly enriched uranium that is shielded—and related safeguards and national security applications. Global security applications include, but are not limited to, neutron radiography of nuclear materials through heavy shielding, e.g., for monitoring dry storage casks for diversion of plutonium in spent nuclear fuel; assay of spent nuclear fuel in a storage facility to estimate plutonium mass; and verification technology for nuclear disarmament treaties both via active interrogation and/or neutron resonance analysis. A highly collimated neutron pulse source will enable high precision neutron radiography of materials. The project aims to model and optimize a novel laser-based, compact, collimated neutron source.

Technical Outcomes

The results of the project show that it is possible to use collisionless-shock to accelerate deuterons in deuterated target with spectral shape favorable for neutron generation by a high intensity laser of current technology.

Low Level Radio Frequency (RF) System for Compact All Solid-state Accelerators for Space Deployments

Michael Holloway
20180741ER

Project Description

This program addresses our ability to power and control a new class of compact, efficient particle accelerator. Driven by a distributed, highly redundant power system, the new accelerators require new approaches towards control of power delivery, performance measurement and optimization. This work is aimed at developing a prototype radiofrequency power system intended for spaceflight, the techniques we develop have potential application to a broad range of accelerator-supported research, development, industrial and medical applications. Within the DOE complex, this includes accelerators intended to support basic and applied research, as well as accelerator-based special nuclear material (SNM) detection systems.

Technical Outcomes

This project successfully completed the Low Level Radio-Frequency (LLRF) design and built and test a prototype for a single RF cavity. We completed and the digital design for controlling the various elements of the LLRF using a space qualified FPGA with a development board. Also, we conducted studies to determine the requirements the for control system necessary to run an all solid state accelerator on a remote platform such as a satellite.

Spallation Neutrons for Radionuclide Production

Jonathan Engle
20160601ECR

Project Description

Our goal is to develop and verify a nuclear data measurement capability needed to estimate purities and yields of needed radionuclides made with spallation neutrons. Presently, no U.S. domestic capability to measure the cumulative formation excitation functions for interesting radionuclides exists above approximately 30 MeV. This means that assessment of the radionuclidic purity achievable by irradiating targets in neutron fluences is difficult to estimate. We will build a capability to assess these reactions in a manner that will benefit the field of radionuclide production and generate nuclear data of interest in studies of dosimetry, accelerator driven systems, and verification of nuclear transport codes.

Next Generation Radiation Hydrodynamics for Astrophysics

Joshua Dolence
20170527ECR

Project Description

A variety of national security challenges require the use of sophisticated multi-physics simulations. The codes used for these simulations must be robust for a diverse set of applications, run efficiently on ever changing hardware, and produce accurate results to enable fruitful insights into the behavior of complicated systems. Radiation transport and coupling to matter has traditionally been one of the most challenging aspects in developing these multi-physics simulation codes. This project will serve to generalize a novel approach for treating radiation, targeting long-standing and fundamental problems in astrophysics: core-collapse supernovae and black hole accretion. These applications, aside from their intrinsic interest in the astrophysics community, have radiation physics as a central player and span a wide range of conditions. The outcomes of this project will include the most sophisticated and accurate simulations of both core-collapse supernovae and black hole accretion performed in the several decades over which modeling efforts have been conducted. In the process, the radiation transport method will have been refined and hardened, preparing it for use in other challenging areas such as those faced in national security applications.

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Richers, S., H. Nagakura, C. D. Ott, J. C. Dolence, K. Sumiyoshi, and S. Yamada. A Detailed Comparison

Gluon Saturation Search with Large Hadron Collider Beauty (LHCb) Experiment

Cesar Da Silva
20170569ECR

Project Description

Gluons are one of the fundamental particles inside protons and neutrons; they are responsible for the strong nuclear force which hold nucleons inside nucleus. Gluon is a boson, which means it can merge in a condensate form, sharing the same energy level, if they are too close to each other. This new form of gluon saturated nuclear matter is up to discovery and can explain many of the behaviors observed in particle and nuclear physics in high-energy collisions at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory and the Large Hadron Collider (LHC) at CERN. The Large Hadron Collider Beauty (LHCb) experiment at LHC is the only experiment in the world which can access unexplored kinematic regions where gluon saturation is expected. This project aims to make the first search and detector prototype of a particle tracker inside the LHCb magnet to extend the experimental coverage in the expected gluon saturated region. The unambiguous discovery of gluon saturation and how nuclear matter behaves in this state will have several implication on particle production in high energy collisions, understanding of the sources of the strong nuclear forces, and can help describe the Universe a few microseconds after the Big-Bang.

Laser-Based Mega Electron Volt (MeV) X-ray Source for Double-Shell Radiography

Sasikumar Palaniyappan
20170573ECR

Project Description

Imaging dense materials requires Mega electron volt x-rays. Traditionally such x-rays are generated by impinging mega electron volt electrons from linear accelerators onto high-Z material such as tungsten or tantalum. However, these linear accelerators are very expensive and large in size. Several applications, such as imaging a National Ignition Facility (NIF) double shell implosion, require a compact mega electron volt x-ray source. This project aims to develop such a compact x-ray source by generating an energetic electron beam using compact intense lasers and impinging those electrons onto a tantalum converter foil. Such a compact x-ray source is an essential tool for mega electron volt x-ray radiography.

Collisionless shock acceleration of carbon ions from 1 μ m-laser-driven near-critical plasma. Submitted to *Nature Physics*. (LA-UR-18-27131)

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Integrated Study of X-ray Free-electron Lasers (XFEL) Performance with High Brightness Bunched Electron Beams

Petr Anisimov
20180535ECR

Project Description

There is a strong national need for high quality light sources at hard x-rays to dynamically image high-Z materials used in nuclear weapons and examine materials in extreme conditions. This work addresses the challenges of Dynamic Materials Performance and Process Aware manufacturing. X-ray free electron lasers operating at a coherent photonic energy gap of the 42+keV region will be used to study multiphase high explosive evolution, dynamic performance of plutonium, surrogate metals and alloys, Turbulent Material Mixing in Variable Density Flows; and Controlled Solidification and Phase Transformations, Predicting Interfacial Microstructure and Strain Evolution, High Explosive Functionality by Design.

Critical Analysis of Neutrinoless Double Beta Decay with Effective Field Theories

Emanuele Mereghetti
20180573ECR

Project Description

Neutrinos are fascinating, elusive elementary particles, and the understanding of their properties holds the keys to answering fundamental open questions in particle physics, such as the origin of matter-antimatter asymmetry in the universe. A particularly pressing question is whether neutrinos are their own antiparticles, which would imply that at a fundamental level "matter number" is not conserved in nature. The definitive answer to this question will come from the observation of neutrinoless double beta decay, an extremely rare nuclear process. The importance of this process is stressed by the decision of the US Nuclear Physics community to identify in the Nuclear Science Advisory Committee's 2015 Long Range Plan "the timely development and deployment of a US-led ton-scale neutrinoless double beta decay experiment" as the highest priority for new projects across all the subfields of nuclear physics. By critically examining the theoretical uncertainties that affect double beta decay, and by developing a very general framework for the interpretation of double beta decay searches, our project will strengthen the case for such a high-profile DOE endeavor.

Theory. (Lansing, Michigan, United States, 2018-07-22 - 2018-07-28). (LA-UR-18-30382)

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Nuclear and Particle Futures

Early Career Research
Continuing Project

New Physics at the Giga Electron Volt (GeV) Scale, with Implications for the Strong Charge-conjugation x Parity (CP) Problem

Daniele Spier Moreira Alves
20180622ECR

Project Description

The high level goal is to explore new dynamics that addresses puzzling properties of the neutron and of the strong interactions, and its implications for the structure of matter and forces, the Higgs boson, and neutrinos. The expected outcome is a further understanding of the role of beyond the Standard Model physics in Giga Electron Volt (GeV) scale dynamics, which could lead to new experimental opportunities and discoveries, directly impacting the mission of DOE SC. This project addresses the challenges defined as high priority scientific goals by the 2014 DOE Particle Physics Project Prioritization Panel (a subpanel of the High Energy Physics Advisory Panel), the 2015 DOE Nuclear Physics Long-Range Plan, and the Laboratory's fiscal year 2018 (FY18) Strategic Investment Plan, specifically in its Nuclear and Particle Futures pillar.

Charged-Particle Stopping Power Measurements in Dense Plasmas

Alex Zylstra
20180567ECR

Project Description

High-energy-density plasmas can generate fast charged particles through fusion reactions. The motion of these charged particles through the plasma depends on how quickly they lose energy and slow down, and modeling the transport of these particles is important for the inertial fusion program and processes in nuclear weapons. This project will perform direct measurements of particle energy loss through plasmas at two conditions, to validate theoretical models.

Technical Outcomes

Platform development work was begun for the measurements of particle energy loss at two conditions, with the actual physics data to be acquired at a later date under a different project due to the early termination of this project with the PI's move to LLNL, where he will continue to support NNSA missions.

Revealing the Particle Nature of Dark Matter with Cosmic Gamma Rays

Andrea Albert
20160641PRD2

Project Description

Most of the mass in the Universe is Dark Matter (DM) of an entirely unknown nature. A strong candidate for dark matter, based on high-energy physics theories, would produce high-energy gamma rays. This project will result in the most sensitive searches for gamma-ray signals from massive DM candidates. These searches will rule out some models of the DM if no signal is detected; however, if a signal is detected then other observations from the High Altitude Water Cherenkov Observatory and Fermi Large Area Telescope will have to be consistent with this signal. This would be a major discovery solving one of the longest standing problems in astrophysics, cosmology, and particle physics. The project also builds capabilities relevant to nuclear weapons research and nuclear nonproliferation through development and analysis of data from complex detectors.

Publications

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Turbulence in Supernova Progenitors

Samuel Jones
20160681PRD4

Project Description

Convection and turbulence are important factors in a wide number of problems, both for academic studies (e.g. supernovae, stars) and core DOE problems of direct national importance (from coal burning to problems in the national ignition facility). This post-doctoral effort seeks to build a bridge between scientists studying the academic problems and scientists working problems of direct national interest. Until recently, groups performing turbulence experiments, code developers at Los Alamos, and code developers in academia have worked separately. The lack of communication between these groups has hampered progress. The postdoc fellow funded through this project will work with all these groups to study convection and turbulence. As he progresses, he will tighten his ties within Los Alamos programs, and at the same time, apply his new knowledge to the academic problem of stellar convection, thereby strengthening collaboration between the Laboratory and the broader scientific community.

\xb3-ray detection in supernova remnants. To appear in *MNRAS*. (LA-UR-18-24048 DOI: 10.1093/mnras/stz536)

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Nuclear and Particle Futures

Postdoctoral Research & Development
Continuing Project

Dark Matter and the Validity of Effective Field Theories

Jessica Goodman
20170661PRD1

Project Description

Discovering and understanding the physics of dark matter is a high priority in high-energy physics. This project will develop new theoretical models of dark matter and confront those against a variety high-energy physics experimental data. This project will develop simplified models for new dark matter physics scenarios in which interactions with Standard Model particles are generated at the quantum (i.e., loop) level. The current and projected sensitivity of the Large Hadron Collider (LHC) experiment to such scenarios will be assessed.

First Principles Approach to Factorization Violation

Duff Neill

20170662PRD1

Project Description

This project advances our understanding of the quantum behavior of the most fundamental building blocks of matter that we know about, protons and the quarks and gluons that they are made of. The project will produce a quantitative theoretical framework to predict the effects of low-energy, long-wavelength gluon radiation between protons as they collide. Such proton collisions are the primary window we have into the nature of their constituents and the fundamental strong force between them. Discoveries of new particles, new forces, and the quantum laws of nature they reveal have underpinned some of the most revolutionary technological advances in the 20th, and now 21st, century. The DOE Office of Science, through the Offices of High-Energy and Nuclear Physics, supports major proton collider experiments in the US such as at the Fermilab accelerator in Illinois and the Relativistic Heavy-Ion Collider at Brookhaven in New York. This project will improve our ability to interpret the results of proton collision experiments at these facilities in terms of the underlying physics. These experiments and theory efforts to support them are highlighted in the National Nuclear Science Advisory Committee's 2015 Long-Range Plan as among the highest scientific priorities in the US.

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- Neill, D. A., W. Waalewijn, L. Zoppi, and A. Papaefstathiou. Phenomenology with a recoil-free jet axis: TMD fragmentation and the jet shape. Submitted to *JHEP*. (LA-UR-18-30361)

Jets in Strongly Interacting Plasmas

Andrey Sadofyev
20170666PRD1

Project Description

Quark-Gluon Plasma (QGP) is a novel state of matter recently discovered in experiments at the Relativistic Heavy-Ion Collider (RHIC) at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN. An extremely dense and hot “fireball” is created in collisions of heavy ions and consists of the elementary constituents of matter, quarks and gluons, otherwise confined into protons and neutrons. It is also subject to the highest known magnetic field in the Universe, giving unique opportunity to study properties of plasmas at these extreme conditions. This research will result in a novel theoretical tool for studying the microscopic properties of strongly interacting matter. It will not only shed light on the phenomena that govern the QGP behavior, but also give insight into system such as the plasmas in the early universe, high-temperature superconductors, and unitary cold atoms. The work will pave the way to implementing modern theoretical methods and will provide guidance for the experimental study of QGP. It also will give valuable insights into energy loss of charged particles and plasma excitations in other extreme environments, relevant to national security applications

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Nuclear and Particle Futures

Postdoctoral Research & Development
Continuing Project

Measurement of (n,g) Cross Sections Crucial for Constraining Stellar Nucleosynthesis

Aaron Couture
20170687PRD3

Project Description

The primary goal of this project is to determine the underlying reactions between the isotopes in stars. This determines the elements we find when we look out into the cosmos, as well as here on earth. In particular, elements heavier than iron have been made by neutrons in stars and stellar explosions. Understanding those reactions tells us about those stars and the cosmos. Many of the most informative reactions take place on unstable isotopes, making laboratory measurements even more challenging. In a similar way to the stellar archeology that tells us about the cosmos through telescopes and satellites, we can use the residue from man-made nuclear explosions to infer information about the yield and design of the device. These capabilities are a core component in DOE/NNSA mission for both Science-Based Stockpile Stewardship and Technical Nuclear Forensics missions. Again, many of the most discriminating reactions take place on unstable isotopes. The measurements performed as part of this project will develop techniques that can then be used to answer these national security questions.

Publications

Prokop, C. J., A. J. Couture, S. Jones, S. M. Mosby, G. Y. Rusev, J. L. Ullmann, and M. Krticka. Measurement of the $^{65}\text{Cu}(n,\gamma)$ cross section using DANCE. Submitted to *Physical Review C*. (LA-UR-19-20879)

Mega Electron Volt (MeV) Gamma-Ray Astronomy: Exploring the Universe in the Nuclear Transition Region

W Vestrand
20170693PRD4

Project Description

The development of more sensitive space-based instruments for the detection of gamma-ray and neutron emission generated by nuclear reactions is important for DOE/NNSA national security programs. This project will develop new tools for imaging sources of gamma-ray and neutron emission that will allow the detection and measurement of sources that are currently too faint to detect. The project will also explore new approaches to the reduction of detector background noise that will enable the construction of more sensitive gamma-ray and fast neutron detectors. Our development of these new tools for on-board Compton gamma-ray imaging and background reduction is likely to influence future designs of Space-based Nuclear Detonation Detection (SNDD) instrumentation.

Publications

- Appel, J. W., A. Ali, C. L. Bennett, R. Bustos, D. T. Chuss, S. Dahal, J. R. Eimer, T. Essinger-Hileman, K. Harrington, J. Iuliano, T. A. Marriage, I. L. Padilla, L. P. Parker, M. Petroff, B. Wang, D. J. Watts, Z. Xu, and L. Zeng. On-sky performance of the CLASS Q-band telescope. Submitted to *Astrophysical Journal*. (LA-UR-18-30124)
- Dahal, S., A. Ali, J. W. Appel, T. Essinger-Hileman, C. Bennett, M. Brewer, R. Bustos, M. Chan, D. Chuss, J. Cleary, T. Engelhoven, P. Fluxa, F. Colazo, J. Couto, K. Denis, R. Dunner, J. Eimer, M. Halpern, K. Harrington, K. Helson, G. Hilton, G. Hinshaw, J. Hubmayr, J. Iuliano, J. Karakla, B. Marquez, T. Marriage, J. McMahon, N. Miller, C. Nunez, I. Padilla, G. Palma, L. P. Parker, M. Petroff, R. Reeves, C. Reintsema, K. Rostrem, M. Sagliocca, K. U-Yen, D. Valle, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan, and L. Zeng. Design and Characterization of Cosmology Large Angular Scale Surveyor (CLASS) 93 GHz Focal Plane. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-24478)
- Gallardo, P., J. W. Fowler, G. Hilton, M. Hasselfield, K. Irwin, S. P. Ho, J. Appel, A. Kusaka, J. A. Beall, T. Essinger-Hileman, H. M. Cho, L. E. Campusano, K. Crowley, S. K. Choi, L. P. Parker, S. Raghunathan, C. D. Reintsema, J. Sievers, S. M. Simon, S. T. Staggs, K. Visnjic, K. W. Yoon, N. Jarosik, M. D. Niemack, G. W. Nixon, M. Nolta, L. A. J. Page, and G. A. Palma. Results from the Atacama B-mode Search (ABS) experiment. 2018. *Journal of Cosmology and Astroparticle Physics*. (09) 5-5. (LA-UR-18-23879 DOI: 10.1088/1475-7516/2018/09/005)
- Harrington, K., J. Eimer, D. Chuss, M. Petroff, J. Cleary, M. DeGeorge, A. Ali, J. W. Appel, C. Bennett, M. Brewer, R. Bustos, M. Chan, J. Couto, K. Denis, R. Dunner, T. Essinger-Hileman, P. Fluxa, M. Halpern, G. Hilton, G. Hinshaw, J. Hubmayr, J. Iuliano, J. Karakla, T. Marriage, J. McMahon, N. Miller, C. Nunez, I. Padilla, G. Palma, L. P. Parker, B. Marquez, R. Reeves, C. Reintsema, K. Rostem, D. Valle, T. Engelhoven, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan, and L. Zeng. Variable-delay Polarization Modulators for the CLASS Telescopes. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-24622)
- Iuliano, J., J. Eimer, L. P. Parker, A. Ali, J. W. Appel, C. Bennett, M. Brewer, R. Bustos, D. Chuss, J. Cleary, J. Couto, S. Dahal, K. Denis, R. Dunner, T. Essinger-Hileman, P. Fluxa, M. Halpern, K. Harrington, K. Helson, G. Hilton, G. Hinshaw, J. Hubmayr, J. Karakla, T. Marriage, N. Miller, J. McMahon, C. Nunez, I. Padilla, G. Palma, M. Petroff, B. Marquez, R. Reeves, C. Reintsema, K. Rostrem, D. Valle, T. Engelhoven, B. Wang, Q. Wang, D. Watts, J. Weiland, E. Wollack, Z. Xu, Z. Yan, and L. Zeng. The Cosmology Large Angular Scale Surveyor Receiver Design. Presented at *SPIE Astronomical Telescopes + Instrumentation*. (Austin, Texas, United States, 2018-06-10 - 2018-06-15). (LA-UR-18-25031)
- Watts, D. J., B. Wang, A. Ali, J. W. Appel, C. L. Bennett, D. T. Chuss, S. Dahal, J. R. Eimer, T. Essinger-Hileman, K. Harrington, G. Hinshaw, J. Iuliano, T. A. Marriage, N. J. Miller, I. L. Padilla, L. P. Parker, M. Petroff, K. Rostem, E. J. Wollack, and Z. Xu. A Projected Estimate of the Reionization Optical Depth Using the CLASS Experiment's Sample Variance Limited E-mode Measurement. To appear in *The Astrophysical Journal*. (2) 121. (LA-UR-18-20165 DOI: 10.3847/1538-4357/aad283)

Shock-accelerated Variable-density Mixing in a Subsonic Cross Flow

Katherine Prestridge
20180714PRD2

Project Description

Accurate predictive simulations of turbulent mixing require experimental data under the relevant flow conditions, because our computation capability requires us to model the smallest scales of mixing—we do not have the capability to simulate all of the important length scales of realistic flows. NNSA/DOE are interested in shock-driven mixing with strong density gradients. This experimental facility and its diagnostics are designed to measure flows in regimes of interest, and the data are used to make improvements to models. The data improve our code capabilities. In addition to the technical outcomes, this facility and team provides training to new scientists on diagnostics for experiments, data analysis techniques, and collaborations among experiments, modelers, and numerical physicists.

Nuclear and Particle Futures

Postdoctoral Research & Development
Continuing Project

Extreme Radiation Magnetohydrodynamics Around Black Holes

Joshua Dolence
20180716PRD2

Project Description

The primary goal of the research is to better understand physical phenomena that occur under the extreme conditions near black holes. In pursuing this goal, expertise and numerical techniques for a range of physical processes of relevance to DOE/NNSA missions will be developed. The expected outcomes include multiple impactful publications and a well-trained early career scientist that will be well-positioned to contribute to DOE/NNSA missions in the long term.

Nuclear and Particle Futures

Postdoctoral Research & Development
Continuing Project

Unraveling Nature's Mysteries at the World's Highest Energy Colliders

Ivan Vitev

20180748PRD3

Project Description

Showers of subatomic particles, called jets, are ubiquitous in nature. For example, cosmic jets are a cornerstone of modern astrophysics and collimated beams of electrons and photons find applications ranging from material science to nuclear medicine. However, nowhere are jets of elementary particles more copiously produced and comprehensively studied than at the modern high energy and nuclear physics collider facilities. This project will develop state of the art theory of jets to interpret experimental data, understand the origin of mass, and unravel the properties of extremely hot and dense state of matter in the early universe. Similar systems are also of interest to national security physics applications.

Publications

Li, A., H. Li, I. Moulton, and H. X. Zhu. The Transverse Energy-Energy Correlator in the Back-to-Back Limit. Submitted to *Physical Review Letters*. (LA-UR-19-20914)

Li, H., and I. M. Vitev. Jet splitting functions in the vacuum and in a QCD medium. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-20679)

Li, H., and I. M. Vitev. Inclusive heavy flavor jet production with semi-inclusive jet functions: from proton to heavy-ion collisions. Submitted to *Journal of High Energy Physics*. (LA-UR-19-20952)

Studying Nuclear Astrophysics and Inertial Fusion with Gamma-rays

Alex Zylstra

20150717PRD2

Project Description

The proposed work has two parts: studying nuclear astrophysics and basic nuclear physics, and developing a unique burning-plasma diagnostic capability for inertial confinement fusion (ICF) implosions. The field of nuclear astrophysics will benefit from high-quality measurements at low energies; the direct applicability of ICF plasmas to conditions in the universe is a unique opportunity to make substantial contributions to our understanding of stellar and big-bang nucleosynthesis. Basic nuclear physics of these few-nucleon systems will be simultaneously studied. This project will result in improved nuclear diagnostics for experiments at National Ignition Facility, which are important for achieving our goal of fusion ignition, in support of stockpile stewardship and fusion energy applications.

Technical Outcomes

This project developed unique capabilities for fundamental science using laser-driven implosions. The primary focus was on astrophysics, with new measurement capabilities developed for studies of reactions relevant to stellar and big-bang nucleosynthesis. Novel types of implosions using liquid fuel layers were also developed and fielded for the first time on the NIF.

Publications

Zylstra, A. Studying nucleosynthesis using high-powered lasers. Unpublished report. (LA-UR-16-24871)

Zylstra, A. Studying Nuclear Astrophysics with Inertial Fusion Implosions. Unpublished report. (LA-UR-18-22785)

Zylstra, A., F. Graziani, S. H. Batha, and B. J. Albright. Stopping Power Workshop Summary. Unpublished report. (LA-UR-16-22332)

Zylstra, A., H. Park, J. Ross, F. Fiuza, J. Frenje, D. Higginson, C. Huntington, C. Li, R. Petrasso, B. Pollock, B. Remington, H. Rinderknecht, D. Ryutov, F. Seguin, D. Turnbull, and S. Wilks. Proton pinhole imaging on the National Ignition Facility. 2016. *Review of Scientific Instruments*. (11) 11E704. (LA-UR-16-23558 DOI: 10.1063/1.4959782)

Zylstra, A., H. W. Herrmann, M. Gatu Johnson, Y. H. Kim, J. Frenje, G. M. Hale, C. Li, M. Rubery, M. W. Paris, A. Bacher, C. Brune, C. Forrest, V. Glebov, R. Janezic, D. McNabb, A. Nikroo, J. Pino, T. Sangster, F. Seguin, W. Seka, H. Sio, C. Stoeckl, and R. Petrasso. Using Inertial Fusion Implosions to Measure the T+3He Fusion Cross Section at Nucleosynthesis-Relevant Energies. 2016. *Physical Review Letters*. (3) 035002. (LA-UR-15-29245 DOI: 10.1103/PhysRevLett.117.035002)

Zylstra, A., H. W. Herrmann, Y. H. Kim, A. McEvoy, M. J. Schmitt, G. M. Hale, C. Forrest, V. Glebov, and C. Stoeckl. Simultaneous measurement of the HT and DT fusion burn histories in inertial fusion implosions. 2017. *Review of Scientific Instruments*. (5) 053504. (LA-UR-17-20368 DOI: 10.1063/1.4983923)

Zylstra, A., H. W. Herrmann, and M. Gatu Johnson. Studying nuclear astrophysics using OMEGA implosions. Unpublished report. (LA-UR-16-22139)

Zylstra, A., J. Frenje, M. Gatu Johnson, G. M. Hale, C. Brune, A. Bacher, D. Casey, C. Li, D. McNabb, M. W. Paris, R. Petrasso, T. Sangster, D. Sayre, and F. Seguin. Proton Spectra from and Fusion at Low Center-of-Mass Energy, with Potential Implications for Solar Fusion Cross Sections. 2017. *Physical Review Letters*. (22) 222701. (LA-UR-17-22452 DOI: 10.1103/PhysRevLett.119.222701)

Zylstra, A., J. Frenje, P. Grabowski, C. Li, G. Collins, P. Fitzsimmons, S. Glenzer, F. Graziani, S. Hansen, S. Hu, M. Gatu Johnson, P. Keiter, H. Reynolds, J. Rygg, F. Seguin, and R. Petrasso. Development of a WDM platform for charged-particle stopping experiments. 2016. *Journal of Physics: Conference Series*. 012118. (LA-UR-15-29128 DOI: 10.1088/1742-6596/717/1/012118)

Zylstra, A., J. Rygg, G. Collins, and R. Petrasso. Charged-particle stopping power and scattering measurements in warm-dense plasma. Unpublished report. (LA-UR-16-22141)

Zylstra, A., R. Rygg, P. Grabowski, S. Hansen, C. Li, J. Frenje, R. Collins, F. Graziani, F. Seguin, R. Petrasso, and R. London. Probing Charged-Particle Stopping Power in Dense Degenerate Plasmas. Unpublished report. (LA-UR-16-26718)

Zylstra, A., S. Le Pape, C. Li, R. Rygg, S. Craxton, and P. McKenty. Proton Backlighter Source Development. Unpublished report. (LA-UR-17-27849)

Precision Theoretical Analysis of Reactions with Protons Polarized in a Strong Magnetic Field

Ivan Vitev
20160645PRD1

Project Description

This project will allow much-improved understanding of the internal structure of protons and neutrons. It will extend the applicability of the theory of strong interactions to reactions with particles polarized by strong magnetic fields. Precision analysis of measurements from the polarized proton experiment at Fermilab will help construct a 3D picture and contribute to the resolution of the longstanding problem about the origin of the nucleon spin. This work addresses DOE's vision for the future of nuclear physics, as well as priorities set for DOE to study the internal structure of nucleons.

Technical Outcomes

This project developed new theoretical techniques to understand the three-dimensional landscape of the nucleon and its relation to the quark orbital angular momentum. Our work included previously neglected quantum correlations between the partons in the nucleon, which are further enhanced in a strong magnetic fields. Pioneering calculations for spin asymmetries in the Drell-Yan process, semi-inclusive deep inelastic scattering, and hyperon production in electron-positron annihilation have resulted in follow up projects and external funding.

Using X-Rays with Protons for a Material-Identification Capability via Proton Radiography

Levi Neukirch
20160652PRD2

Project Description

A single source of x-rays produces a wide range of energies, which often degrades the quality of an x-ray image. We will exploit this characteristic of x-ray sources to make simultaneous images from different energies in the x-rays spectrum. The attenuation of x-rays of different energies can be used to identify the materials present, so the images can be combined to make a 2D map of materials. The images can be fast enough to capture the details of plumes, jets, and ejecta produced in explosively driven systems. We will then further combine x-radiography with proton radiography for an even more sensitive pixel-by-pixel material identification diagnostic of dynamic systems. This technique will help answer very important questions about materials transport in shock physics experiments, such as what are the constituents of gas plumes and ejecta, and tell us where these constituents originated. Even a proof-of-principle demonstration of the technique with a static manufactured model will produce a high-impact publication of an important novel diagnostic.

Technical Outcomes

A Director's funded postdoctoral fellow converted to a Scientist within the physics pRad (Proton Radiography) team and developed an integrated model of a Bremsstrahlung x-ray source, test objects, and detectors to generate simulated radiographs. Objects and a filtered detector stack were fabricated and tested at the Laboratory x-ray sources, with analysis ongoing. This work also helped develop proton energy loss radiography based on proton time-of-flight measurements.

Publications

Pettit, R. M., L. P. Neukirch, Z. Yi, and A. N. Vamivakas.

Coherent control of a single nitrogen-vacancy center spin in optically levitated nanodiamond. 2017. *Journal of the Optical Society of America B*. (6) C31. (LA-UR-17-20272 DOI: 10.1364/JOSAB.34.000C31)



Science of Signatures

Using Extinct Radionuclides for Radiochemical Diagnostics (U)

Hugh Selby
20160011DR

Project Description

The goals of the Extinct Radionuclide System (ERS), that is, the integrated measurement, simulation and analysis tools for debris diagnostics, are simple but offer significant positive impact to all missions that employ radiochemical debris data. The single most important goal is to develop the suite of diagnostically useful measurement signatures that have been lost to decay. Validation of the measurements against known examples is the corollary of the main goal and will prove the feasibility of ERS concept. Successful development of the ERS will mark a completely new capability to address a number of NNSA missions. In essence, anything that one would do with fresh debris can now be done with old debris. This has major implications for the NNSA's main mission, Stockpile Stewardship. This statement can be understood by considering that all data employed in modern Stewardship is decades old and reflects the precision and accuracy of that time. The ERS allows for much more data and much higher precision. Such improvements will provide the data backstop for more confident stewardship assessments. These same ERS tools can be applied to other missions in the National Security endeavor, including treaty monitoring and verification.

Technical Outcomes

The project was successful. All major goals were achieved. Outcomes of the project will be published in an upcoming special issue of Defense Research Review. Follow-on funding has been obtained from internal and external sponsors.

Publications

Hanson, S. K., A. D. Pollington, C. R. Waidmann, W. S. Kinman, A. M. Wende, J. L. Miller, J. Berger, W. J. Oldham, and H. D. Selby. Measurements of Extinct ⁹⁵Zr and ⁹⁷Zr Fission Products in Old Nuclear Bomb Debris: Determination of the Yield of the Trinity Nuclear Test 70 Years Later. Submitted to *Science*. (LA-UR-16-20179)

Hanson, S. K., A. D. Pollington, C. R. Waidmann, W. S. Kinman, A. M. Wende, J. L. Miller, J. Berger, W. J. Oldham, and H. D. Selby. Measurements of extinct fission products in nuclear bomb debris: Determination of the yield of the Trinity nuclear test 70 y later. 2016. *Proceedings of the National Academy of Sciences*. (29) 8104-8108. (LA-UR-16-22956 DOI: 10.1073/pnas.1602792113)

10 Gigahertz Bandwidth Synthetic Aperture Radar (SAR) Technology Development for Satellite Deployment

Bruce Carlsten
20160013DR

Project Description

We will develop a radio frequency (RF) amplifier with order-of-magnitude higher power and bandwidth than possible with conventional technology at extremely high frequency to enable ultra high resolution imaging for urgent national security missions. RF amplifier technology has a performance limitation at high frequency because sizes shrink, including the size of the electron beam needed for RF amplification. It has been long recognized in the RF amplifier technical community that a sheet electron beam will be needed to bypass this limitation, but previous research has shown that sheet beams with conventional RF structures lead to over-moding. This project proposes to demonstrate a high-frequency RF amplifier using novel high-dielectric constant ceramics. These ceramics will allow the development of RF amplifier designs that eliminate mode competition yet have unprecedented wide bandwidths.

Technical Outcomes

Overall, this project completed over 90% of its scope, including understanding the design trade-offs and high-frequency potential of a dielectric traveling-wave tube (TWT), the design of the first practical dielectric TWT, development of the fabrication steps needed for assembling a dielectric TWT, and fabricating it (testing not initiated). We also demonstrated 10-GHz of spread spectrum centered at 33.25 GHz and the development and testing of the first synthetic aperture radar using range-resolved data.

Publications

Carlsten, B. E., E. I. Simakov, K. Nichols, and D. Shchegolkov. Emittance Effects on Gain in W-Band TWTs. 2016. *IEEE Transactions on Electron Devices*. (11) 4493-4498. (LA-UR-17-24412 DOI: 10.1109/TED.2016.2612583)

Marksteiner, Q. R., N. Yampolsky, and B. E. Carlsten. Analytical Calculations of the Energy Spread from the Microbunching Instability in the MaRIE XFEL. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A:*

Accelerators, Spectrometers, Detectors, and Associated Equipment. (LA-UR-18-29118)

Simakov, E. I., B. E. Carlsten, F. L. Krawczyk, K. Nichols, and M. R. A. Zuboraj. Design and Fabrication of a Ka-Band Dielectric-Loaded Traveling-Wave Tube. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-18-29670)

A. Zuboraj, M. R., and B. E. Carlsten. Beam Transport and Beam-Current Loss in Emittance-Dominated High-Frequency Tubes. Submitted to *IEEE Transactions on Electron Devices*. (LA-UR-19-21597)

Fieldable Chemical Threat Mapping by Multi-Modal Low Magnetic Field Nuclear Magnetic Resonance Signatures

Robert Williams
20170048DR

Project Description

Over the past 90 years we have successfully made chemical agents more lethal, harder to destroy, and easier to obtain and use. Today, thousands of chemicals have the potential to be used as weapons of mass destruction. By extending Los Alamos National Laboratory's extensive expertise in high field Nuclear Magnetic Resonance (NMR) signature detection and ultra-low magnetic field relaxometry and Magnetic Resonance Imaging, our team has taken an innovative approach using multi-modal NMR signatures to unequivocally characterize and identify Chemical Warfare Agents (CWAs), their precursors and degradation compounds, as well as related Chemical Threat Agents (CTAs) and emerging threats. A transformative, innovative, and portable technology detects vulnerabilities and threats through unique, multiple Nuclear Magnetic Resonance (NMR) signatures that conclusively identify CWAs and other emerging threats allowing them to be mitigated. Our new measurement capabilities and strategies will map human activities in manufacturing and/or the use of toxic chemicals, pesticides, pharmaceuticals, and explosives as well as assist in responding to the accidental release of such chemicals or the intentional release by terrorists. With the ever-changing national and global security environment, these advances will mitigate vulnerabilities and keep pace with the rapidly evolving security environment that is affected by hazardous chemical misuse.

Catalytic Hydroboration. To appear in *Science*. 874-884. (LA-UR-18-24664 DOI: 10.1021/acscatal.8b04096)

Dub, P. The Effect of M-L Antiferromagnetic Coupling in Catalysis. Submitted to *Science, Science Advances*. (LA-UR-18-25395)

Dub, P., and J. C. Gordon. What Does the Net Retention of the N-H functionality in the Noyori Asymmetric Hydrogenation Reaction Mean for Catalysis Science?. Submitted to *Nature Reviews Chemistry*. (LA-UR-18-24550)

Gan, X. Y., D. C. Kaseman, S. Saxena, J. E. Millstone, and A. Gamble Jarvi. Evolution of Surface Copper(II) Environments in Cu Se Nanoparticles. To appear in *Chemistry of Materials*. (20) 7313-7321. (LA-UR-18-28650 DOI: 10.1021/acs.chemmater.8b03967)

Nelson, T. R. LDRD Data Sheet Template. Unpublished report. (LA-UR-17-31085)

Publications

Baumann, D. O., J. C. Gordon, and R. F. Williams. Peptoid Siderophore Analogues. Submitted to *Actinide Research Quarterly*. (LA-UR-18-31782)

Dub, P. Dearomatization and Functionalization of Terpyridine Ligands Leading to Unprecedented Zwitterionic Meisenheimer Aluminum Complexes and Their Use in

Agile Spectral Reconnaissance from CubeSats

Steven Love
20170055DR

Project Description

Remote chemical analysis by spectral remote sensing is an extremely powerful tool for both national security and earth science problems. Deploying this capability in space, however, has traditionally demanded national-level investment and many-year development efforts. This project seeks to enable a paradigm shift to rapidly deployable, inexpensive constellations of CubeSats. These fully functional miniaturized satellites are small enough to hold in your hand, game changingly inexpensive to launch, and carry ultra-compact spectral imagers that ultimately could provide comparable sensing capability with far greater agility and far lower cost. This project jumpstarts this vision by rapidly building and launching a high-performance CubeSat-based hyperspectral imager, operating in the ultraviolet/visible spectral region, to perform targeted mapping of key signature gases. This first demonstration focuses on earth science problems: volcanic gas monitoring for eruption prediction and greenhouse gas tracking via the easily detected proxy gas nitrogen dioxide. However, with anticipated improvements in CubeSat pointing accuracy, CubeSat-based instruments capable of detecting gases and materials of relevance to proliferation detection and other national security problems should be possible. This project lays the groundwork for future low-cost and versatile multi-CubeSat monitoring constellations.

Publications

Theiler, J. P., B. R. Foy, C. L. Safi, and S. P. Love. Onboard Cubesat Data Processing for Hyperspectral Detection of Chemical Plumes. Presented at *SPIE Defense + Commercial Sensing*. (Orlando, Florida, United States, 2018-04-15 - 2018-04-19). (LA-UR-18-23005)

Atomtronics: A New Approach to Sensing, Signal Processing, and Signal Analysis

Malcolm Boshier
20180045DR

Project Description

The project addresses three challenges facing the intelligence and defense communities: navigation when global position system (GPS) is unavailable or denied, unscrambling mixtures of radio signals received by multiple antennas (Blind Source Separation, or BSS), and determining the security of cryptography systems that rely on the presumed hardness of finding the prime factors of a large number. Our proposed solutions are based on atomtronics, the emerging science of circuits created from atoms flowing inside guides. We expect to demonstrate a compact atomtronic rotation sensor that outperforms all existing technologies and therefore improves the accuracy of inertial navigation. We plan to build a prototype atomtronic signal processing circuit that can perform BSS. Finally, we will build an atomtronic device that finds the prime factors of numbers larger than any factored to date on quantum computers.

Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces

Abul Azad
20180062DR

Project Description

Modern communication, sensing, and surveillance systems rely heavily on the utilization of the electromagnetic spectrum for collecting information, controlling instruments, and making decisions. Our proposed spatio-temporal modulated metasurfaces will result in a revolutionary design paradigm that will enable the effective control and manipulation of electromagnetic waves, and hence play a critical role in attaining enhanced performance of electromagnetic systems. In particular, we will apply this technology to small satellite platforms, an emerging geo-spatial capability for remote sensing and imaging which are a key component of Los Alamos National Laboratory mission space in Science of Signatures. However, they are intrinsically constrained in size, weight, and power, and are in dire need of revolutionary design paradigms to enable dramatically increased performance. This project underpins the Laboratory mission in Science supporting National Security, and advances sensing capabilities for space situational awareness in Global Security. The main anticipated outcomes of this research are reprogrammable microwave metasurface antennas for active beam steering and wavefront correction, and control over their transmission and reception characteristics through tailored modulations in space and time.

Publications

Chang, C. C., H. Chen, W. J. de Melo Kort-Kamp, J. Nogan, T. S. Luk, A. K. Azad, A. J. Taylor, D. A. R. Dalvit, and M. Sykora. High-Temperature Refractory Metasurfaces for Solar Thermophotovoltaic Energy Harvesting. To appear in *Nano Letters*. acs.nanolett.8b03322. (LA-UR-18-27846 DOI: 10.1021/acs.nanolett.8b03322)

Chen, H., C. C. Chang, A. J. Taylor, Z. Zhao, and S. Fan. Achromatic linear-to-circular polarization conversion

based on off-resonance reflective metasurfaces. Submitted to *Science*. (LA-UR-18-31108)

Chen, X., S. Ghosh, Q. Xu, C. Ouyang, Y. Li, X. Zhang, Z. Tian, J. Gu, L. Liu, A. K. Azad, J. Han, and W. Zhang. Active control of polarization-dependent near-field coupling in hybrid metasurfaces. Submitted to *Applied Physics Letters*. (LA-UR-18-29890)

Cheong, S. W., D. Talbayev, V. Kiryukhin, and A. Saxena. Broken symmetries, non-reciprocity, and multiferroicity. 2018. *npj Quantum Materials*. (1) 19. (LA-UR-18-20267 DOI: 10.1038/s41535-018-0092-5)

Chowdhury, D. R., A. K. Azad, G. Kumar, and S. J. M. Rao. Ultrafast Relaxation of Charge Carriers Induced Switching in Terahertz Metamaterials. To appear in *Journal of Infrared, Millimeter, and Terahertz Waves*. (12) 1211-1220. (LA-UR-18-30111 DOI: 10.1007/s10762-018-0547-6)

R. Dalvit, D. A., F. Intravaia, D. Oelschläger, D. Reiche, and K. Busch. Rolling Quantum Friction. Submitted to *Physical Review Letters*. (LA-UR-18-29152)

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The Fundamental Physical Interpretation and Exploitation of Stable Isotope Fractionation (U)

Samuel Clegg
20180066DR

Project Description

This project will theoretically and experimentally investigate the mechanisms responsible for the fractionation of stable isotopes. Stable isotopes are long-lived, non-radioactive atoms. Stable isotopes are exceedingly sensitive indicators of the source of a material and are widely used within the atmospheric chemistry, geochemical, planetary, environmental, forensic, and climate change communities. However, interpretation of stable isotope ratios is limited to empirical analysis without much detailed theoretical understanding. The proposed work will provide the fundamental tools and models necessary to relate stable isotopic signatures to specific processing steps used in their production.

Publications

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Emerging Challenges in Space and Earth Science

Reinhard Friedel
20180475DR

Project Description

This project provides national science research & education services that benefit a wide range of Los Alamos National Laboratory's national security programs in global security, energy and climate security and space situational awareness, and the modeling capability in the stockpile stewardship program. This includes university research outreach and student / postdoc research programs, which are the technical heart of this project. This project further provides funding for new ideas and programs that may play a large part in the future DOE/ NNSA mission. Support for innovative small work also plays a large role in the Lab's retention of technical talent.

Publications

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Holmes, R. M., and D. Palmer. Extreme background-rejection techniques for the ELROI optical satellite license plate. 2019. *Review of Scientific Instruments*. (4) 814-825. (LA-UR-18-28957 DOI: 10.1364/AO.58.000814)

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Kalintsev, A., A. Migdisov, H. Xu, R. C. Roback, and J. Brugger. Uranyl speciation in sulfate-bearing hydrothermal solutions up to 250 °C. Submitted to *Geochimica et Cosmochimica Acta*. (LA-UR-19-20322)

Kroeniger, K., F. De Roo, P. Brugger, S. Huq, T. Banerjee, and M. Mauder. Effect of Secondary Circulations on the Surface-Atmosphere Exchange of Energy at an Isolated Semi-arid Forest. To appear in *Boundary-Layer Meteorology*. (LA-UR-17-30829 DOI: 10.1007/s10546-018-0370-6)

Kunegel-Lion, M., D. W. Goodsman, and M. A. Lewis. When managers forage for pests: Functional response applications to human-pest management. Submitted to *American Naturalist*. (LA-UR-17-30015)

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- Lin, Y., Z. Zhang, Z. Zhou, and T. Chen. ADAPTIVE FILTERING FOR EVENT RECOGNITION FROM NOISY SIGNAL: AN APPLICATION TO EARTHQUAKE DETECTION. Presented at *International Conference on Acoustics, Speech, and Signal Processing*. (Brighton, United Kingdom, 2019-05-12 - 2019-05-12). (LA-UR-18-30687)
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- Paris, M. W., V. Cirigliano, and S. M. Shalgar. Collective neutrino oscillations with the halo effect in single-angle approximation. Submitted to *Journal of Cosmology and Astroparticle Physics*. (LA-UR-19-20928)
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Integrated Biosurveillance

Benjamin McMahon
20150090DR

Project Description

We will apply three types of diagnostics to characterize emergence of disease and antibiotic resistance in an immunocompromized population living in the high-disease-burden area of western Kenya. This project will lay the foundations to achieve our long-term technical goals of situational awareness for global pathogen circulation and emergence, thereby addressing national security missions in the area of biological threat reduction. We will apply three types of diagnostics to characterize emergence of disease and antibiotic resistance in an immune-compromised population living in the high-disease-burden area of western Kenya. Our approach involves biomarker discovery, assay development, and assay deployment of three complementary infectious disease assays on a human population. Overall information integration and process optimization will result from both statistical analysis and development and application of realistic epidemiological models. If successful, this work could enable characterization of emerging diseases in the high-disease-burden region where they emerge.

Technical Outcomes

Several facets of integrative biosurveillance was demonstrated in Siaya, Kenya. Biomarker based assays were developed, optimized, and favorably demonstrated for three of the largest sources of fatality from bacterial infection: Salmonella, Staphylococcus, and Tuberculosis. Appropriate statistical methodological methods and mechanistic models were demonstrated to quantify both the benefit of such diagnostics and identify genetic determinants of outcome in the children. Salmonella isolates were analyzed for evolution of genomics, virulence, antimicrobial resistance, metabolism, and clinical impact.

Publications

Fenimore, P. W., C. A. Manore, J. M. Hyman, N. W. Hengartner, S. Y. Del Valle, R. M. Ribeiro, and B. H. McMahon. The role of resource limitations, learning to reduce transmission,

and re-introduction, in controlling the current West African Ebola epidemic. Submitted to *PLoS Neglected Tropical Diseases*. (LA-UR-15-20357)

Frauenfelder, H., R. D. Young, and P. W. Fenimore. A Wave-mechanical model of neutron scattering. Submitted to *Physical Review E*. (LA-UR-15-26544)

Kubicek-Sutherland, J. Z., D. M. Vu, A. Noormohamed, H. M. Mendez, A. C. Hengartner, K. E. Klosterman, H. A. Bridgewater, J. M. Ongecha, D. J. Perkins, N. A. Doggett, B. H. McMahon, and H. Mukundan. Direct detection of bacteremia by exploiting host-pathogen interactions of lipoteichoic acid and lipopolysaccharide. Submitted to *Nature Microbiology*. (LA-UR-18-22478)

Kubicek-Sutherland, J. Z., D. M. Vu, H. Mendez, S. Jakhar, and H. Mukundan. Detection of Lipid and Amphiphilic Biomarkers for Disease Diagnostics. 2017. *Biosensors*. (3) 25. (LA-UR-17-24316 DOI: 10.3390/bios7030025)

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Kubicek-Sutherland, J. Z., H. Mukundan, and A. C. Hengartner. Membrane Insertion for Direct Detection of Lipoteichoic Acid. *Transactions of the Materials Research Society of Japan*. (4) 101-105. (LA-UR-17-20290 DOI: 10.14723/tmrj.42.101)

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Chikungunya challenge. 2018. *BMC Infectious Diseases*. (1) 245. (LA-UR-16-26565 DOI: 10.1186/s12879-018-3124-7)

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Vu, D. M., R. M. Sakamuri, W. R. Waters, B. Swanson, and H. Mukundan. Detection of Lipomannan in Cattle Infected with Bovine Tuberculosis. *Analytical Sciences*. (4) 457-460. (LA-UR-17-21083 DOI: 10.2116/analsci.33.457)

Vu, D. M., R. M. Sakamuri, W. R. Waters, and H. Mukundan. Detection of Lipomannan in Cattle Infected with Bovine Tuberculosis. Submitted to *Analytical Sciences*. (LA-UR-17-24010)

Enabling Anticipatory Analytics for Data Fusion Applications

Kendra Van Buren
20180088DR

Project Description

This work aims to provide technology to significantly advance nuclear safeguards, which provides credible assurance in the timely detection of the diversion of nuclear material and assures that there is no undeclared nuclear material or activities. The most substantial return-on-investment to catapult Los Alamos National Laboratory's (LANL) capabilities forward is to integrate our strengths in sensing technology with what Big Data has to offer. To achieve this goal, it is absolutely necessary to generate and demonstrate the use of experimental data to address the problem. We will generate these experimental data at the international safeguards schoolhouse located at the Technical Area (TA)-66 facility at LANL, and develop the network infrastructure necessary to store and analyze the data. Doing so will provide the framework necessary to deploy to other LANL facilities that are extremely relevant to monitor processes related to special nuclear material.

Safeguards Symposium. (Vienna, Austria, 2018-11-05 - 2018-11-05). (LA-UR-18-28226)

Technical Outcomes

This project demonstrated the ability to deploy, collect, store, and analyze experimental data relevant to nuclear safeguards at Los Alamos National Laboratory's (LANL) international safeguards schoolhouse. Data analysis using supervised machine learning methods and time series analysis showcased the feasibility of using classification models with safeguards-relevant data streams. These results demonstrate the potential to develop accurate models for activity characterization under realistic operational conditions.

Publications

Hou, E. M., K. A. Miller, and A. O. I. Hero. Anomaly Detection for Nuclear Facility Monitoring. Presented at *Consortium for Verification Technology (CVT) Workshop*. (Ann Arbor, Michigan, United States, 2018-10-31 - 2018-10-31). (LA-UR-18-30107)

Miller, K. A., K. L. Van Buren, J. R. Frigo, M. Zeyen, J. P. Sackos, P. M. Mendoza, and A. P. Wright. Disparate Data Integration for Advanced Facility Monitoring. Presented at *IAEA*

Probing Critical Behavior in Hydraulic Injection Reservoirs and Active Seismic Regions

Paul Johnson
20160144ER

Project Description

Conspicuously, seismicity rates in the mid-west United States have dramatically increased over the last 10 years, corresponding to the rapid growth of unconventional oil and gas production and the associated fluid waste injection. A moderate or large magnitude earthquake located in or near a population center could be potentially catastrophic. If a probe existed for the critical stress state at locations in which earthquakes may occur, preventative action (such as termination of pumping) could be taken. We propose that dynamically triggered microearthquakes can be used as a probe of critical stress state (faults near failure) within injection reservoirs and active tectonic regions, and aim to develop the methodology to quantify the new probe. This work could dramatically advance earthquake hazard analysis for both natural and anthropogenic earthquakes.

Technical Outcomes

This project developed and demonstrated a method to calculate the stress tensor field with seismic and gravity data, using a joint geophysical inversion and finite element modelling. In our study area, Oklahoma, we determined that the tectonic and gravitational components of the stress field are of similar magnitude. This is an improvement over existing methods based on borehole measurements and earthquake focal mechanisms because we calculate stress throughout the study area rather than at a point.

Publications

- Chai, C., A. A. Delorey, P. A. Johnson, and M. Maceira. The State of Stress in Oklahoma. Submitted to *Geophysical Research Letters*. (LA-UR-18-25838)
- van der Elst, N., P. A. Johnson, A. A. Delorey, and D. Shelly. Fortnightly modulation of San Andreas tremor and low-frequency earthquakes. Submitted to *Proceedings of the National Academy of Sciences*. (LA-UR-16-22323)

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- Johnson, P. A. Machine Learning Predicts Laboratory Earthquakes. 2017. *Geophysical Research Letters*. (18) 9276-9282. (LA-UR-16-26108 DOI: 10.1002/2017GL074677)
- McBrearty, I. W., A. A. Delorey, and P. A. Johnson. Pairwise Association of Seismic Arrivals with Convolutional Neural Networks. Submitted to *Seismological Research Letters*. (LA-UR-18-29660)
- Scuderi, M., P. A. Johnson, B. Carpenter, and C. Marone. Poromechanics of stick-slip frictional sliding and strength recovery on tectonic faults. 2015. *Journal of Geophysical Research: Solid Earth*. (10) 6895-6912. (LA-UR-16-22578 DOI: 10.1002/2015JB011983)

Radio Frequency Scintillation Prediction Driven by Direct Measurement of Ionospheric Spatial Irregularities

Max Light
20160231ER

Project Description

Scintillation, or distortion and degradation of a radio signal as it passes through the ionospheric plasma, is a concern for space-based nuclear detection. This project will help determine the viability of a new scintillation prediction method. There is currently no global system to measure electron density at the spatio-temporal scales required for scintillation prediction. This project will provide a system architecture and proof-of-concept for such a system. Once implemented, measurements from the proposed system will aid in answering global scintillation questions and could be part of a global scintillation forecasting system. The ability to accurately predict scintillation effects with our model will advance the design of space-based sensors used to detect signals generated from a nuclear detonation.

Technical Outcomes

In order to predict scintillation effects globally, the local irregularity spectral density (ISD) must be known. Theoretically-derived ISD functions based on synoptic measurements of ground-based radars, rockets carrying plasma diagnostic instruments, and satellite RF beacons are currently employed in scintillation models. The stochastic component at any given time or location is typically not known. This work presents the technique we developed and initial results to empirically determine the ISD.

Publications

Lay, E. H. Ionospheric Irregularities and Acoustic/Gravity Wave Activity Above Low-Latitude Thunderstorms. 2018. *Geophysical Research Letters*. (1) 90-97. (LA-UR-17-30883 DOI: 10.1002/2017GL076058)

Lay, E. H., P. A. Parker, M. E. Light, C. S. Carrano, S. Debchoudhury, and R. A. Haaser. Mid-latitude ionospheric irregularity spectral density as determined by ground-based GPS receiver networks. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-18-24228)

Lay, E. H., P. A. Parker, M. Light, C. S. Carrano, S. Debchoudhury, and R. A. Haaser. Midlatitude Ionospheric Irregularity Spectral Density as Determined by Ground-Based GPS Receiver Networks. 2018. *Journal of Geophysical Research: Space Physics*. (6) 5055-5067. (LA-UR-18-21184 DOI: 10.1029/2018JA025364)

Lay, E. H., and I. Azeem. Acoustic gravity waves in the ionosphere during the 2017 total solar eclipse event. Unpublished report. (LA-UR-16-28966)

Narrow Spectrum Gamma-Ray Production Through Inverse Compton Scattering with a Free-Electron Laser

Frank Krawczyk
20160459ER

Project Description

This project will determine the fundamental limitations to very narrow gamma-ray production through inverse Compton scattering. This is needed for the future capability to detect special nuclear material through nuclear resonance fluorescence. The technical goals are to demonstrate a novel inverse Compton scattering (ICS)/ free-electron laser (FEL) hybrid approach to generating MeV gamma rays with spectral widths of 0.1% and less and to develop a validated predictive capability through detailed measurements at the Lawrence Livermore accelerator facility. We will be able to produce high flux gamma rays with an order of magnitude narrower spectral widths than ever before, allowing us to experimentally investigate subtleties and the interdependencies of the various physical phenomena leading to gamma ray spectral broadening.

Technical Outcomes

Based on proven performance of an Energy Recovery Linac (ERL) as narrow-band Inverse Compton Scattering (ICS) source at KEK, Japan, this project developed an optimized ERL for remote SNM detection. We developed an optimized compact ERL system combined with advantages of Free-Electron Lasers as the photon source. This provides a new technical solution with compact foot-print with an increased potential for achieving narrow band-width high-flux ICS gamma output, as it avoids limitations from other prior attempts.

Range-Resolved Measurement of Atmospheric Greenhouse Gases for Treaty Verification and Climate Science

Brent Newman
20160462ER

Project Description

This project will demonstrate a novel scheme to measure atmospheric gas concentrations in the stratosphere between 15 and 30 kilometer (km) altitude. This measurement technique can be flown in a satellite and may support future greenhouse gas treaty verification. The technical goal of this project is to verify our hypothesis that we can use a W-Band approach to interrogate the stratosphere for volume-constrained spectroscopy of atmospheric gases. Using available hardware, we will separately verify the two key elements in this hypothesis: (1) the Rayleigh reflection of aerosols in the stratosphere between 15 and 30 km altitude at W-band is large enough so a practical spectroscopy instrument can be built, and (2) by measuring the differential absorption of a specific gas rotational resonance at slightly different altitudes, we can determine the gas concentration at that altitude. Both climate science (in particular modeling of greenhouse gases) and future greenhouse gas emission treaty verification will greatly benefit from this new technology.

Ramani, S. Microwave remote sensing for atmospheric chemistry. Unpublished report. (LA-UR-18-28667)

Technical Outcomes

Conducted outdoor radiance measurements with vector network analyzer to evaluate hardware performance suitable for W-band spectroscopy. Investigated radiometry for measuring stratospheric ozone emissions. Completed a W-band radiometer receiver design and tested and programmed a software defined radio for use as a portable radiometer. For the first time, conducted deuterium measurements using a mini-FTS. Conducted a comparative analysis of satellite and ground-based NO₂ emissions providing scaling relations for understanding transport of this pollutant in the atmosphere.

Publications

Bishopberger, K. A., and S. Ramani. W-Band Noise Floor Measurements. Unpublished report. (LA-UR-17-20942)

Novel Antennas Based on Atomic Magnetometers

Malcolm Boshier
20160518ER

Project Description

We will use new atomic magnetometer technology to develop compact high-performance receiving antennas. The overall technical goal is to show that newly developed atomic magnetometer technology can realize low-frequency receiving antennas with an unprecedented combination of high sensitivity and compact size. Applications of these devices include communication underground, through buildings, and under water; receiving signals from low frequency beacons; and remotely diagnosing machinery operating in an underground facility.

Technical Outcomes

This project developed the world's first portable atomic magnetometer that can operate in real-world field environments. We showed that this device can function as a compact antenna for encoded messages transmitted using very low frequency radio waves. With the addition of extra coils to cancel ambient magnetic fields, the atomic magnetometer antenna should deliver state of the art sensitivity in outdoor and underground environments.

Publications

Savukov, I. M. High-sensitivity operation of single-beam optically pumped magnetometer in a kHz frequency range. 2017. *Measurement Science and Technology*. (3) 035104. (LA-UR-16-24444 DOI: 10.1088/1361-6501/aa58b4)

Accumulator for Low-Energy Laser-Cooled Particles

Kevin Mertes
20160584ER

Project Description

The technical base of accumulators and injectors for high-energy particles can be molded into exotic experiments or medical tools. Analogous elements, we will show, can also be made for ultracold matter, for use in a wide and newfound range of research. Accumulators are special tools of high-energy physics (HEP) that catch and overlap batches of particles into dense packets. Accumulator principles, however, are not exclusive to HEP and may be formed for the decidedly low-energy particles of laser-cooled atoms and molecules, as indicated by our calculations. We propose to build an accumulator for cold atoms and demonstrate its capacity for gathering more cold particles than possible by conventional means and concentrating them to very high densities. With greater familiarity and adoption, accumulators could provide a foundation for applications of ultracold matter in navigation, precision measurement, remote sensing, and chemical detection.

Technical Outcomes

This project created an ultra-cold chemistry apparatus capable of manipulating atoms with laser light. The system is a better starting point for quantum enhanced sensors. Together with a theoretical program this system can be a vehicle for many body physics measurements by providing opportunities for experimental measurements of important parameters such as scattering lengths, interaction strengths, resonant interactions and tunneling via external fields which can be used to verify and refine theory.

Publications

Mertes, K. M., and Y. Suzuki. Vacuum Texture: A New Interpretation of Quantum Mechanics and a New Loophole for Bell's Inequality Measurements that preserves Local Realism and Causality. Submitted to *Physical Review Letters*. (LA-UR-19-22136)

Walking the Road from Impacts to Seismic Sources for Celestial Bodies

Carene Larmat
20170109ER

Project Description

The goal of this project is to facilitate future seismic missions to a multitude of planets and moons. Decades of seismic exploration on Earth has provided high-resolution images of its buried features, and we know that important clues to natural resources of other planets will reside in their interior. However, data return from extraterrestrial seismic missions is highly dependent on how efficient are impacts to generate seismic waves. The level of uncertainty of current models translates in high risk explaining the low number of seismic missions launched by NASA so far. This view is changing as the Discovery program gears towards planets beyond Mars. This research aims to provide a new generation of numerical Bolide impact models for rocky planets. These models will leverage on unique modeling capabilities developed at Los Alamos to capture the high-strain high-energy physics involved in modeling of Underground Nuclear Explosions (UNEs). Of note, the new material models developed will extend our nuclear monitoring ability to unconventional geologic environments (i.e. other than US and Russian test areas), which will help extend DOE's Research and Development efforts into other regions in support of US national security interests.

Publications

- Larmat, C., P. Lognonn\xc3\xa9, V. Rakoto, I. Daubar, and F. Karakostas. Inversion of Meteor Rayleigh Waves on Earth and Modeling of Air Coupled Rayleigh Waves on Mars. 2018. *Space Science Reviews*. (8) 127. (LA-UR-18-25160 DOI: 10.1007/s11214-018-0566-6)
- Larmat, C., Z. Lei, E. E. Knight, E. Rougier, P. Lognonne, F. Karakostas, and M. Froment. FINAL REPORT IC PROJECT w17_seismicsources " Walking the road from impacts to seismic sources for celestial bodies". Unpublished report. (LA-UR-19-22152)

Three-Dimensional Nuclear Quadrupole Resonance Imaging

Petr Volegov
20170141ER

Project Description

This work will result in a new method to non-invasively detect and image illicit substances (namely explosives and narcotics) at a chemically specific level. While many other imaging techniques exist, none are able to positively identify specific chemical compounds, making our approach a unique tool for substance detection. With immediate national security applications in airport security, improvised explosive device (IED) detection and removal, and drug trafficking, there is a large application space for our technology. Our principal goal is to demonstrate the first 3-Dimensional image with our two proposed techniques and determine the ultimate physical limits of our approach. Specific to NNSA, our research has the potential to look inside the bulk high explosives of our nuclear warheads to address questions about aging and quality control of the manufacturing process to ensure the safety and suitability of our stockpile for years to come.

High Energy Lightning: Understanding Relations Between Energetic Particles and Lightning Discharges in Thunderclouds

Xuan-Min Shao
20170179ER

Project Description

This project directly addresses DOE/NNSA's space-based nuclear detonation detection missions, as well as the nation's newly developed ground-based nuclear forensics missions. Lightning-related electromagnetic pulse (EMP) and gamma/x-ray emission signatures are often similar to those of atmospheric nuclear explosions and are unwanted background interference for these systems. Better understanding of their signatures and the underlying physics is important to reducing the possible false alarms for these systems. Los Alamos National Laboratory's ground-based EMP observation and advanced simulation play a critical role in providing prompt nuclear weapon performance information for a national-level forensics mission. However, without actual nuclear tests it is difficult to validate the sensor and the simulation performance. Fortunately, EMP and gamma emissions produced by cosmic ray showers and lightning are similar (in a small scale) in physics to that of a nuclear explosion, especially at the exponential multiplication stage, and can be used to validate the United States Prompt Detection System (USPDS) sensor and simulation.

Conference on Atmospheric Electricity. (Nara, Japan, 2018-06-17 - 2018-06-22). (LA-UR-18-23483)

Shao, X. M., C. Ho, M. P. Caffrey, P. S. Graham, W. B. Haynes, G. S. Bowers, H. Rasoul, D. Smith, B. L. Dingus, and W. G. Blaine. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations of Lightning Discharges: Revealing New Physics Insights Into Breakdown Processes. 2019. *Journal of Geophysical Research: Atmospheres*. (18) 10-10. (LA-UR-18-24675 DOI: 10.1029/2018JD029096)

Publications

Bowers, G. S., X. M. Shao, W. G. Blaine, B. L. Dingus, D. M. Smith, M. Schneider, and M. McCarthy. Simulation of the High Altitude Water Cherenkov (HAWC) Observatory & Gamma-ray Observations During Overhead Thunderstorms (GODOT) instrument to Relativistic Runaway Electron Avalanche (RREA) gamma-ray enhancements. Presented at *16th International Conference on Atmospheric Electricity (ICAE)*. (Nara, Japan, 2018-06-17 - 2018-06-22). (LA-UR-18-23454)

Shao, X. M., C. Ho, G. S. Bowers, W. G. Blaine, B. L. Dingus, M. P. Caffrey, P. S. Graham, W. B. Haynes, and D. Smith. Broadband RF interferometric and polarization observations of lightning discharges correlated with gamma flux detection. Presented at *XVI International*

Laser Radiochronometry

Alonso Castro
20170199ER

Project Description

The goal of this project is to demonstrate the development of a new method for dating nuclear materials, i.e., the determination of the date when a nuclear material, such as uranium or plutonium, was first manufactured and purified. This new method will improve upon existing radiological dating methods such as mass spectrometry because it is fast, inexpensive, and will be able to date materials without signal interferences from isotopes of similar masses, such as Plutonium-241 (^{241}Pu) and Americium-241 (^{241}Am).

A Novel Ultrasound Tomography Technique for High-Resolution Imaging

Lianjie Huang
20170203ER

Project Description

This research will advance the Laboratory's world-leading acoustic-wave and elastic-wave capabilities, which are crucial for addressing various challenges in energy and environmental security, nuclear security (monitoring weapon components), and public health. With this project, we endeavor to develop the first transrectal ultrasound tomography technique to accurately distinguish malignant from benign prostate tissues, and aggressive from indolent or nonaggressive prostate cancers. Results from this project could fill a technology gap identified by the U.S. Preventative Services Task Force for new imaging techniques; in fact, there is great opportunity for multi-mission impact due to the technology's safe (non-ionizing radiation), cost-effective, and portable imaging modality.

Publications

- Huang, L., K. Gao, and Y. Huang. Transrectal ultrasound-waveform tomography using plane-wave ultrasound reflection data for prostate cancer imaging. Presented at *2018 SPIE Medical Imaging*. (Houston, Texas, United States, 2018-02-12 - 2018-02-15). (LA-UR-18-21057)
- Huang, L., Y. Huang, and K. Gao. Transrectal ultrasound imaging using plane-wave, fan-beam and wide-beam ultrasound: Phantom results. Presented at *2019 SPIE Medical Imaging meeting*. (San Diego, California, United States, 2019-02-17 - 2019-02-17). (LA-UR-19-21584)
- Shin, J., L. Huang, and J. T. Yen. Spatial Prediction Filtering for Medical Ultrasound in Aberration and Random Noise. To appear in *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*. (10) 1845-1856. (LA-UR-17-30593 DOI: 10.1109/TUFFC.2018.2860962)
- Shin, J., Y. Lou, J. T. Yen, and L. Huang. Spatial Prediction Filtering for Increased Penetration Depth in Synthetic Aperture Ultrasound. Presented at *2017 IEEE International Ultrasonics Symposium*. (Washington, D.C., District Of Columbia, United States, 2017-09-06 - 2017-09-09). (LA-UR-17-27566)

Strontium Bose-Einstein Condensate Atom Interferometer with Matter Wave Circuits

Changhyun Ryu
20170218ER

Project Description

Inertial navigation is essential in many national security missions. Although global position system (GPS)-based navigation can be used in ideal situations, when GPS service is denied or unavailable, an independent, accurate, inertial sensor is needed. Traditional technologies have reached their limit in sensitivity and a new approach has been sought. Inertial sensing with an atom interferometer is a promising new direction to improve sensitivity in sensing of rotation and acceleration toward the goal of long distance navigation without GPS input. We will develop a novel inertial sensor with atoms trapped in a waveguide made of laser beams. Since atoms are trapped inside waveguides, the interrogation time can be very long and this increases sensitivity accordingly. The successful completion of this project will demonstrate the highest sensitivity in sensing of rotation and acceleration with waveguide atom interferometer. This will make it possible to develop a portable compact inertial sensor for many national security missions. This research is relevant to DOE/NNSA missions of national security science in developing novel sensing technologies for national security missions.

Fluctuating Domains in Antiferromagnets for Sensing and Switching Applications

Vivien Zapf
20170288ER

Project Description

Technology is moving beyond simple ferromagnets, where all the individual electron spins align with each other. New computing, sensing, communication and energy technologies are increasingly using antiferromagnets and more complex magnetic structures, where the different spins point in different directions and break various symmetries. As these useful magnets become more complex, it becomes challenging to study them. In particular, we need to understand defects, domains, and fluctuations in antiferromagnets and other complex magnets. It is well established that domains control the functionality of ferromagnets. Domains are likely very common in antiferromagnets as well, however they have historically been difficult to study. Here we explore how the new generation of magnetic field and X-ray technologies at DOE and NNSA facilities in conjunction with world-class theoretical efforts can be applied to understanding domains and fluctuations in antiferromagnets. This work extends our fundamental understanding of technologies related to communication, energy, data storage and manipulation and sensing.

P. Dai, A. H. Nevidomskyy, C. L. Hunag, and E. Morosan. Anomalous metamagnetism in the low carrier density Kondo lattice YbRh₃Si₇. Submitted to *Physical Review X*. (LA-UR-18-30067)

Zapf, V. Multiferroic Metal-Organic Materials. Unpublished report. (LA-UR-18-21705)

Publications

Chikara, S., V. Zapf, J. Eckert, S. Lin, N. C. Smythe, J. Singleton, B. L. Scott, E. Krenkel, and C. Batista. Multiferroic behavior via a spin state transition. Submitted to *Nature*. (LA-UR-17-29041)

Kim, J. W., V. Zapf, M. Jaime, N. Harrison, X. Ding, S. W. Cheong, H. T. Yi, Y. Chai, Y. Sun, A. Hansen, and E. D. Mun. Metastable states in the frustrated triangular compounds Ca₃Co_{2-x}MnxO₆ and Ca₃Co₂O₆. 2018. *Physical Review B*. (2) 024407. (LA-UR-17-28067 DOI: 10.1103/PhysRevB.98.024407)

Rai, B. K., V. Zapf, J. Singleton, S. Chikara, X. Ding, I. W. H. Oswald, R. Shoenemann, V. Loganathan, A. M. Hallas, H. B. Cao, M. Stavinoha, H. Man, S. Carr, K. Benavides, J. Y. Chan, Q. R. Zhang, D. Rhodes, Y. C. Chiu, L. Balicas, A. A. Aczel, Q. Huang, J. W. Lynn, J. Gaudet, D. A. Sokolov,

Life on the Edge: Microbes in Rock Varnish

Chris Yeager
20170414ER

Project Description

This project supports DOE's Energy Security mission by conducting basic research on exoelectrogenic processes (the extracellular electron transfer pathways that allow certain microorganisms to transfer energy between intracellular chemical energy stores and extracellular solids) under harsh conditions. Additionally, this research benefits NNSA's mission in nonproliferation because elemental signatures in rock varnish can be used to characterize past atmospheric depositional events. By integrating Los Alamos capabilities and expertise in geochemistry, space science, and microbiology we aim to: 1) identify and interpret the microbial species and processes involved in the habitation and/or formation of rock varnish; 2) identify organic biosignatures that, in concert with trace element and mineralogy, can be used to conclusively distinguish the biogenic and abiogenic origins of terrestrial Mn-rich surfaces; 3) determine the role of light-dependent Fe/Mn redox chemistry in sustaining life in rock varnish. Each of these goals in and of themselves has important implications for our understanding of how life on Earth has evolved to capture and harness energy from the physical environment, and will aid in our search for similar processes on Mars. Knowledge gained from this research will benefit further technological advances in DOE-relevant fields ranging from bioenergy to solar energy to bioremediation.

Quantum-Dot-Based Infrared Photodetectors with Picosecond Temporal Resolution Operating at Room Temperature

Istvan Robel
20170435ER

Project Description

The principal goal of this project is to develop inexpensive, high-efficiency, and high-time-resolution infrared photodetectors based on semiconductor quantum dots, a class of nanomaterials with size-tunable optical and electronic properties. Such technologies could find applications for surveillance, remote sensing, and spectral imaging.

Elpasolite Planetary Ice and Composition Spectrometer (EPICS): A Low-Resource Combined Gamma-Ray and Neutron Spectrometer for Planetary Science

Daniel Coupland
20170438ER

Project Description

The Elpasolite Planetary Ice and Composition Spectrometer (EPICS) will provide a transformational advance in the orbital investigation of the composition of planetary bodies, including asteroids, moons, Mars, and the inner planets. The elpasolite scintillators and other new technologies in EPICS enable for the first time combined neutron and gamma-ray spectroscopy with a single detector, yielding a substantial reduction in instrument size, mass, power, and complexity for future planetary science missions. Planetary science provides high-profile positive press to the Laboratory, raising our scientific visibility and attracting new talent. EPICS will also revitalize synergy between planetary science and national security in space. Neutron and gamma-ray planetary science instruments have significant design synergy with instrumentation for the US Nuclear Detonation Detection System (USNDS) program and other national security missions; staying engaged in scientific instrument development is critical for retaining talent, remaining abreast of new technologies, and improving future USNDS instrument designs.

Mesick, K. E., D. D. S. Coupland, S. F. Nowicki, and L. C. Stonehill. The Effects of Radiation Damage on CLYC Performance. Submitted to *Proceedings of the IEEE*. (LA-UR-17-30435)

Nowicki, S. F., L. C. Stonehill, D. D. S. Coupland, and K. E. Mesick. Development of an Elpasolite Planetary Science Instrument. Submitted to *IEEE Nuclear Science Symposium Conference Record*. (LA-UR-16-29261)

Publications

S. Coupland, D. D., K. E. Mesick, S. F. Nowicki, L. C. Stonehill, and S. D. Dibb. Thermal Variance Investigation of Cs₂LiLa(Br,Cl)₆:Ce. Presented at *IEEE Nuclear Science Symposium and Medical Imaging Conference*. (Atlanta, Georgia, United States, 2017-10-23 - 2017-10-23). (LA-UR-17-30406)

Mesick, K. E., D. D. S. Coupland, L. C. Stonehill, S. T. West, D. T. Beckman, N. Dallmann, S. F. Nowicki, W. Feldman, and S. A. Storms. Elpasolite Planetary Ice and Composition Spectrometer (EPICS): A Low-Resource Combined Gamma-Ray and Neutron Spectrometer for Planetary Science. Presented at *2018 IEEE Nuclear Science Symposium and Medical Imaging Conference*. (Sydney, Australia, 2018-11-10 - 2018-11-10). (LA-UR-19-20081)

Imaging Neural Dynamics With Ultra-Low Field Magnetic Resonance Imaging (MRI)

Per Magnelind
20180058ER

Project Description

This project will provide a new neuroimaging capability that will aid in different aspects of increasing the knowledge about the most complex system we know – the human brain. An increased fundamental understanding of the brain would have important implications in the vast field of neuroscience (e.g. within National Institutes of Health – NIH), and could have importance for national security by enhancing human performance through methods such as transcranial electrical stimulation and magnetic stimulation, which are of interest to numerous Department of Defense (DoD) sponsors, such as the Defense Advanced Research Projects Agency (DARPA).

Atomic Structure of Actinides

Igor Savukov
20180125ER

Project Description

Knowledge of the properties of actinide atoms is central to Los Alamos National Laboratory mission applications. In particular, atomic properties, such as energy levels and transition rates, are needed for spectroscopy-based applications, such as detection of actinide atoms and enrichment characterization, and for plasma modeling. Currently, there are no theories adequate for this task. This project will develop an accurate atomic structure theory that will be capable of generating data needed in various applications.

Publications

Savukov, I. M., and P. M. Anisimov. Accurate configuration-interaction many-body-perturbation theory La II electric-dipole transition probabilities. Submitted to *Physical Review A*. (LA-UR-18-30155)

Novel Multichannel Atomic Magnetometer

Young Jin Kim
20180131ER

Project Description

This project will result in the development of a low-cost, compact, rugged, high-sensitivity multichannel atomic magnetometer (AM) module that will significantly improve the current multichannel technology. We anticipate broad applications in fields ranging from medicine to national security. In magnetoencephalography (MEG), the sensitivity and resolution will be improved, and with increased positioning flexibility we envision the first size-adjustable pediatric system. The spatial resolution of magnetic imaging can be improved by adding an array of flux guides (FGs) to facilitate neurosurgical planning and studies of cognitive/perceptual responses. This method will have applications in nano-particle detection, important for biosecurity and medical diagnostics, such as early stage cancer detection. Other applications of our AM module include explosive detection via nuclear quadrupole resonance (NQR) and magnetic resonance imaging (MRI). For example, by replacing the multichannel SQUID sensors with the AM module, a MagViz system can be made non-cryogenic to facilitate deployment in airports. The same replacement can be done for anatomical brain imaging applications.

Zhu, Y., I. M. Savukov, Y. Gao, and C. Hilty. Frequency Resolved Detection of Nuclear Spin Optical Rotation at Low Field. Submitted to *JPCL*. (LA-UR-18-22153)

Publications

Kim, Y. J., I. M. Savukov, and S. G. Newman.

Magnetocardiography with a 16-channel fiber-coupled single-cell Rb optically pumped magnetometer. Submitted to *Applied Physics Letters*. (LA-UR-19-21746)

Kim, Y. J., and I. M. Savukov. A Portable 16-channel Magnetic Sensor for Human Magnetocardiographic Experiments. 2018. *International Journal of Engineering and Science Invention*. (10) 54-57. (LA-UR-18-28670)

Kim, Y. J., and I. M. Savukov. Highly sensitive multi-channel atomic magnetometer. Presented at *2018 IEEE Sensors Applications Symposium*. (Seoul, Korea, South, 2018-03-12 - 2018-03-14). (LA-UR-17-29859)

Proton Radiography for Advanced Cancer Therapy

Michelle Espy
20180238ER

Project Description

More than two dozen proton therapy centers now operate in the US, taking advantage of the centimeter precision while minimizing the radiation absorbed in nearby healthy tissue. Even more precise proton treatments could target tumors on the order of a millimeter in size, or to tumors close to sensitive tissues, if relativistic proton beams (~1GeV) were used. The future of proton beam therapy will be at high energy, with direct, positive impact in treating the most difficult cancers, including some that may have otherwise been deemed untreatable, and those in the most radiation-sensitive, pediatric patients. Fully exploiting the precision of the higher-energy protons will require imaging both the patient and the dose deposition in real-time, on location, to ensure radiation accurately targets the tumor during each treatment. Fortunately, the same relativistic protons used for treatment can also be used to image tumors in a patient, as well as track treatment delivery. We propose to use the LANSCE Proton Radiography Facility (pRad) to demonstrate imaging of small tagged tumors in mice with sufficient resolution and low enough dose to guide precise relativistic proton beam therapy. This work could profoundly influence the future development of proton therapy worldwide.

Publications

- Freeman, M. S., E. F. Aulwes, M. A. Espy, J. F. Hunter, P. E. Magnelind, F. E. Merrill, F. R. Trouw, and D. Tupa. Direct Proton Detection for Therapy Guidance and Treatment Planning. Submitted to *Medical Physics*. (LA-UR-18-30411)
- Freeman, M. S., M. A. Espy, P. E. Magnelind, F. G. Mariam, F. E. Merrill, D. Tupa, and C. H. Wilde. Proton Radiography for Relativistic Proton Beam Therapy. Presented at *SPIE Medical Imaging*. (Houston, Texas, United States, 2018-02-12 - 2018-02-16). (LA-UR-18-20428)

OrganiCam: A High-Sensitivity Radiation-Hardened Imaging Organic Detector For Space and Programmatic Applications

Roger Wiens
20180244ER

Project Description

This is a dual-purpose project with applications for outer solar system and for high-radiation areas on Earth such as nuclear reactor cores or an accident area such as Fukushima. We plan to build a time-resolved fluorescence camera and spectrometer (OrganiCam) that will be able to observe and distinguish organic and mineral (e.g., heavy-element) fluorescence. In tune with the NASA applications, we will study and develop plans for an instrument that can survive and operate in a highly radioactive environment. Robots like the “Little Sunfish” now exploring the insides of the Fukushima reactor show that instruments of this type can be highly beneficial in surveying damage in a nuclear contamination zone. Careful use of electronic and optical components are required for such an environment and so our project will focus significant effort for this capability.

Engineering the Universal Bacterial Sensor

Harshini Mukundan
20180387ER

Project Description

Rapid point of care detection of infectious diseases is a critical requirement for the Department of Defense, both for the health of the deployed troops and for prevention of biological terrorism. This universal platform and the fieldable and technical simplicity will advance our capability. Also, emerging and antimicrobial resistance is a major threat to national health security, and identifying bacterial infections at the point of care will become increasingly important. This work addresses the first technical challenge identified in the National Biosurveillance strategy, released by the White House in 2012. The uniqueness of this platform is its ability to use the Los Alamos National Laboratory developed lipoprotein capture assays to identify ALL bacterial infection without prior knowledge- making it invaluable in biological threat and border protection screening situations.

Publications

Mukundan, H., and S. Y. Del Valle. Zika virus forecasting and prediction studies: a systematic review and evaluation of forecasting research during a public health emergency of international concern. Submitted to *PLOS Medicine*. (LA-UR-18-30805)

Noninvasive Thermal Mass Flow Meter for Safeguards

Rollin Lakis
20180575ER

Project Description

A fundamental component for the implementation of nuclear safeguards is the reliable monitoring of nuclear material production and waste generation. A major cause of concern in nuclear-non-proliferation is that currently available monitoring strategies usually monitor the process in a few or even a single key location and, for this reason, might not be effective in enforcing safeguards in nuclear production facilities. The goal of this work is to create a low-cost, non-invasive, spoof-resistant, internet of things enabled mass flow meter for safeguards monitoring of process fluids in nuclear production facilities. At this stage, the flowmeter will be developed for uranium hexafluoride (UF₆). The low cost and noninvasive nature of the proposed meter enables the installation of a network of mass flow meters distributed in a systematic manner throughout the flow sheet at critical locations. Importantly, this network would be independent of the operator and would not rely upon shared data streams. The approach we are currently proposing for the non-invasive monitoring of UF₆ gas can be extended to the monitoring of other relevant nuclear process gas and liquids used in nuclear production facilities. For this reason, the project is directly relevant to a broad set of DOE/NNSA/Nuclear Nonproliferation programs.

Point of Care Enabling Technologies(PoCET): Magnetically Coupled Valves and Pumps

Pulak Nath
20170026ER

Project Description

This project is enabling the development of the "liquid logic" technology, which is essentially the reduction of common laboratory processes into handheld platforms that are fully automated and deployable for point of care applications. Proposed work supports the "forward deployment" theme of the Los Alamos Science of Signature pillar. From medical diagnostics to nuclear forensics, the capabilities developed with this project will support a wide range of applications. Microfluidics have experienced remarkable growth with thousands of patents/publications in the last 15 years. Nevertheless, in most cases we get "chip-in-a-lab" as opposed to "lab-on-a-chip," due to large peripherals such as pumps, valves, tubes, electrical/optical components, and sensors. Our focus is to develop miniaturized magnetically coupled microfluidic valves, pumps, and their novel driver mechanism. These platforms will enable truly integrated microfluidic platforms that can carry out complex operations in a pocket size platform, which otherwise would require significant laboratory space with current technologies.

Technical Outcomes

This project developed a self-contained, liquid handling approach integrating disposable microfluidic cards, magnetically-coupled valves/pumps, and novel valve/pump driver technologies. Two versions of the drivers have been demonstrated: (1) Battery powered; and (2) Self-powered. These integrated microfluidic platforms are suitable to carry out complex laboratory operations in a portable and miniaturized format. Demonstration of proof of principle included fully automated serial dilution, microfluidic droplet generation, and simulated steps to execute automated DNA extraction.

Publications

Nath, P. LDRD ER (20170026ER) Final Report: Point of Care Enabling Technologies (PoCET): Magnetically Coupled Valves & Pumps. Unpublished report. (LA-UR-18-29406)

Inspecting America's Aging Infrastructure with Muon Radiography

J Durham

20170402ER

Project Description

As our country's infrastructure continues to age and deteriorate, America is increasingly subject to economic losses from process downtime as well as loss of competitiveness in the global industrial market. Los Alamos National Laboratory has developed a new, unique method to non-destructively evaluate industrial components, using only naturally occurring background radiation from space called "cosmic ray muons." Using these particles, we can produce tomographic images of pipes, valves, concrete, and other object that can be subject to aging and failure. Unlike x-rays, this method does not rely on artificial sources of radiation that may give workers or the public unnecessary exposure. Muons are also highly penetrating, enabling inspections of (for example) pipes that are covered by insulation while they are in use. For a typical x-ray or ultrasound inspection, insulation must be removed prior to inspection, and the process using that pipe must be stopped. Since muons can image deterioration through insulation, there is no downtime associated with this technique. This new inspection technique can be applied to power plants, petrochemical refineries, and multiple other industrial sites. Reduced process downtime and increased confidence in our country's infrastructure will result in economic benefit to the United States.

Technical Outcomes

This project developed a small, lightweight muon detector with high efficiency. As opposed to typical muon radiography systems, this instrument is easily portable by hand. This potentially expands the applicability of muon radiography to the inspection of small parts (i.e. pipes) in areas that are difficult to access with large equipment, such as refineries. This small system also serves as a prototype for developing larger man-portable systems that may be useful in nuclear emergency response.

Coherent Radio Frequency Collection Through Computation for CubeSat Constellations

Zachary Baker
20170583ER

Project Description

The goal of this project is to change how we think about and build arrays of satellites. Traditional radio collection vehicles required large dish receivers; this means large, expensive satellites. Our approach breaks the large satellite into many small apertures and then computationally recombines the observations of the small satellites. The key promise of "agile space" is that a medium number of low-cost vehicles orbited can provide similar functionality but with multiple eggs in multiple baskets. These clusters of small satellites are very hard to target, "cheap" to replace, and provide higher coverage over Earth for longer periods of time with increased survivability

Technical Outcomes

This project successfully demonstrated the "Coherence through Computation" approach with on-orbit collects using both ground-based transmitters with satellite collection, and space-based transmitters with ground collection. A key take-away is to demonstrate that precise time and position knowledge is not necessary to form a beamforming array, which has the potential to change how we build satellites. In particular, we can build smaller, cheaper, lower power satellites, replacing the precision of the collect with ground-based correction.

Publications

Baker, Z. K., J. L. Woodring, J. E. Payne, N. Dallmann, and W. Junor. Accelerated Aperture Synthesis from Free-flying Collectors. Presented at *IEEE High Performance Extreme Computing Conference*. (Boston, Massachusetts, United States, 2018-09-25 - 2018-09-25). (LA-UR-18-24534)

Baker, Z. K., N. Dallmann, and W. Junor. Aperture Synthesis from Free-flying Collectors without Accurate Metrology. Presented at *IEEE Aerospace*. (Big Sky, Montana, United States, 2018-03-03 - 2018-03-03). (LA-UR-18-21471)

Baker, Z. K., N. Dallmann, and W. Junor. Aperture Synthesis from Free-flying Collectors without Accurate Metrology.

Presented at *IEEE Aerospace*. (Big Sky, Montana, United States, 2018-03-03 - 2018-03-03). (LA-UR-17-29518)

Baker, Z. K., V. B. Ramakrishnaiah, J. L. Woodring, N. Dallmann, and W. Junor. Acceleration on Heterogeneous Architectures for Synthesis of Coherent Sparse Arrays. Presented at *IEEE Aerospace Conference*. (Big Sky, Montana, United States, 2019-03-02 - 2019-03-02). (LA-UR-18-29886)

Ramakrishnaiah, V. B., and Z. K. Baker. Accelerating the Signal Alignment Process in Time-Evolving Geometries using Python. Presented at *The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC18)*. (Dallas, Texas, United States, 2018-11-11 - 2018-11-16). (LA-UR-18-27904)

Very Low Frequency (VLF) Mode Generation and Propagation in Space Plasmas

Bruce Carlsten
20180287ER

Project Description

This project will extend the foundational understanding of generating and propagating Very Low Frequency (about 10 kilohertz) plasma electromagnetic modes in the ionosphere/magnetosphere with a combination of theory, simulation tool development, modeling, and validation with both an upcoming satellite experiment and a highly relevant laboratory experiment. This work supports an urgent, high-priority, national security mission that Los Alamos National Laboratory is uniquely positioned to address with its broad capabilities in nuclear weapons phenomenology, space technologies, compact nuclear reactors, compact accelerators, and beam-plasma interactions. A high-altitude nuclear explosion would create artificial radiation belts with charged particles that in turn would damage satellites. These charged particles can be precipitated into the atmosphere by scattering them off very low frequency whistler waves - a rough estimate of required very low frequency power for ensuring accelerated satellite mortality can be reduced to the equivalent of a few extra years of orbit time is on the order of 100 kW for a few months. The proposed work will develop the tools needed to evaluate different Radiation Belt Remediation schemes for optimizing an Radiation Belt Remediation architecture while investigating novel phenomena in ionospheric very low frequency wave generation and propagation.

Technical Outcomes

This project developed the necessary tools to predict, guide, and eventually interpret Very Low Frequency (about 10 kHz) RF emission experiments from the Air Force Demonstration and Science Experiments mission which will be launched in early FY19. This work is foundational to, and supports, the development of a larger Laboratory capability in radiation belt remediation to mitigate a catastrophic loss of US satellites in the case of a high-altitude nuclear detonation.

Teng, S., J. Zhao, X. Tao, S. Wang, C. Kletzing, G. D. Reeves, H. O. Funsten, and H. E. Spence. Observation of Very Oblique Lower Band Chorus Generated by Nonlinear Three Wave Interaction. Submitted to *Geophysical Research Letters*. (LA-UR-18-31204)

Publications

Full-Field Ultrasound for In-process Inspection of Additively Manufactured Parts

Adam Wachtor
20180402ER

Project Description

This work supports the national security mission by improving the capability to produce mission-critical parts through additive manufacturing. Additive manufacturing allows for the production of unique components without the need for significant preparation and tooling costs seen in traditional fabrication processes. These advances in non-destructive evaluation for in-process additive manufacturing will lead to active feedback and control of the additive manufacturing process and benefit quality control. This in turn will allow for the production of reliable components in-house that support stockpile life-extension programs and retrofits and provide low-cost handling and tooling fixtures for fabrication services.

Technical Outcomes

Performed the first full part, 3D ultrasonic diagnostic measurements of an additively manufactured (AM) metal built non-invasively during the AM process. These measurements were acquired by performing full-field ultrasonic scans of each deposition layer throughout the AM process and assembling the 2D response maps together to produce a 3D response volume. Novel LANL developed technology (acoustic wavenumber spectroscopy – R&D 100 2014) made it possible to perform these measurements without interfering with the AM process.

Advances in Multi-Phenomenology Event Identification and Location

Jonathan Maccarthy
20180527ER

Project Description

This work addresses the challenge of detecting and locating a clandestine nuclear explosion in the absence of existing supporting data from the site. We will improve our ability to use seismic and atmospheric sensor data to detect and locate an event in a new region. We expect that new waveform detection methods will outperform existing template-based detection methods, and that improved physics-based atmospheric transport modeling uncertainties will lead to a more accurate representation of the uncertainty in the event location. An improved ability to monitor new regions for nuclear events will contribute to DOE/NNSA nonproliferation and forensics efforts.

Technical Outcomes

This project simulated a large suite of atmospheric releases in Oklahoma City on a cluster, and learned about model stochasticity and our ability to emulate higher fidelity models. We have developed the software to build a constrained QUIC design, and have ideas for building a suitable emulator. We have tested a nonlinear waveform matching method on simulated seismic data, and found improved detection ability at the expense of heavy computational cost and additional parameter tuning.

Nonlinear Elastic Wave Measurements for Diagnosing Aging in Pentaerythritol Tetranitrate

Carly Donahue
20180578ER

Project Description

As the nuclear stockpile ages, limited quantities of aged detonators are available for surveillance purposes to assess performance degradation. The ability to predict and diagnose aging in pentaerythritol tetranitrate (PETN) pellets is of paramount interest to the detonator community. However, current evaluation methods can be time consuming, hard to perform in situ, and do not necessarily produce meaningful information. We propose to develop nonlinear elastic wave propagation measurements as diagnostic tools for PETN aging. Such techniques are promising because of their ability to probe microstructure characteristics as well as wave propagation characteristics, which are fundamental parameters governing sensitivity and function time. Activating a nonlinear wave based metric could drastically reduce the burden on the stockpile for surveillance parts. Additionally, the non-destructive nature of the technique implies that surveillance could occur more frequently and in situ, which would strengthen nonproliferation efforts as well as further understanding of how natural aging of PETN occurs. Ultimately, what we learn by developing technologies using the US stockpile can be applied to other types of explosives such as those that might be used by other proliferant states.

Technical Outcomes

This project successfully demonstrated that NRUS can be used to measure the nonlinear hysteric parameter in small pressed pellets of PETN. Furthermore, PETN pellets that were artificially aged by heating in an oven at 80C for 4, 7, and 10 weeks showed a larger average values of nonlinearity than the pristine pellets that were not artificially aged. These results indicate that NRUS is a promising tool for diagnosing damage in PETN.

Publications

Donahue, C. M., D. S. Moore, and P. A. Schulze. Nonlinear Resonant Ultrasound Spectroscopy for Nondestructive

Evaluation of Thermally Aged Small Pressed Pellets. Presented at *Quantitative Nondestructive Evaluation*. (Burlington, Vermont, United States, 2018-07-14 - 2018-07-14). (LA-UR-18-28955)

Schulze, P. A., J. T. Mang, C. M. Donahue, and C. B. Skidmore. Connecting Novel Microstructure Characterization Techniques for Pentaerythritol Tetranitrate (PETN) Pellet Aging to Performance. Presented at *16th International Detonation Symposium*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-20). (LA-UR-18-25684)

Development of a Compton Imager for Planetary Science Gamma-ray Spectroscopy

Suzanne Nowicki
20180657ER

Project Description

The pixelated cadmium-zinc-telluride (CZT) detector technology and the methods developed as part of this project could be leveraged for national security applications. Our technique could be used in a similar way on Earth to detect nuclear events from a drone or similar platforms to locate the source of the event.

Technical Outcomes

It was shown that the CZT based instrument can be used for gamma-ray spectroscopy to measure the abundance of important elements such as H, C, O, Na, Mg, Al, Si, P, S, Cl, K, Ca, It, Fe, Th and U. Through simulations and experimental methods, we demonstrated that the spectral performance of the instrument approaches that of HPGe with significantly reduced SWaP and improved spatial resolution.

Publications

- Hoover, A. S., J. R. Tutt, S. F. Nowicki, and G. W. Mckinney. Radiation Transport Calculations Supporting the Development of a Compton Imager for Planetary Science Gamma-ray Spectroscopy. Presented at *SORMA XVII*. (Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-14). (LA-UR-18-21734)
- Nowicki, S. F., G. W. Mckinney, and J. R. Tutt. Simulation of Galactic-Cosmic-Ray induced Neutron Production on Mars with MCNP6. Presented at *SORMA XVII*. (Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-14). (LA-UR-18-21504)

Experimental Demonstration of Hyperspectral Intensity Correlation Interferometry

David Thompson
20180658ER

Project Description

Geosynchronous satellites are critical to the nation's national security and economic interests, occupying strategic real estate in orbit around the earth. Understanding of their operations through ground-based imaging is a high priority for various commercial, DoD and IC agencies. However imaging of geosynchronous satellites from the ground is very difficult; with current techniques extremely larger and more expensive telescope systems than currently exist would be required. This project will perform an initial laboratory demonstration of Hyperspectral Intensity Correlation Interferometry (HICI), a technique that could enable imaging of small and faint objects like geosynchronous satellites using much simpler and lower cost ground-based optical systems. Once confirmed, we expect that there will be interest in developing the HICI technique further, leading to larger systems that can begin to actually contribute to pure science and national security imaging needs.

Technical Outcomes

This project demonstrates important aspects of hyperspectral intensity correlation interferometry (HICI), a technique for imaging small, dim astronomical objects by measuring time correlations between photons at different spatial locations. This technique is insensitive to atmospheric turbulence and could produce clear images using large, cheap mirrors to collect light. This project has successfully demonstrated ICI measurements in the lab which agree with theoretical predictions, using a large array of photon-counting detectors for the first time.

Publications

Holmes, R. M., C. T. Weaver, and D. Palmer. ELROI: A license plate for satellites that anyone can read. Presented at *Small Satellite Conference*. (Logan, Utah, United States, 2018-08-04 - 2018-08-09). (LA-UR-18-25426)

Holmes, R. M., D. Palmer, and C. T. Weaver. Progress on ELROI satellite license plate flight prototypes. Presented at *SPIE*

Defense + Commercial Sensing. (Orlando, Florida, United States, 2018-04-15 - 2018-04-15). (LA-UR-18-22381)

Holmes, R. M., M. M. Victora, R. F. Wang, and P. G. Kwiat. Past, present, and future experiments in single-photon vision. Presented at *SPIE Defense and Commercial Sensing*. (Orlando, Florida, United States, 2018-04-16 - 2018-04-16). (LA-UR-18-22536)

Palmer, D., and R. M. Holmes. Extreme background-rejection techniques for the ELROI optical satellite license plate. 2019. *Review of Scientific Instruments*. (4) 814-825. (LA-UR-18-28957 DOI: 10.1364/AO.58.000814)

Experimental Signatures for Dynamic Plutonium Hydriding

Brian Scott
20180725ER

Project Description

This work will provide signatures for plutonium hydriding at ultrafast time scales, from femtoseconds to microseconds. These signatures are of importance to planned experiments that will follow the dynamic hydriding of plutonium. Specifically, this work will directly address challenges in the DOE/NNSA Nuclear Weapons arena.

Technical Outcomes

This project successfully measured in-situ Raman signatures for PuH₂ and PuH₃ species on a plutonium metal surface under 1 atm of H₂ and 120 degrees Celsius. We also successfully calculated Raman and IR modes, and ground state structures for PuH₂ and PuH₃ using density functional theory (DFT+U), and these results show good agreement with our experimentally measured modes.

Overturning a Staple of Radiation Belt Physics: Explaining the Formation of the Inner Electron Belt

Gregory Cunningham
20180731ER

Project Description

Following a high-altitude nuclear explosion, or HANE, radioactive fission fragments will beta-decay and produce electrons that can become trapped in Earth's surrounding magnetic field. The trapped electrons can interact with sensitive components on satellites, especially those in low-Earth orbit, disabling those components or the entire satellite. The national security community does not have well-validated and robust tools that are capable of predicting the number of trapped electrons that will become trapped after a HANE, nor the evolution of the trapped electron population in the hours, days and months following a HANE. Nature provides us with a surrogate for this process since electrons with similar energies can be suddenly inserted into the inner radiation belt, and slowly decay afterward. We will build a model for the evolution of trapped electrons that are inserted into the inner radiation belt through natural processes originating in the sun and validate it with data from a NASA satellite, Van Allen Probes. Our model will be capable of predicting the evolution of the artificially introduced electrons following a HANE assuming that their initial distribution can be predicted from a different code.

estimated at the Van Allen Probes footprints from the World-Wide Lightning Location Network database. Submitted to *Geophysical Research Letters*. (LA-UR-19-21524)

Technical Outcomes

The lifetime of electrons following a high-altitude nuclear explosion at low latitudes is thought to be controlled by electromagnetic waves from ground-based transmitters and lightning-generated whistlers, which scatter electrons into the atmosphere so that they no longer pose a threat to space assets. This project included these waves in our radiation belt model to determine whether they explain observations at $L < 1.26$ after Starfish and found that they make a small difference at those very low altitudes.

Publications

Cunningham, G. S., J. F. Ripoll, T. Farges, and E. H. Lay.
Maps and statistics of lightning-generated wave power

Actionable Intelligence for Maintenance and Reliability through Sensor Data

Neil Loychik
20180735ER

Project Description

This project will develop the measurement system and analytical techniques to monitor and explore vast quantities of data produced by the emerging industrial internet of things (IIoT) with applied learning from actual Laboratory assets. The Laboratory manages more than 13,000 rotating-machines, including pumps, compressors, fans, etc., which produce fault signatures in sound, vibration, thermal, or other sensor data not typically captured in plant operation logs. Utilizing this data for equipment reliability is difficult because machinery faults are rare occurrences and unique signatures depend on machinery size, parts, and usage. Our innovation is the focus on operating conditions, such as pump flow and efficiency, instead of specific failure signatures. Focusing on conditions provides an immediate benefit; an efficiency detector would provide immediate energy savings. Potential applications for this research are high. This could make existing operations, including those related to the maintenance of the nuclear stockpile, safer and more reliable without the investment into new infrastructure equipment. Outside of the Laboratory, IIoT methods could improve the efficiency and reliability of the entire United States manufacturing base.

Technical Outcomes

Los Alamos has established capability to take industrial internet of things (IIoT) measurements. The earliest results show that equipment vibration correlates with operational parameters like flow and efficiency from fluid handling devices such as pumps, fans, blowers, and compressors. With further development, this relationship makes viable a low-cost sensor network that can improve the safety and reliability of the American industrial base and if generally deployed, reduce electrical consumption by an estimated 5 to 10%.

Integrating Los Alamos National Laboratory Developed Visual Analytics for Forecasting Infectious Disease Outbreaks

Tracy Erkkila
20180743ER

Project Description

When faced with biological threats, our ability to provide early warning, situational awareness, and decision support will depend on whether we can rapidly and accurately detect threat pathogens in clinical and environmental samples. Retrieval and integration of multiple sources of information are required in order to provide high confidence models for prediction, early warning and forecasting of disease events. Reliable and automated on-demand analytics are key components to such biosurveillance efforts. We are proposing to integrate two of our tools, Analytics for Investigation of Disease Outbreaks (AIDO) and Next Generation Genome Analytics for Biosurveillance (GenoSurv) to develop a novel forecasting functionality. While these tools are independently very useful and are offered as stand-alone tools in DTRA's Biosurveillance Ecosystem (BSVE), in combination they offer the potential for a novel and powerful means of disease prediction and forecasting of infectious disease outbreaks. Our work will advance infectious disease surveillance and forecasting by: 1) enabling high confidence predictions based on pathogens involved in past and present disease outbreaks, 2) empowering medical responders to issue early warnings of potential disease outbreaks, and 3) improving responders' ability to determine the most effective courses of action to prevent or mitigate effects of an outbreak.

Technical Outcomes

This project successfully developed Application Programming Interfaces for both the Analytics for Investigation of Disease Outbreaks (AIDO) and GenoSurv apps that now enables users to browse and correlate data and information between the applications. This capability can be used to further investigate new approaches of integrating genomic data with historical outbreak data with the aim to more accurately forecast and predict the length and severity of infectious disease outbreaks.

Publications

Rosenberger, W. E., G. Fairchild, A. R. Daughton, N. Velappan, L. A. Castro, R. Priedhorsky, F. M. Altherr, E. N. A. Generous, E. K. Cloyd, A. R. Vaidya, E. L. Abeyta, A. Deshpande, L. A. Naranjo, A. D. Hollander, G. Vuyisich, A. M. Lillo, and M. E. Chitanvis. Analytics for Investigation of Disease Outbreaks: Web-Based Analytics Facilitating Situational Awareness in Unfolding Disease Outbreaks. To appear in *Journal of Medical Internet Research - Public Health and Surveillance*. (1) e12032. (LA-UR-18-28570 DOI: 10.2196/12032)

Geospatial Change Surveillance with Heterogeneous Data

Amanda Ziemann
20180529ECR

Project Description

The work in this project enables the development and application of meaningful geospatial change detection from heterogeneous satellite data streams. This is a longstanding challenge in the science and national security communities, as identified by DOE/NNSA and NGA. The capability developed in this project will leverage multiple satellite sensors, and integrate them across time to surveil particular areas. The case study is the detection of Siberian methane craters through a sophisticated change surveillance approach, and the understanding of these craters is important as they have significant climate implications. The methane craters serve as a proxy for nonproliferation and proliferation detection applications. The expected outcome is a capability that can ingest a constant stream of multi-sensor satellite imagery for a targeted area of interest, and perform both automated cueing and broad area search.

Publications

Theiler, J. P., and A. Ziemann. Background estimation in multispectral imagery. Presented at *OSA Hyperspectral Imaging and Sounding of the Environment*. (San Jose, California, United States, 2019-06-25 - 2019-06-27). (LA-UR-19-21593)

Using Solar-analog Stars to Understand Extreme Space Weather

Lisa Winter
20180533ECR

Project Description

Flaring stars continue to be a source of transient emission detected by the space based X-ray monitors. This project will benefit our Space Nuclear Detonation Detection mission by better understanding the nature of the transient background signals which our instruments may see. Further, this project will benefit our national security mission by providing better understanding of space weather and its threat to United States infrastructure (e.g., by causing large-scale power grid blackouts and failure of satellite systems). This project will help establish limits on these risks for how extreme and how frequently extreme space weather occurs.

Technical Outcomes

This project used the first and only X-ray observations of the solar-analog stars discovered by NASA's Kepler Space Telescope and compared their stellar magnetic activity levels with historic magnetic activity in the Sun. Results suggest that the occurrence rate of super-flares for the Kepler-derived super-flare-producing solar-analog stars is likely higher than the occurrence rate for our Sun. Further study is needed to assess the implications of these extreme space weather conditions on Earth.

Establishing a Scientific Understanding for the Generation of Radiofrequency Signals from High Explosives

Kendra Van Buren
20180589ECR

Project Description

Radio-frequency (RF) measurements offer the potential to diagnose properties of high explosives (HE) during detonation. Despite the wealth of experimental results published in the last three decades, no predictive capability of RF production currently exists because the theoretical understanding of how intrinsic properties (density, composition, porosity, piezoelectric content, etc.) of HE might contribute to RF production is to a great extent incomplete. This research project will help to close this gap through a combination of experiments, signal processing, and simulation capability to explore the extent to which RF emissions can be used to reliably assess HE detonation. Establishing a scientific understanding of HE properties that contribute to RF emissions will stimulate its reliable use as a novel diagnostic for hydrodynamic testing. This, in turn, offers the potential to yield novel metrics for the validation of both HE models and integrated simulations. It will also set the stage to implement computational models of RF generation, which are currently not available in Advanced Scientific Computing (ASC) codes.

Tracking Ultrafast Morphology Changes in Solid Explosives During a Detonation using Visible Laser Speckle

Pamela Bowlan
20180597ECR

Project Description

Our weapons stockpile relies entirely on a small number of secondary high explosive materials, such as octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Energetic materials exhibit a unique and complex interplay of shock physics, chemistry, kinetics and thermodynamics, giving rise to the highly coherent phenomenon of detonation. Even after decades of research there are still significant uncertainties in our ability to predict and control when and how energetic materials release energy, which has serious implications for safety and performance of explosives. One reason is that, while chemical kinetics are understood in gases and liquids, much less is known about how reactions proceed within a crystalline lattice. Secondly, events like detonation, where a bulk material can go from ambient conditions to pressures of Gigapascals (GPa) and temperatures of ~ 4000 kelvin (K) within a nanosecond (ns) are extremely difficult to measure. While studying explosives with visible lasers has been avoided in the past since they are highly scattering powders, our innovation is to use the resulting laser speckle as an instantaneous probe of a material's morphology during detonation. This technique will reveal important basic science facts missing from current models about how the extreme temperatures and pressures which lead to detonation are generated in explosive materials.

Discovering Biosignatures in Manganese Deposits on Mars

Nina Lanza
20160606ECR

Project Description

On Earth, high concentrations of manganese are associated with life and environments supportive of life. Our goal is to identify key signatures pointing to a biological origin for manganese-rich materials so they may be identified on Mars by rovers. The objective of this project is to determine what chemical and mineralogical signatures can uniquely identify manganese-rich materials as biological in origin using Mars rover payload instruments. If these signatures are identified on Mars, they will address one of the highest priority goals of the planetary science community: clear evidence of past or present microbial life on Mars.

Technical Outcomes

This project identified key trace elements for biotic Mn minerals with LIBS and time-resolved luminescence, and established that the trace element abundance of Mn minerals may indicate the redox state of Mn. Additionally, we have identified important Raman spectral features for biotic and abiotic Mn minerals. We have improved the accuracy of univariate Mn quantification in LIBS data. We have also developed a machine learning based tool to identify rock targets with coatings.

Publications

Oyen, D. A., and N. L. Lanza. Interactive Discovery of Chemical Structure in ChemCam Targets Using Gaussian Graphical Models. Presented at *Workshops of the International Joint Conference on Artificial Intelligence*. (New York City, New York, United States, 2016-07-09 - 2016-07-09). (LA-UR-16-24519)

Developing a Compact Portable Muon Tracker for Non-Destructive Evaluation

Elena Guardincerri
20160629ECR

Project Description

This project proposes to design and build a modular muon tracker for radiographing thick structures and imaging denser objects inside those structures. The tracker will be capable of recording data and tracking muons with a good angular resolution. We will characterize our detectors by measuring the accuracy of the muon tracks reconstructed from the data, and we will leak test the drift tubes periodically and evaluate their long-term performances.

Technical Outcomes

This project was able to manufacture modules of lightweight drift tubes that could be easily transported and assembled in a tracking system around the structure to be imaged. The tracking system itself was not completed due to problems with the readout electronics. The project initiated a collaboration with a group of instrumentation experts at the University of Pennsylvania and devised a path forward to complete the system once funds are secured.

Publications

Blasi, C., R. D'Alessandro, L. Bonechi, E. Guardincerri, and V. Vaccaro. Detecting metal elements inside the dome of Santa Maria del Fiore in Florence using cosmic ray muons. Submitted to *IOP Conference Series: Materials Science and Engineering*. (LA-UR-18-31487)

Guardincerri, E., J. D. Bacon, N. Barros, C. Blasi, L. Bonechi, A. Chen, R. D'Alessandro, J. M. Durham, M. Fine, C. Mauger, G. Mayers, C. Morris, F. M. Newcomer, J. Okasinski, T. Pizzico, K. O. Plaud-Ramos, D. C. Poulson, M. B. Reilly, A. Roberts, T. Saeid, V. Vaccaro, and R. Van Berg. Imaging the dome of Santa Maria del Fiore using cosmic rays. Submitted to *Philosophical Transactions of the Royal Society A. Mathematical, Physical and Engineering Sciences*. (LA-UR-18-31558)

Deep Learning for Multispectral and Hyperspectral Target Detection in Remote Sensing Data

Monica Cook
20170537ECR

Project Description

Target identification from remote sensing imagery is already recognized as a potential solution to a number of high-profile national security problems and DOE/NNSA missions. The goal of this research is to improve upon current results in order to extend this utility to other applications of great importance. We expect by the end of this research to understand how deep learning can be utilized to improve current performance in target detection from remote sensing imagery. The product will be a processing chain that can analyze large volumes of spectral remote sensing imagery quickly and efficiently using deep learning to achieve improved target identification results. Using new techniques to resolve current challenges will improve the accuracy of a solution that will continue to be demanded to solve important problems.

Technical Outcomes

The outcome of this project is a hybrid deep learning approach to target detection in remote sensing imagery. This work has shown the potential for the application of deep learning in the exploitation of remote sensing data and has laid the foundation to continue to improve these techniques with the goal of applying them to a broad range of mission areas.

Additive Manufacturing of Composite Lithium Containing Neutron Scintillators

Brenden Wiggins
20160678PRD4

Project Description

We will develop and demonstrate the additive manufacturing of a composite neutron scintillator for the first time. The resulting material is expected to enable a new class of neutron detectors needed for a wide range of national-security applications. Key metrics of success include the scintillator performance and the projected manufacturing cost. We anticipate that the resulting composite scintillator will out-perform any other neutron detector in terms of gamma-ray rejection and sensitivity per volume. We also anticipate that the projected scintillator manufacturing cost will make this novel detection approach economically competitive with existing neutron detectors such as Helium-3 (He-3) tubes.

Publications

- Wiggins, B. W., A. Favalli, M. Iliev, K. D. Ianakiev, and M. P. Hehlen. Computational investigation of arranged scintillating particle composites for fast neutron detection. To appear in *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. 17-23. (LA-UR-18-21568 DOI: 10.1016/j.nima.2018.10.165)
- Wiggins, B. W., M. Iliev, A. Favalli, K. D. Ianakiev, and M. P. Hehlen. Developments in additive manufacturing of arranged scintillating particle composites for fast neutron detection. Presented at *SPIE optics and photonics 2018*. (San Diego, California, United States, 2018-08-19 - 2018-08-23). (LA-UR-18-25504)

Full-Field Characterization of the Micromechanical Cues Associated with the Breakdown of the Cytoskeleton During Cancer Metastasis

David Mascarenas
20170694PRD4

Project Description

Dr. Martinez's work focuses on the measurement of the full-field structural dynamics of micro/nano scale objects. This work could have significant impact on DOE/NNSA missions. First, it could potentially be used to characterize new nano materials which underpins a number of manufacturing, global security and science missions of Los Alamos National Laboratory. It could also aid in the engineering of new microscale sensors such as those needed to inspect extremely confined spaces in nuclear facilities. The work could potentially also have a significant impact on the health aspect of global security challenges. It is possible that the new signatures that are discovered as a result of the application of this technique could be used to develop new treatments for a variety of health problems. It could also be applied to help engineer the mechanisms and materials used in the development of surrogate organs such as the Athena organ-on-a-chip.

Publications

- N. Liao, A. S., H. Mukundan, C. R. Farrar, D. D. L. Mascarenas, P. Nath, Y. Yang, and B. Martinez. Full-Field Mode Shape Identification of Vibrating Structures From Compressively Sampled Video. Presented at *International Modal Analysis Conference*. (Orlando, Florida, United States, 2019-01-28 - 2019-01-28). (LA-UR-18-29902)
- Martinez, B., C. R. Farrar, Y. Yang, H. Mukundan, P. Nath, and D. D. L. Mascarenas. Poking the Genome: BioMechano Signal Transduction and Cancer Metastasis. Submitted to *Poking the Genome: BioMechano Signal Transduction and Cancer Metastasis*. (LA-UR-18-27063)
- Nath, P., B. Martinez, Y. Yang, C. R. Farrar, H. Mukundan, and D. D. L. Mascarenas. Experimental Modal Analysis of Tumorigenesis and Cancer Metastasis. Presented at *International Modal Analysis Conference*. (Orlando, Florida, United States, 2019-01-28 - 2019-01-28). (LA-UR-18-29913)

How Biological Communities Can Unlock Hidden Signatures of Environmental Change

Jeanne Fair
20180715PRD2

Project Description

The Science of Signatures (SOS) pillar links the Laboratory's capability to pressing national needs in the Laboratory's primary mission areas of National Security Science, Global Security, and Emerging National Challenges. It does so by developing a scientific understanding of the origin and evolution of signatures and backgrounds, new measurement techniques and strategies for signature identification, and new analysis and interpretation tools for development of knowledge from these signatures. This project seeks to identify signatures of biological communities from the microbiome to forest communities in response to environmental change. Application of biological community signatures is relevant to global health security and threat reduction with pathogen detection as well as environmental change over time.

fledging success of two passerines. Submitted to *Oikos*. (LA-UR-18-31593)

Wysner, T. E., A. W. Bartlow, C. D. Hathcock, and J. M. Fair. Long-term phenology of two North American secondary cavity-nesters. Submitted to *Ecology & Evolution*. (LA-UR-18-30750)

Publications

Bartlow, A. W. Histological findings in wild rodents of the Great Basin. Submitted to *Western North American Naturalist*. (LA-UR-19-22174)

Bartlow, A. W., and S. J. Agosta. Phoretic dispersal: review and synthesis of a common but understudied species interaction. Submitted to *Journal of Animal Ecology*. (LA-UR-19-22175)

Bartlow, A. W., and T. Vickers. Solving the mystery of an outbreak using the One Health concept. Submitted to *American Biology Teacher*. (LA-UR-19-22173)

Fair, J. M., A. W. Bartlow, C. A. Manore, C. Xu, K. A. Kaufeld, S. Y. Del Valle, A. Ziemann, and G. Fairchild. Forecasting Zoonotic Infectious Disease Response to Climate Change: Mosquito Vectors and a Changing Environment. Submitted to *Veterinary Sciences*. (LA-UR-19-22170)

Musgrave, K. S., A. W. Bartlow, and J. M. Fair. The effects of long-term environmental change on blowflies and

Improving Public Health by Linking Virus Genetic Evolution and Epidemic Spread

Thomas Leitner
20180751PRD3

Project Description

This project aims to develop models, methods, and applications based on the basic evolutionary biology of human viruses to better understand the epidemiology of human viral diseases and, ultimately to help intervene to reduce the burden of disease. Using public health data, including thousands of HIV sequences sampled from real populations, we will develop a computational framework to routinely retrieve virus sequence data (and associated metadata) from public health surveillance systems, apply standard and novel genetics and epidemiological models, and produce automated reports of HIV evolution and spread. This project ties in with the DOE/NNSA National Security mission of forecasting and predicting biological threats. We focus specifically on the US HIV epidemic, working together with the Colorado and Michigan health departments, but our general framework will also be useful, with adaptations, in preventing other pathogen threats, such as Avian Flu, Ebola, Dengue, Zika and other rapidly evolving pathogens. Thus, this project strongly ties in with 'Pathogen Detection and Countermeasures' as well as 'Information Collection, Surveillance, and Reconnaissance' and 'Non-Nuclear Forensics' (as we will reconstruct the hidden who-infected-whom network).

An Atomtronic Rotation Sensor

Malcolm Boshier
20180753PRD3

Project Description

This research will develop one approach to creating a so-called waveguide Sagnac atom interferometer. This device acts as an exquisitely sensitive rotation sensor. Rotation sensors are a key component of inertial navigation systems (INS). The atom interferometer sensor could potentially improve positioning accuracy with INS by an order of magnitude. Such an advance would be viewed as extremely important by agencies within DOD and the Intelligence Community (IC) who need precise positioning when Global Positioning System (GPS) is unavailable or denied. The device may also function as an accelerometer or gravimeter, which can be useful for detecting underground facilities relevant to non-proliferation and for finding mineral and oil deposits relevant to fossil fuels.

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