Los Alamos National Laboratory

Laboratory Directed Research and Development

FY19 Annual Progress Report

Los Alamos
NATIONAL LABORATORY
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Structure of this Report

The Laboratory Directed Research and Development (LDRD) annual report for fiscal year 2019 (FY19) provides summaries of each LDRD-funded project for the fiscal year, as well as full final reports on 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 summaries for continuing projects appear first, followed by project summaries and technical outcomes for projects that ended in FY19.

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.

Publications identified throughout the project summaries that are marked with an "*" are confirmed to be peer reviewed publications.

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Leadership Perspectives

"LDRD is central to Los Alamos's science, technology, and engineering strategy as articulated in our Laboratory Agenda, and I cannot imagine being successful without it. Our LDRD objectives of advancing mission agility, technical vitality, and workforce development 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 and future prospects from LDRD Program Director Bill Priedhorsky

"LDRD has doubled our commitment to [the] new generation of talent through our Early Career Research component. The quality of ideas coming into LDRD by these new people is a significant asset to the program. I hope everyone reading this will join me in advocating for these bright, creative minds who will lead our country in addressing the evolving and uncertain international security environment."
– **Bill Priedhorsky**, LDRD Program Director

Now 13 years into my service as LDRD Program Director, I continue to be impressed every day by what LDRD delivers to this great Laboratory. LDRD at LANL is responsible for soliciting, evaluating, and executing high-risk, high-reward research proposals that create innovative or technical insights related to NNSA core capabilities. With our complex and well-engineered program, we continuously grow such insights in both depth and breadth.

The goals of LDRD are to advance mission agility, technical vitality, and workforce development. LDRD continues to optimize its delivery of these goals by evolving with Laboratory and external changes. Given mission challenges such as 30 pits per year, LDRD has re-emphasized the Mission Foundations Research component, doubling the number of FY20 starts in response to a strong set of proposals relevant to nuclear and non-nuclear manufacturing and testing. Additionally, the Laboratory Agenda sets priorities for Nuclear Security and Mission-Focused Science, Technology & Engineering; this led to a set of Director's Initiative projects, proposed by Agenda item owners and subject to the same rigorous peer review as all LDRD.

The annual influx of new staff to the Laboratory has doubled since 2015. The trend of over 1,000 hires a year is anticipated to remain steady in the years to come. In response, LDRD has doubled our commitment to this new generation of talent through our Early Career Research component. The quality of ideas coming into LDRD by these new people is a significant asset to the program. I hope everyone reading this will join me in advocating for these bright, creative minds who will lead our country in addressing the evolving and uncertain international security environment.

Despite these changes, the heart of LDRD (2/3 of the FY20 portfolio) remains strategically-guided Directed Research and bottom-up Exploratory Research. Directed Research will evolve for FY22 to include the new Weapons Systems capability pillar as a sixth LDRD Focus Area. I expect to see the trend for greater confluence of mission and mission-enabling work to continue to grow.

Success for LDRD is success for the Laboratory. I feel honored to be part of helping build this success – idea by idea, project by project, person by person.

Retrospective and future prospects from LDRD Deputy Director Laura Stonehill

> "Unlike the other DOE laboratories, NNSA laboratories do not perform basic research as a core mission; thus LDRD is crucial to innovation, recruitment, and retention at Los Alamos."
> – **Laura Stonehill**, LDRD Program Deputy Director

Having joined the Los Alamos LDRD Program Office as the new Deputy Program Director early in fiscal year 2019, I am now more focused than ever on the future of this program, the Laboratory, and our Nation. Indeed, LDRD is an investment in the nation's future, ensuring mission support that lies beyond the planning horizon of current Laboratory programs.

The combination of strategic guidance and bottom-up peer review-based competition positions LDRD to provide a stream of capabilities for mission agility and world-class science and engineering excellence. Notably, the Exploratory Research component, a largely bottom-up process, will be thoughtfully evolved in a refresh process in FY20, the first since 2014, to ensure that it will deliver the right balance of technical capability for the FY22 proposal cycle.

Every day I am struck by the degree of rigor LDRD exercises at every stage of a project–from selection through transition. For example, the LDRD Program tracks project progress through reports and regular project appraisals. This process identifies those few projects that require attention and revectoring, but also assures us that the overwhelming majority of LDRD work is excellent or outstanding, assessed against our LDRD goals of mission agility, technical vitality, and workforce development.

The impact from this rigor is evident in many of the metrics you will see throughout this report. While LDRD was funded with just 5.3% of the Laboratory budget in FY19:

- 59% of all postdocs at the Laboratory were partially supported by LDRD. LDRD is critical to supporting these post-doctoral researchers as they transition to staff and programmatic work.
- 47% of LANL publication citations were derived from publications supported by LDRD.
- 22% of R&D 100 awards given to DOE went to Los Alamos, half with LDRD roots.

These are just a few examples of the success realized by this program.

Unlike the other DOE laboratories, NNSA laboratories do not perform basic research as a core mission; thus LDRD is crucial to innovation, recruitment, and retention at Los Alamos. Your support of LDRD at Los Alamos helps sustain our ability to deliver agile solutions to the nation's current and future security threats.

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 FY19 with approximately 5.3% 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 seven components with distinct institutional objectives: Directed Research (DR), flagship investments in mission solutions; Exploratory Research (ER), focusing on a single discipline or capability; Early Career Research (ECR), cultivating the Laboratory's workforce; Postdoctoral Research and Development (PRD), recruiting bright, qualified scientists and engineers; Mission Foundations Research (MFR), addressing mission problems through applied science and engineering; Director's Initiatives (DI), bolstering growth areas according to strategic objectives within the Laboratory Agenda; and Center Research (CR), organized around scientific themes.

In FY19, the LDRD program funded 340 projects with total costs of $130.8 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 Office holds a reserve each year to make modest investments that address new opportunities. In FY19, the beginning-of-year reserve budget was approximately $11M, most of which was committed well before year-end.

Director's Initiatives

LDRD Director's Initiatives are strategic efforts first implemented in FY19. The Initiatives focus on strategic objectives within the Laboratory Agenda. In FY19, LDRD funded four DI projects, responding to three Agenda objectives. For example, $1M was planned for a Dynamic Mesoscale Materials project. This project will continue into fiscal year (FY) 2020.

The senior Laboratory leaders responsible for each objective work with the LDRD Program Office and the Deputy Director for Science, Technology, and Engineering to identify strategic growth areas and potential projects. Director's Initiatives may be executed as either special calls or special projects. Proposals are required and held to the same standards of peer review as other investment components.

FY19 Laboratory Agenda Objectives Supported by LDRD Director's Initiatives

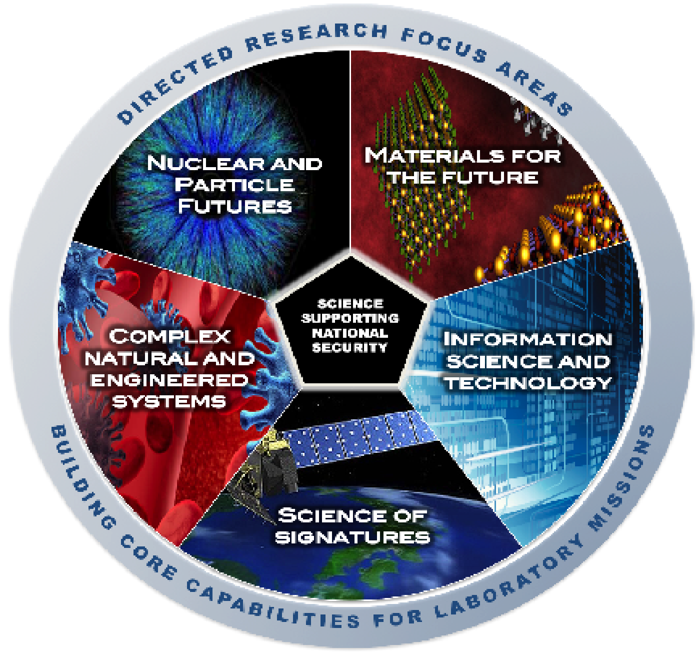
Anticipate threats to global security; develop and deploy revolutionary tools to detect, deter, and respond

Advance accelerator science, engineering, and technology to enable future stewardship capabilities

Develop and implement an integrated nuclear energy and materials initiative

Directed Research

The DR component makes long-range investments in multidisciplinary scientific projects in key competency or technology-development areas. In FY19, LDRD funded 45 DR projects, which represents approximately 49% 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 the Complex natural and Engineered Systems Focus Area that was not included in the pillars until FY20. 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 FY19 Strategic Investment Plan, published Lab-wide.



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

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 FY19, LDRD funded 143 ER projects, which represents approximately 32% of the program's research funds. Exploratory Research projects are funded up to $345K 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 in them.

Exploratory Research builds new technical staff competencies in key strategic disciplines that ready the Laboratory to address current and future national missions. This ER PI is advancing engineering design and manufacturing to produce more efficient processes for handling aqueous nuclear materials.

Exploratory Research Technical Categories

Atomic, Molecular, Quantum and Optical Sciences (AMQOS)
Biological Sciences (BIOS)
Chemical Sciences (CHEM)
Computational and Numerical Methods (CNM)
Computer Science, Mathematics, and Data Science (CMD)
Defects and Interfaces in Materials (DIM)
Earth, Planetary and Space Sciences (EPS)
Emergent Phenomena in Materials Functionality (EPM)
Engineering Applications (ENG)
High-Energy Density, Plasma, & Fluid Physics (HPF)
Measurement Science, Instruments & Diagnostics (MID)
Nuclear & Particle Physics, Astrophysics & Cosmology (NPAC)

Mission Foundation Research

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 FY19, the LDRD program funded 12 MFR projects, which represents approximately 3% of the program's research funds. MFR projects are typically funded at $160K over 8 months (phase 1), with an additional $700K awarded over 16 months for those projects selected to continue (Phase 2).

FY19 MFR Phase 1 Projects

Title	Problem Statement
Non-Destructive Analysis and Surveillance of SAVY and Hagan Containers used for Nuclear Material Storage	Manufacturing Process Agility and Innovation
High Efficiency Automated Leaching of Gloveboxes (HEAL-GB)	Manufacturing Process Agility and Innovation
Customized Materials to Attenuate Ionizing Radiation	Advanced manufacturing for non-SNM Nuclear Explosive Package materials and components
Modeling an Artificial Radiation Belt of Ionized Fission Fragments After a HANE	Impact of a High-Altitude Nuclear Explosion
A simplified design and advanced manufacture for expedited explosive hydrodynamic testing and equation of state development using extreme scaling (U)	Advanced manufacturing for non-SNM Nuclear Explosive Package materials and components
The Effect of Prompt Neutrons on Electronics	Impact of a High-Altitude Nuclear Explosion
Modeling EMP-E3B and Its Disturbed Atmospheric Environment	Impact of a High-Altitude Nuclear Explosion
Imager-Based Qualification and Control of Metallic Additive Manufacturing Processes	Manufacturing Process Agility and Innovation

FY18 MFR Phase II Projects, Continued from FY18

Project Title	Problem Statement
Additive Re-Manufacturing Guided by Process and Hydrodynamic Modeling	Advanced manufacturing for non-SNM Nuclear Explosive Package components and materials
Noninvasive Thermal Mass Flow Meter for Safeguards	Analytics for WMD Monitoring
Disrupting Actinide Aqueous Processing: Additively Manufacturing High-Speed Counter-Current Chromatography Devices	Manufacturing Process Agility and Innovation
New Methods for Producing Stockpile Equivalent High Explosive Components	Advanced manufacturing for non-SNM Nuclear Explosive Package components and materials

Centers Research

The National Security Education Center (NSEC) promotes science and engineering education and research through Strategic Centers, academic partnerships, and student and postdoctoral programs. Aligned with the LDRD vision, the NSEC vision is to develop the nation's next-generation workforce and leadership talent and to serve as an incubator for the introduction of emerging science and technology into DOE and NNSA missions.

Strategic Centers organized under NSEC support a broad spectrum of interdisciplinary science that underpins the Laboratory's mission in national security. Collaborations established through the Centers provide Laboratory programs with a systematic infusion of new ideas, people, and contacts both inside and outside the Laboratory. For example, collaborative work with universities fosters top-quality research at the Laboratory in the more basic or fundamental aspects of fields that map into existing and/or emerging mission areas of the Laboratory. The Centers also introduce students and postdocs to the scientific interests of the Laboratory. The Centers nucleate new research areas at the interface between emerging frontiers in the scientific community and the Laboratory's national security mission and are instrumental in anticipating future needs.

Commensurate with this shared vision, LDRD has made a commitment to partner with the Centers. LDRD funds the Centers Rapid Response research and development program that supports short-term, rapid-turnaround high-risk ideas or feasibility studies. Three of the Centers have formal postdoctoral programs funded through LDRD, targeting strategic areas where new staff members are recruited at the PhD level. In FY19, the LDRD program funded 9 CR projects, which represents approximately 5% of the program's research funds.

This Seaborg postdoctoral fellow is partially funded by LDRD. Consistently, over half the postdocs at the Laboratory are funded at least 10% by LDRD.

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 FY19, LDRD funded 85 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 FY19, LDRD supported 64 Director's and 18 Distinguished fellows (1 Director's fellow was 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 by continuing the PRD project, post-conversion, until its originally planned end date (In FY19, the LDRD program continued support for 2 former Director's postdoc fellows who converted to staff prior to FY19).

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 FY19 the LDRD program supported 59% of the 632 postdocs who spent at least part of the year at the Laboratory.

LDRD Postdocs Receive 2019 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.

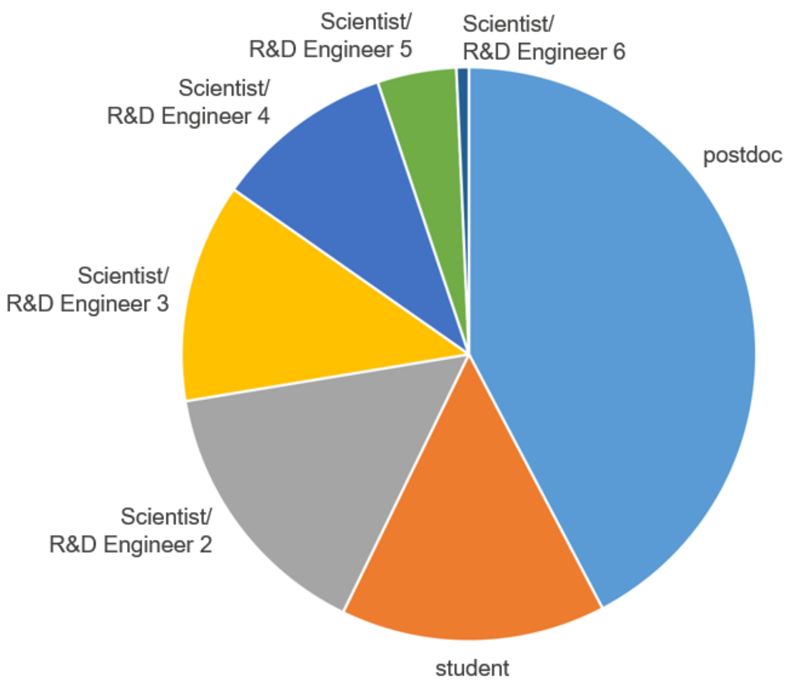
Conrad Goodwin was recognized for his outstanding contributions to the field of actinide chemistry. Conrad is currently a J. Robert Oppenheimer Distinguished Fellow working on "Unusual Oxidation States and Covalency-Tuning in Transuranic Molecules."

Christina Steadman was recognized for pioneering studies of algae epigenetics. Previously a Director's Postdoctoral Fellow, Christina is now a staff member in the Bioenergy and Biome Sciences (B-11) group. Christina is currently a co-investigator on two Directed Research projects.

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 FY19, the LDRD program funded 42 ECR projects, which represents approximately 5% of the program's research funds. This included 18 new starts, continuing the significant increase started in FY18. ECR projects are funded up to $218K per year for two years.

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.



LDRD Participation
(Hours charged in FY19)
Postdocs, students, and staff at the level Scientist/R&D Engineer 2 contribute the majority of hours to LDRD projects. LDRD is essential to retaining this critical demographic.

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–technical vitality, mission agility, and workforce development. 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 FY19, 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 play an important role in the year 2 project appraisal. 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- and third-year DR projects appraised in FY19 was 4.4, or "excellent." The average score rose to the "excellent/outstanding" range for final appraisals (4.5), pointing to the efficacy of the appraisal process to help PIs maintain high quality 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.

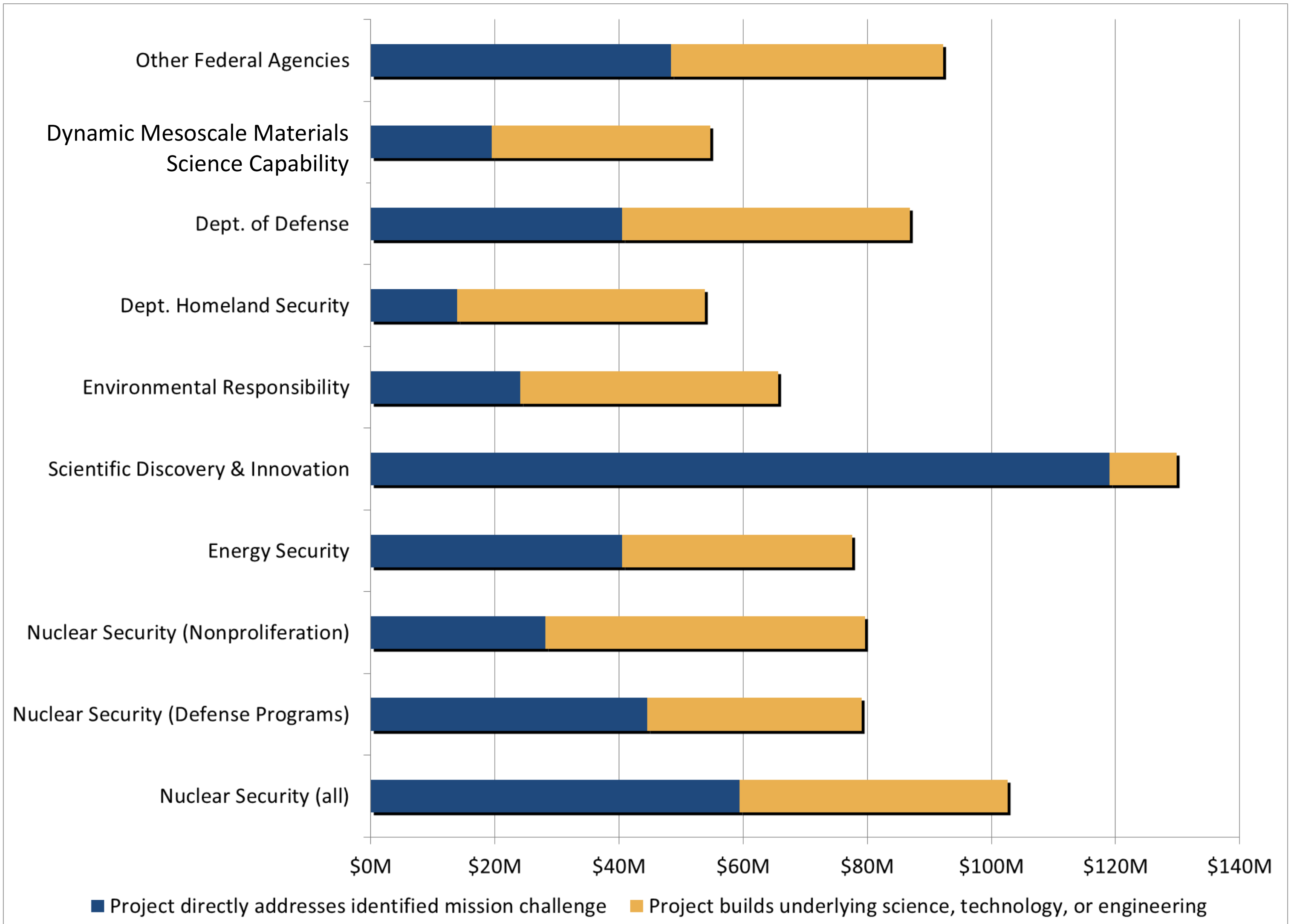
Continuing ER projects are appraised at the start of their second and third years. ECR projects are appraised midway through their second (last) year. The LDRD Program Office collaborates with the technical divisions to conduct project appraisals.

In addition to formal project appraisals, the LDRD program leaders meet informally with PIs. The purpose of these one-on-one meetings is to give PIs individualized feedback.

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 FY19 LDRD Portfolio ($M)

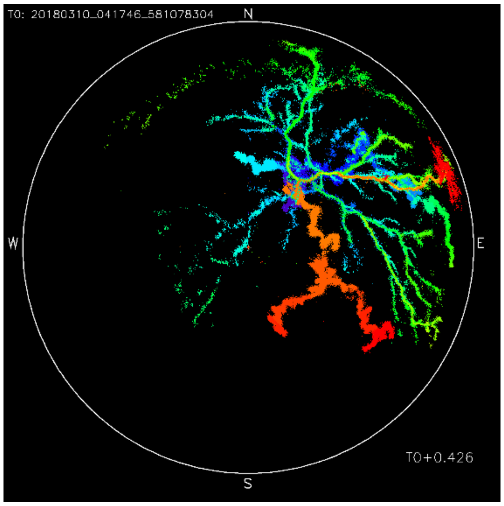


First and foremost, Los Alamos LDRD projects are required to address one or more of the DOE or NNSA mission areas. Due to the nature of basic R&D, the work may also benefit the mission challenges of other Federal agencies. The sum of the total LDRD investment in relevant missions is far greater than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

Multi-Mission Impact

Due to the basic science nature of most LDRD projects, the work often proves relevant to several missions and agencies.

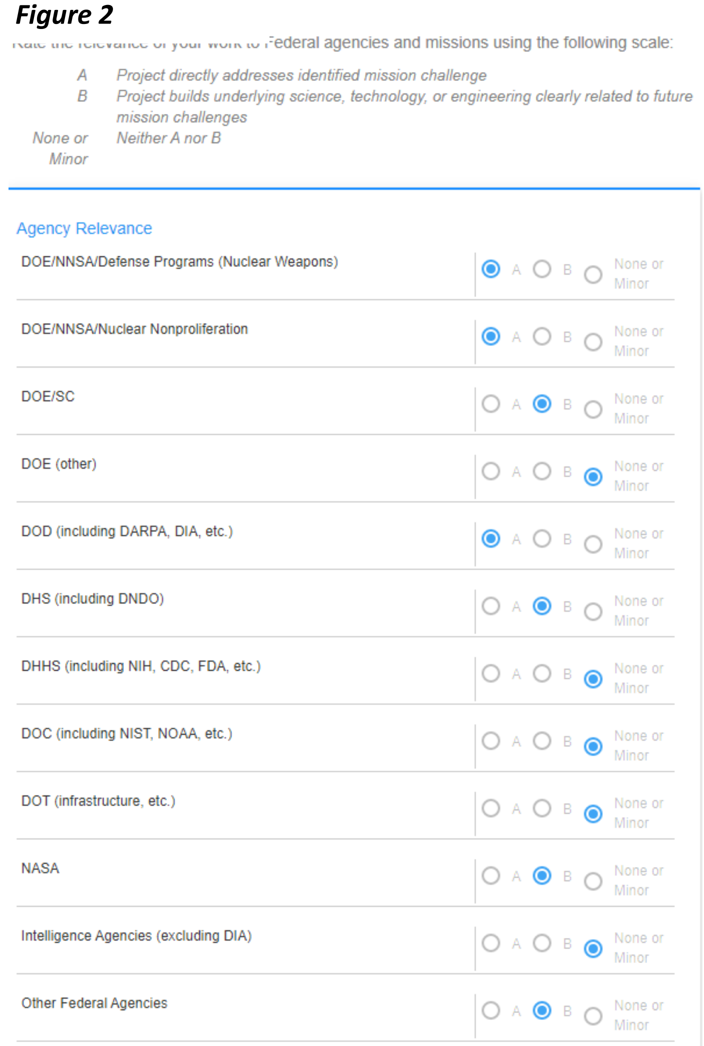
Figure 1



For example, PI Xuan-Min Shao is exploring the connection between the intense electromagnetic pulse and energetic particle emissions from lightning discharges in order to better understand the corresponding signals in atmospheric nuclear explosions. While there have been recent advances in lightning research, Shao and his team are digging into the many fundamental questions that remain unanswered and are of interest not only to science programs, but also to defense and nuclear nonproliferation programs. The signatures under study are unwanted background interference for systems that monitor nuclear emissions. Better understanding these signatures and the underlying physics is critically important to reduce possible false alarms and to validate simulations of the United States Prompt Diagnostic System for prompt nuclear weapon performance information. (20170179ER, “High Energy Lightning: Understanding Relations between Energetic Particle and Lightning Discharges in Thunderclouds.”)

Figure 1: *LDRD researcher Xuan-Min Shao and his team obtained this lightning image with a radio frequency interferometer at the High-Altitude Water Cherenkov (HAWC) Gamma-Ray Observatory. The Los Alamos HAWC Observatory, designed to observe the most energetic objects in the known universe, is on a mountaintop and well-situated for observing lightning. The colors from purple to red show the time sequence.*

Figure 2



ederal agencies and missions using the following scale:

A Project directly addresses identified mission challenge
B Project builds underlying science, technology, or engineering clearly related to future mission challenges
None or Minor Neither A nor B

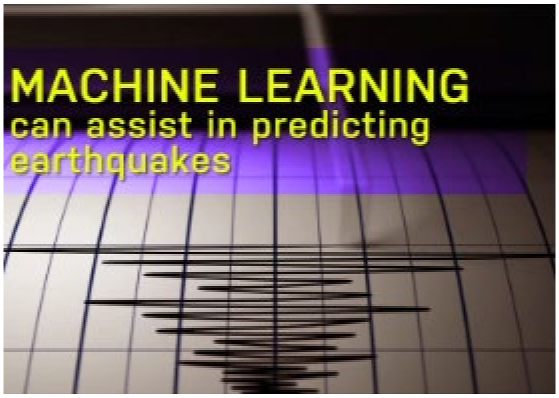
Agency Relevance

Agency	Selection
DOE/NNSA/Defense Programs (Nuclear Weapons)	A
DOE/NNSA/Nuclear Nonproliferation	A
DOE/SC	B
DOE (other)	None or Minor
DOD (including DARPA, DIA, etc.)	A
DHS (including DNDO)	B
DHHS (including NIH, CDC, FDA, etc.)	None or Minor
DOC (including NIST, NOAA, etc.)	None or Minor
DOT (infrastructure, etc.)	None or Minor
NASA	B
Intelligence Agencies (excluding DIA)	None or Minor
Other Federal Agencies	B

Figure 2: *LDRD data sheets include an analysis of mission relevance in which the PI indicates direct, underlying and clearly related, or no relevance to federal agency missions, nuclear security and national defense, energy security, environmental stewardship, and areas of scientific discovery and innovation.*

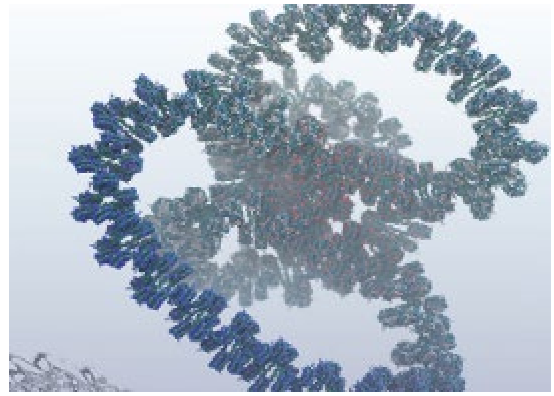
Science News

Here's a look at just a few of the Laboratory's top science stories from 2019, 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. Click any of the images below to read the news.



Could machine learning be the key to earthquake prediction?
Geophysicist Paul Johnson leads a team at Los Alamos National Laboratory pioneering the use of machine learning to analyze seismic signals revealing the deep physics of earthquakes with the ultimate goal of forecasting them.

READ MORE Smithsonian



First-ever simulation of an entire gene
Researchers at Los Alamos National Laboratory created the largest simulation to date of an entire gene of DNA, a feat that required one billion atoms to model and will help researchers to better understand and develop cures for diseases like cancer.

READ MORE POPULAR MECHANICS

READ MORE Discover MAGAZINE

NASA's new nuclear reactor could change space exploration
Experts at Los Alamos National created a high-power, next-generation nuclear reactor for space exploration. The reactor, called Kilopower, is the size of a paper towel roll and is in a protective case the size of a tall trash can.

2018 R&D 100 FINALIST

Since 1978 Los Alamos has won more than 162 of the prestigious R&D 100 Awards, and in 2019 it took nine. Five of the awards have roots in LDRD and represent the program's investments in science, engineering, and technology impacting the broader scientific community.

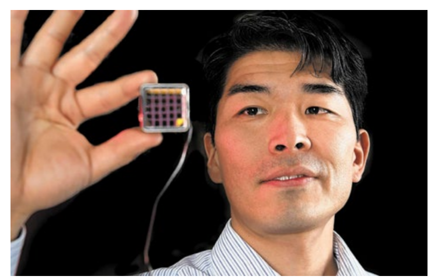
ALFa LDS: Autonomous, Low-Cost, Fast Leak Detection System

ALFa LDS is a featherweight platform that is small enough to be deployed on a drone but powerful and intelligent enough to minimize fugitive leaks across the entire network of natural gas extraction, production and consumption. This technology has roots in an LDRD project from 2011 (20110081DR).

Photo: Manvendra Dubey with the gas detection system mounted on a drone.

Informational Video: [ALFa LDS]

Atomic Armor



This radical new type of coating is dubbed "atomic armor." Made from two-dimensional, ultrathin crystal materials, atomic armor can be applied in a skin-like layer to a particularly sensitive device without hindering its performance. This technology has roots in an LDRD project from 2015 (20150394DR).

Photo: Hisato Yamaguchi examines a material for night vision goggles that is coated with atomic armor. The coating will protect the goggles against corrosive gases.

Informational Video: [Atomic Armor]

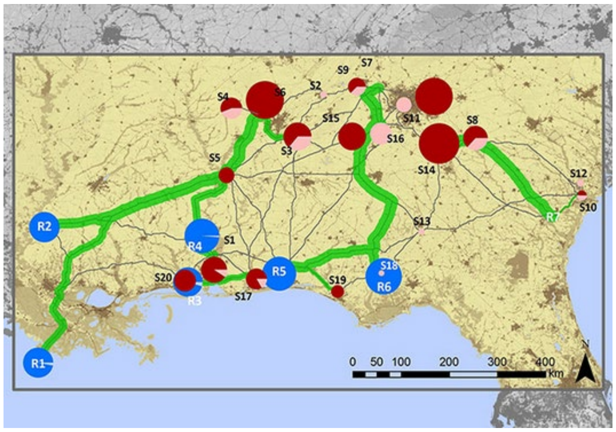
Severe Contingency Solver

The Severe Contingency Solver is a new software that reliably predicts how damage from hurricanes, ice storms, earthquakes, and other extreme events will restrict power delivery from utility grids. It is the only software available—commercially or open-source—that reliably supports analysis of extreme events that cause widespread damage. This innovation builds on the basic science conducted in an LDRD project from 2010 (20100030DR).

Photo: Carleton Coffrin, a computer scientist at Los Alamos, developed the Severe Contingency Solver software to help government agencies better plan for power outages caused by extreme events.

Informational Video: [Severe Contingency Solver]

SimCCS2.0



SimCCS$^{2.0}$ is an open-source software package that industry, researchers, and government can use to design CO_2 capture and storage infrastructure that optimally links CO_2 sources (such as power plants) with CO_2 sinks (such as saline aquifers and depleted oil fields) to reduce industry carbon footprints and maximize revenues. This technology has roots in an LDRD project from 2014 (20140002DR).

Photo: Example output from the software. (Source: Los Alamos National Laboratory)

Informational Video: [SimCCS2.0]

SPLASH: Smart Platforms Leveraging Automated Sample Handling

SPLASH is a fully customizable, miniature liquid handling platform technology that can execute sequential operations involved in complex laboratory processes. Its electricity-free, pocket-sized variants bring automated sample preparation and processing to the point of need and resource-limited settings. This technology has roots in an LDRD project from 2017 (20170026ER).

Informational Video: [SPLASH]

Los Alamos National Laboratory consistently delivers significant technological advances. In FY19 U.S. Department of Energy researchers won 41 of the 100 awards given out by R&D World Magazine, and **22%** of DOE’s awards went to Los Alamos National Laboratory technologies. As noted above, LDRD plays a significant role in developing these technologies, often laying the groundwork that is realized many years later.

Performance Metrics

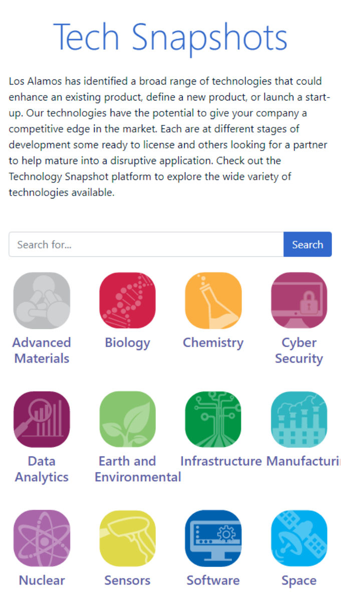
The LDRD program is a key resource for addressing the long-term science and technology goals of the Laboratory, as well as enhancing the scientific capabilities of Laboratory staff. Through careful investment of LDRD funds, the Laboratory builds its reputation, recruits and retains excellent scientists 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				
	FY16	**FY17**	**FY18**	**FY19**
LANL Patents	88	43	51	53
LDRD Supported	19	9	10	20
% due to LDRD	22%	21%	20%	38%

Invention Disclosures				
	FY16	**FY17**	**FY18**	**FY19**
LANL Disclosures	133	117	109	118
LDRD Supported	69	24	40	39
% due to LDRD	52%	21%	37%	33%



"Tech Snapshots" on many of these technologies can be found on the Richard P. Feynman Center for Innovation web site. For example, search: "Atomic Armor" and download a pdf handout that includes the benefits and market opportunities for this R&D 100 winning technology.

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.

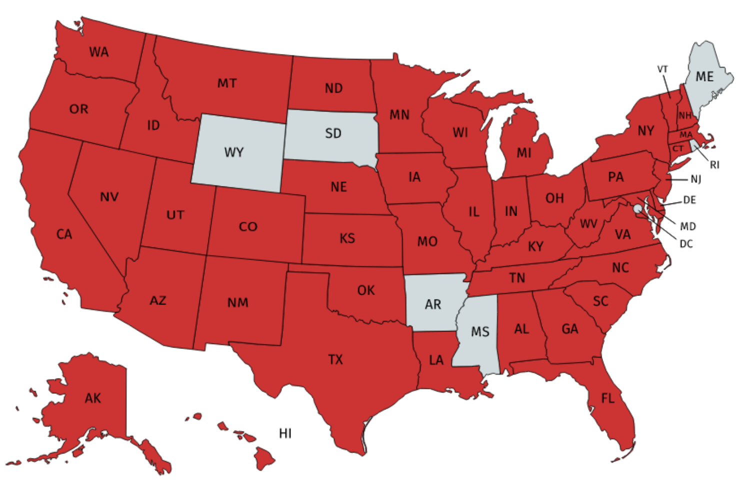
Postdoc Support				
	FY16	**FY17**	**FY18**	**FY19**
LANL Postdocs	501	497	556	632
LDRD Supported >10%	272	263	281	376
% due to LDRD	54%	53%	51%	59%

Postdoc Conversions				
	FY16	**FY17**	**FY18**	**FY19**
LANL Conversions	80	69	81	87
LDRD Supported >10%	47	37	37	39
% due to LDRD	59%	54%	46%	45%

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.

Recent LDRD external collaborators within the United States come from 45 states and Washington DC. (Data from FY18 and FY19.)



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 frequency they were cited. In 2019, nearly half (47%) of citations of LANL publications were derived from publications supported by LDRD.

Publications				
	FY16	**FY17**	**FY18**	**FY19**
LANL Pubs	1968	2001*	2100	2066
LDRD Supported	426	525*	613	714
% due to LDRD	22%	26%	29%	35%

Citations				
	FY16	**FY17**	**FY18**	**FY19**
LANL Citations	24043	15360	6357	5484
LDRD Supported	8104	4991	2379	2580
% due to LDRD	34%	33%	37%	47%

*FY17 data corrected 3/12/20. Percentage LDRD did not change.

LDRD Researcher Wins JICRD Best Paper Award

LDRD researcher Malcolm Boshier and guest scientist Dana Berkeland have been awarded this year's Science and Technology Best Paper in the Journal of Intelligence Community Research and Development (JICRD). In the paper, "A Survey of Environmental Magnetic Field Noise and Mitigation Techniques," Boshier and Berkeland tabulate the magnitudes and frequencies of noise sources and discuss the anticipated effects on signal collection. They also describe various techniques to mitigate these noise sources during and after data collection, in particular looking at several data processing techniques. JICRD is a multidisciplinary science and technology journal that covers a wide range of topics affecting the intelligence landscape. Since its founding in the late 1990's, JICRD has provided the intelligence community (IC) with a mechanism for peer review and a venue to securely publish sensitive research findings. LA-UR-19-22116

Left to right: Corin R. Stone, Deputy Director of National Intelligence, Strategy & Engagement; Malcolm Boshier, LDRD researcher; Dana Berkeland, Los Alamos National Laboratory Affiliate; and Pamela Duke, Assistant Director of National Intelligence for Transformation & Innovation.

Professional Awards and Recognition

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 FY19 received many prestigious awards, honors, and recognitions.

Top Los Alamos LDRD Researchers Honored with Presidential Early Career Awards

On July 2, 2019 President Donald J. Trump announced the recipients of the 2019 Presidential Early Career Award for Scientists and Engineers. The award is the highest honor bestowed by the United States Government to outstanding scientists and engineers who are beginning their independent research careers and who show exceptional promise for leadership in science and technology. Two people from Los Alamos National Laboratory won this award, both of whom have led Early Career LDRD projects.

Abigail Hunter's research focuses on understanding and modeling nanoscale deformation mechanisms in metals. She is a leading expert in phase field modeling of dislocation-based deformation behaviors. A primary goal of her work is to better understand defect physics at the mesoscale and then use this information to develop more physically informed continuum-scale material models that must integrate into large-scale, parallel codes used for predictive science at Los Alamos. Hunter has participated in LDRD as a PI for both Early Career Research and Exploratory Research.

Shea Mosby's research at Los Alamos has focused on nuclear reactions relevant for applications using a variety of detector systems at the Los Alamos Neutron Science Center. He started at the Laboratory studying neutron capture using the Detector for Advanced Neutron Capture Experiments. Mosby recently began investigating novel approaches to measuring neutron-induced reactions for radioactive isotopes, which preclude traditional measurement techniques. Mosby has participated in LDRD as a PI for Early Career Research.

LDRD Researchers Work Recognized with Gears of Government President's Award

Photo: NASA and NNSA engineers lower the wall of the vacuum chamber around the Kilowatt Reactor Using Stirling TechnologY (KRUSTY) system. The vacuum chamber is later evacuated to simulate the conditions of space when KRUSTY operates.

In FY19, the joint NNSA/NASA Kilopower team won a Gears of Government Award for their profound contributions to the lives of the American people. Each May, the award is presented by the Executive Office of the President. The Kilopower project team is led by NASA's Glenn Research Center in partnership with NASA's Marshall Space Flight Center; the Department of Energy's (DOE) National Nuclear Security Administration (NNSA); and NNSA's Los Alamos National Laboratory, Y-12 National Security Complex, and Nevada National Security Site (NNSS).

The Los Alamos National Laboratory team is led by LDRD researchers **Pat McClure** and **Robert Reid**. The work leading to this achievement can be traced back to two projects funded by LDRD in 2012 and 2013.

Read the announcement on the NNSA web site.

Four of Five LDRD scientists elected 2019 APS Fellows Have Received LDRD Funding

Five LANL scientists were elected Fellows of the American Physical Society (APS). Scott Hsu, Alan Hurd, Katherine Prestridge, Richard Van de Water, and Hans Herrmann were chosen for their "exceptional contributions to the physics enterprise." Fewer than one half of one percent of APS members are elected as Fellows each year. Notably, four of the five are currently leading LDRD projects or have received LDRD funding in the recent past.

These LDRD scientists represent top physics contributions made at the Laboratory. Van de Water said of the award, "The thrill of doing science is an award itself, an APS Fellowship honor makes it that much better."

"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

About the LDRD APS Fellows

Hans Herrmann was cited for “pioneering the use of Cherenkov radiation techniques for high energy gamma spectroscopy applications at the National Ignition and Omega Laser Facility.”

Scott Hsu was cited for “seminal experiments elucidating the physics of merging plasmas and jets spanning hydrodynamic to magnetized, self-organized behavior, thus impacting basic plasma physics, plasma astrophysics, and innovative fusion concept development.”

Katherine Prestridge was cited for “thoughtfully designed experiments on shock-driven mixing and turbulence, and for developing advanced flow diagnostics that bring insights to the understanding of mixing in extreme flows.”

Richard Van de Water was cited for “outstanding contributions to solar-neutrino and short-baseline accelerator-neutrino physics experiments that have shed new light on neutrino properties and have provided evidence for physics beyond the Standard Model.”

LDRD Chemist Jennifer Hollingsworth named 2019 AAAS Fellow

Jennifer A. Hollingsworth of the Center for Integrated Nanotechnologies was honored as a Fellow in the American Association for the Advancement of Science (AAAS) for her work in materials chemistry.

“We’re thrilled that Jennifer is receiving this well-deserved honor and joining the ranks of Los Alamos staff that are AAAS Fellows. Not only is Jennifer an outstanding researcher but also she is deeply committed to community engagement and STEM education,” said **John Sarrao**, director for Science, Technology & Engineering.

Hollingsworth, a specialist in optical nanomaterial synthesis, characterization and application, has been an LDRD researcher since her first Exploratory Research project in 2002. She is being honored specifically for her discovery and development of non-blinking giant quantum dots, spanning pioneering contributions to materials chemistry, photophysics of excited-state processes in nanomaterials, and applications in optoelectronics. She is currently pursuing work in photonics through an LDRD postdoctoral research and development project.

The American Association for the Advancement of Science (AAAS) is the world’s largest general scientific society. AAAS awarded the distinction of Fellow to 443 of its members this year. These individuals have been elevated to this rank because of their efforts toward advancing science applications that are deemed scientifically or socially distinguished.

The Long-Term Impacts of LDRD Investment

Following this section, you will find project summaries for continuing projects and projects that ended in FY19. Sometimes it is easy to predict from a project's description what the impact of the research will be. Additionally, the previous sections of this overview provide some illustration of how LDRD research has been received by the scientific community and the media. Arguably, the most interesting stories are about the long-term impacts of LDRD, be it a single project or the sustained investment in a capability over time.

The long-term goals of LDRD are to advance mission agility, technical vitality, and workforce development. Of the three, workforce development is perhaps the most challenging. With pending retirements and the increased operations tempo requirements stemming from the 2018 Nuclear Posture Review, the NNSA laboratories have accelerated their effort to hire the nation's best—the combined hiring effort across the NNSA labs is to add an estimated one thousand scientists, technical specialists, and post-doctoral students to the workforce annually. This pace of hiring is expected to continue.

In this time of rapid hiring, LDRD serves as an important pipeline for R&D talent. LDRD offers top-tier potential scientists and engineers from leading academic institutions the chance to hone their research skills and apply their education to mission-oriented research. LDRD is especially critical in supporting post-doctoral researchers as they transition to staff and programmatic work (see Performance Metrics). LDRD also serves as a driver for staff productivity, allowing post-doctoral researchers, as well as other technical staff awaiting clearance, to conduct meaningful research that impacts national security; this is particularly true for new hires in the weapons programs.

The stories below shine a light on the value of sustained investment in the Laboratory's workforce by building on historic expertise, present talent, and our future needs.

Historic expertise: LDRD Research on explosive safety carries the legacy forward

LDRD's Predicting High Explosive Safety Under Impacts (20180100DR) Team pictured with one of the pioneers of the Los Alamos High Explosive Crystal Laboratory.

Recent technological advances pioneered by LANL are transforming explosives research and serve as the springboard for innovations in current LDRD research. New in situ diagnostic capabilities, including those at advanced light sources, are enabling the community to answer long-standing, fundamental questions regarding materials' responses in dynamic extreme environments like never before.

In a two-day event February 20-21, 2019 LDRD researchers shared what they are doing to bolster prediction of High Explosive (HE) safety under impacts. Day 1 included a formal review of relevant program needs (i.e. within the Lab's Weapons Engineering and Weapons Physics Associate Level Directorates, Joint Munitions and Advanced Scientific Computing Programs, and the Department of Defense). Day 2 included a formal appraisal of the LDRD Directed Research (DR) project "Boom or Bust? Predicting Explosive Safety under Impact," as well as presentations of several related LDRD DR projects.

"We are in exciting times! I didn't think I'd see anything like this in HE mesoscale mechanics research in my career," said LDRD principal investigator Kyle Ramos, describing how experimental and theoretical capabilities have dramatically advanced in recent years.

Notably, the project review included one of the pioneers (since retired) of the Laboratory's High Explosive Crystal Laboratory, Howard Cady. Both LDRD principal investigators Kyle Ramos and Marc Cawkwell spoke with heartfelt respect and appreciation for the enduring legacy of Howard and others who initiated the HE Crystal Lab, circa 1970s.

"The pioneers began asking important questions," said Ramos. "Much of the work remained speculative for many years because the diagnostics were lacking to probe the microstructure scale response during impact."

Nearly 50 years later, LDRD became the vehicle for Ramos and others to bridge the research of the past with the present technical advances.

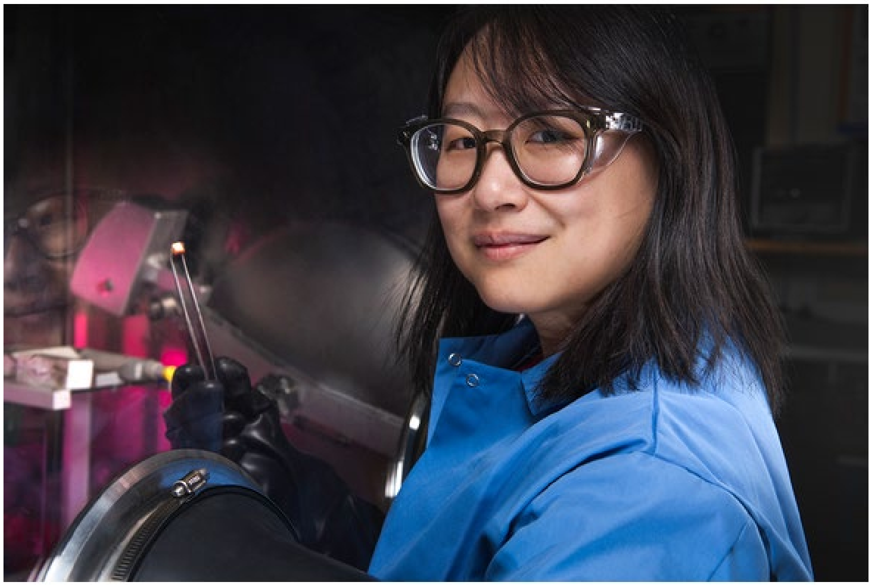
"LDRD allowed us to apply current capabilities and understanding to build on the work of Howard and others and to answer questions that would otherwise remain unanswered," said Ramos. These answers will in turn allow prediction of explosive safety under impact, which is critical to the Laboratory's ability to carry out Weapons Mission."

LDRD principal investigators Kyle Ramos (left) and Marc Cawkwell (right) with one of the pioneers of the Los Alamos High Explosive Crystal Laboratory, Howard Cady (center)

Tie to Missions

Enhanced energetic materials modeling will generate long-term savings in production, deployment, and accident/threat scenario assessments for DoD, DOE, DHS, and NASA.

Present talent: Early career researcher thrives through LDRD collaborations



LDRD researcher Wanyi Nie holds a perovskite crystal in an argon-filled glovebox. Nie will build a new semiconducting device capable of detecting gamma rays and x-rays using the crystal.

LDRD researcher **Wanyi Nie** (Materials Synthesis and Integrated Devices, MPA-11) believes her ideas are within reach at Los Alamos. She attributes her success largely to the collaborations she made through LDRD. A physicist and materials scientist by training, Nie loves learning about quantum mechanics and wants in on the chemists' conversations, she said, because they are the most fun.

"Early career staff don't have extensive networks of collaborators that senior scientists may have," she said. "We want to find places to share our science, we want to meet colleagues who study things we haven't thought of, and overall we want opportunities to grow. Participating as a member of a thriving, complex, interdisciplinary team through LDRD gave me access to collaborators in a variety of fields."

Nie attributes her drive to the fact that she's an early-career researcher.

"We have the motivation, passion, and willingness to take the risks to try and push the frontiers of science," she said, describing herself and her fellow junior scientists.

This drive is exactly what LDRD seeks to tap into. In 2013, Nie participated as a co-investigator on the LDRD Directed Research project, "Organic Electronic Materials: Designing and Creating Functional Interfaces" (20120019DR). She began studying this crystalline material known for its ability to absorb and transmit energy from light (photovoltaic capabilities).

The PI of that project, theorist **Sergei Tretiak** (Physics and Chemistry of Materials, T-1) heard about Nie from a colleague who said Nie had a "magic touch" that could boost a solar cell from 3% to 6% efficiency. Tretiak said he was just joking when he wondered what would happen if Nie started from a 10% solar cell. But less than a year later, Nie fabricated solar cells with 18% efficiency, having started literally from scratch in the unfamiliar world of organic-inorganic perovskite materials.

Six years later, Nie became the Co-PI on Tretiak's Directed Research project, "Rational Design of Halide Perovskites for Next Generation Gamma-ray Detection" (20180026DR). The team has proved fruitful, producing startling results and earning publications in journals such as *Nature* and *Science*.

“Wanyi is a fantastic collaborator: she is readily stepping up to your ground and ‘speaks in your language’ – clearly postulating the problems her experiment needs help with,” Tretiak said. “On many occasions these were the best examples of theory-experiment collaborations I ever had in the course of my entire research career.”

Tretiak, Nie and their team have discovered that perovskites can have a myriad of valuable properties. The crystals are not only sensitive to light, but also to magnetic fields, x-rays, and gamma rays: all valuable inputs for detectors or information storage. Each perovskite also has certain outputs like light or electricity. Nie has expanded the definition of what a halide-perovskite semiconductor can do. She uses her understanding of the unique qualities of each perovskite to imagine and produce new devices.

One of Nie’s goals is to produce perovskite detectors that nondestructively observe a variety of signals. Most detectors absorb, and therefore destroy, the signal they are designed to recognize. Other applications she envisions include an x-ray camera enabled by inexpensive and highly sensitive crystals and low-energy-consuming information storage and more-robust encryption technology using the team’s magnetically sensitive perovskites.

Tie to Missions

A primary outcome of this project is the demonstration of a proof-of-concept room-temperature operated gamma-ray detector, which will address several NNSA mission relevant programs at Los Alamos National Laboratory such as stockpile stewardship, nuclear deterrence, and space sensing.

Future needs: Preparing the quantum workforce

Three LDRD researchers, while early in their careers themselves, are leading an effort to prepare the quantum workforce of the future. Lukasz Cincio, Carleton Coffrin, and Patrick Coles (see bios below) – are program leads for the Los Alamos Quantum Computing Summer School, a program intended to address the workforce shortage in this important field.

Everyone has heard of quantum computers and their potential to shape our future, says Cincio. From quicker financial analysis to better medicine for cancer treatment, they could solve problems much faster than classical computers. But quantum computing is still only in its infancy. It is a subject that, for the most part, doesn’t exist in universities. It’s still new enough that it doesn’t have many people who are researching it in order to help it reach its full potential.

Which is why, Cincio says, Los Alamos established the Quantum Computing Summer School. He wrote about it in the Aug. 11 Lab Science column published in the Albuquerque Journal.

- The 10-week immersive program — now in its second year — accepts students from all over the world from a variety of disciplines.

- The school brings in some of the world’s leading quantum computing experts as speakers, as well as people from big tech companies (Google, Microsoft) that are working on their own quantum computers.

- Students get the rare experience working directly on quantum computers. Their projects may focus on hybrid quantum-classical algorithms and optimizing algorithms.

Quantum computing is a revolutionary new form of computing that leverages the bizarre characteristics of quantum mechanics to solve problems faster than is possible with classical computing.

“If you have a classical supercomputer that can simulate a molecule with at most 10 atoms, then you would have to double the size of that supercomputer just to simulate 11 atoms,” said Patrick Coles. You kind of hit a wall because your computer has to grow exponentially just to add atoms.

Coles and Cincio are part of an interdisciplinary team funded by LDRD to “tame the defects of quantum computing” (20190065DR). They are pursuing a key step in getting algorithms to run effectively. For more information on the school, visit the Los Alamos National Laboratory public web site.

Tie to Missions

The work of quantum computers could, in the future, help scientists tackle some of our most challenging mission problems. For example, it could help us create better drugs by simulating interactions among molecules or it could help us understand how the nuclear material inside bombs is behaving. The Quantum Computing Summer School is focusing on creating a workforce that is ready for that future.

About the LDRD Researchers

Lukasz Cincio's research interests lie at the interface between Condensed Matter Physics and Quantum Information Theory. While previously funded by LDRD as a J.R. Oppenheimer Distinguished Postdoctoral Fellow, Cincio worked on a scalable, numerical tool to enable insights into two-dimensional quantum systems (20160643PRD2). Cincio was honored with a Los Alamos 2018 Postdoctoral Distinguished Performance Award, honoring outstanding postdoc achievements that significantly impact the Laboratory’s status in the scientific community. He is currently a scientist in the Physics and Condensed Matter and Complex Systems group, as well as a current investigator on the Directed Research project “Taming Defects in Quantum Computers” (20190065DR) and Co-Principal Investigator on the Directed Research project “Quantum Chemistry using Quantum Computers” (20200056DR).

Carleton Coffrin is a computer scientist currently leading two LDRD projects that will end in FY19 – “Large-Scale Nonlinear Optimization via Cloud Computing” (20170574ECR) and “Physics-Based Machine Learning for Electric Power Outage Prediction” (20190630ER, Reserve). Coffrin developed the Severe Contingency Solver for Electric Power Transmission Analysis software to help government agencies better plan for power outages caused by extreme events. In addition to his quantum work, Coffrin is also an LDRD investigator on “"Towards Memristor Supremacy with Novel Machine Learning Algorithms” (20190195ER).

Patrick Coles is currently leading an Early Career Research project, “Machine Learning of Quantum Computing Algorithms” (20180628ECR). He is striving to develop automated software that optimizes quantum algorithms for applications like drug design and data analysis. He is also a current investigator on the Directed Research projects “Taming Defects in Quantum Computers” (20190065DR) and “Quantum Chemistry using Quantum Computers” (20200056DR).

The next section of this report includes project summaries 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 summaries for continuing projects appear first, followed by project summaries and technical outcomes for projects that ended in FY19.

Complex Natural and Engineered Systems

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

Journal Articles

*Ferrier, M. G., B. Stein, S. E. Bone, S. K. Cary, A. S. Ditter, S. A. Kozimor, J. S. Lezama Pacheco, V. Mocko and G. T. Seidler. The coordination chemistry of Cm , Am , and Ac in nitrate solutions: an actinide L -edge EXAFS study. 2018. *Chemical Science*. **9** (35): 7078-7090. (LA-UR-18-22688 DOI: 10.1039/C8SC02270D)

Kozimor, S. A., K. E. Aldrich, C. Eiroa Lledo, L. M. Lilley, V. Mocko, B. Stein and N. H. Lam. PREPARATION OF AN ACTINIUM-228 GENERATOR. Submitted to *Inorganic Chemistry*. (LA-UR-19-31448)

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Eiroa Lledo, C., D. H. Woen, A. C. Akin, N. H. Anderson, K. Bennett, E. R. Birnbaum, A. V. Blake, M. Brugh, E. Danielou Dalodiere, S. A. Kozimor, L. M. Lilley, V. Mocko, S. L. Thiemann, F. D. J. White, E. F. Dorman, M. G. Ferrier, D. K. Hamlin, Y. Li and D. S. Wilbur. DEVELOPMENT OF A SOLID-STATE SUPPORT FOR SEPARATING ASTATINE-211 FROM BISMUTH. Submitted to *Inorganic Chemistry*. (LA-UR-19-31728)

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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.

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Xu, H., X. Guo, C. Chung, J. T. White, J. N. Mitchell, H. Boukhalfa, A. J. Gaunt, A. Migdissov, G. Wang, P. Yang, E. R. Batista and A. Navrotsky. Calorimetric Studies of Actinide Compounds. Presented at *LDRD DR Project Appraisal Meeting*, Los Alamos, New Mexico, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20543)

Posters

Baker, J. L., J. T. White, R. C. Roback, C. Park and H. Xu. High-Pressure Structural Behavior and Bulk Modulus of U3Si5. Presented at *2019 COMPRES Annual Meeting*, Big Sky, Montana, United States, 2019-08-02 - 2019-08-05. (LA-UR-19-27177)

Chung, C., X. Guo, J. T. White, A. T. Nelson, A. Shelyug, H. Boukhalfa, R. C. Roback, A. Navrotsky and H. Xu. Enthalpies of Formation and Phase Stabilities of U-Si Materials. Presented at *ThermoCon Workshop 2018*, Pullman, Washington, United States, 2018-07-23 - 2018-07-23. (LA-UR-18-26568)

Kalintsev, A., A. Migdissov, H. Xu, R. C. Roback and J. Brugger. U(VI) speciation in hydrothermal carbonate-bearing fluids up to 250 \xc2\xbaC. Presented at *Migration 2019*, Kyoto, Japan, 2019-09-15 - 2019-09-20. (LA-UR-20-21350)

Liu, M., Q. Kang and H. Xu. Modelling of Uranium Dioxide Corrosion under Flow Conditions. Presented at *AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31438)

Migdissov, A. Hydrothermal Studies of Actinides at LANL (EES-14): Predictive Capabilities for Repositories, Nuclear Reactors, Environmental, and Non-Proliferation Science. . (LA-UR-18-21516)

Nisbet, H. D., A. Migdissov, H. Xu, X. Guo, V. van Hinsberg, A. Williams-Jones, H. Boukhalfa and R. C. Roback. An experimental investigation into the behavior of thorium in aqueous solution at elevated temperature. Presented at *LANL Student Symposium 2018*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-26874)

Xu, H., A. Migdissov, H. D. Nisbet, A. Kalintsev, N. F. van Hartesveldt, J. L. Baker, H. Boukhalfa, R. C. Roback, R. Mayanovic, D. Dhakal and N. Akram. Speciation, Stability and Mobility of Uranium and Thorium in Hydrothermal Environments. Presented at *GSA Annual Meeting*, Phoenix, Arizona, United States, 2019-09-22 - 2019-09-22. (LA-UR-19-29065)

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 disproportionally 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

Journal Articles

Cao, Z., P. J. J. Wolfram, C. Friedrichs, J. C. Rowland and Y. Zhang. A Data-driven Approach to Predict Sediment Settling Velocity. Submitted to *Joint Special Issue on Coastal Hydrology and Oceanography for Water Resources Research and Journal of Geophysical Research: Oceans*. (LA-UR-19-25788)

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)

*Tasseff, B., R. Bent and P. Van Hentenryck. Optimization of Structural Flood Mitigation Strategies. 2019. *Water Resources Research*. **55** (2): 1490-1509. (LA-UR-18-21506 DOI: 10.1029/2018WR024362)

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)

Wang, S., R. W. Bent, C. J. Coffrin, S. Eksioglu and S. Mason. A Scenario-Based Algorithm for Joint Chance-Constrained Programs with Finite Support and Feasible Integer Recourse. Submitted to *Computers and Operations Research*. (LA-UR-19-29356)

Ward, N., B. Bond-Lamberty, V. Bailey, D. Butman, E. Canuel, H. Diefenerfer, N. Ganju, M. Goni, C. Hopkinson, T. Khangaokar, A. Langley, N. G. McDowell, A. Myers-Pigg, R. Neumann, C. Osburn, R. Price, J. C. Rowland, A. Sengupta, M. Simard, M. Tzortziou, R. Vargas, P. Weisenhorn and L. Windham-Myers. Representing the Function and Sensitivity of Coastal Interfaces in Earth System Models. Submitted to *Nature Communications*. (LA-UR-19-31990)

Zhang, Y., J. C. Rowland, C. Xu, P. J. J. Wolfram, D. Svyatsky, J. D. Moulton, M. Marani, A. D'Alpaos, Z. Cao and D. Pasqualini. Intercomparison of eco-geomorphologic models: Toward a unified view of hydro-eco-geomorphological process sensitivities for coastal wetland evolution. Submitted to *Journal of Geophysical Research: Earth Surface*. (LA-UR-19-28502)

Presentation Slides

Francom, D. C., N. M. Urban and D. Pasqualini. Storm Surge Model Emulation and Sensitivity Analysis using Bayesian Adaptive Splines. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-28 - 2019-07-28. (LA-UR-19-27244)

Pasqualini, D., N. M. Urban, J. C. Rowland, J. D. Moulton, P. J. J. Wolfram, C. Xu, R. W. Bent, D. W. Goodsman, D. C. Francom, H. Nagarajan, B. A. Tasseff, B. Li and B. A. Vega-Westhoff. Preparing Our Coastlines for Climate Security Threats. Presented at *AGU Fall 2018*, Washington, DC, District Of Columbia, United States, 2018-12-10 - 2018-12-15. (LA-UR-18-31515)

Rowland, J. C. ModEx and landsurface processes: Thoughts on matching models, scales, and process-based observations. . (LA-UR-19-29437)

Tasseff, B. A., C. J. Coffrin and R. W. Bent. WaterModels.jl: An Open-source Framework for Exploring Water Network Optimization Formulations. Presented at *2019 INFORMS Annual Meeting*, Seattle, Washington, United States, 2019-10-20 - 2019-10-23. (LA-UR-19-30453)

Tasseff, B. A., R. W. Bent and P. Van Hentenryck. Cutting Planes for Global Optimization of Water Distribution Network Design. Presented at *2019 INFORMS Annual Meeting*, Seattle, Washington, United States, 2019-10-20 - 2019-10-23. (LA-UR-19-30452)

Urban, N. M., A. M. Barthel, R. W. Bent, M. Berdahl, D. S. Comeau, M. Dinniman, D. C. Francom, D. A. S. Foster, M. W. Hecht, A. Jonko, J. Klinck, G. Leguy, B. Li, W. H. Lipscomb, C. Little, J. D. Moulton, B. T. Nadiga, D. Pasqualini, J. C. Rowland, R. Sriver, E. Steig, B. A. Tasseff, C. Veneziani, T. Verma, S. Wang, W. Weijer, P. J. J. Wolfram and C. Xu. Synthesizing climate uncertainties and decision making in complex interdependent coastal systems. Presented at *Sea Level Hotspots from Florida to Maine*, Norfolk, Virginia, United States, 2019-04-23 - 2019-04-23. (LA-UR-19-24103)

Urban, N. M., D. Pasqualini and J. C. Rowland. Coastal energy-water-land interactions and adaptation. Presented at *Energy Modeling Forum: Analyses of Multi-sector Energy and Environmental Dynamics Workshop*, Snowmass, Colorado, United States, 2018-10-18 - 2018-10-18. (LA-UR-18-30324)

Urban, N. M., D. Pasqualini and J. C. Rowland. Adaptation science at LANL: High-fidelity endogenous modeling of coastal energy-water infrastructure adaptation. Presented at *Snowmass Workshop: Analyses of Multi-sector Energy and Environmental Dynamics*, Snowmass, Colorado, United States, 2018-07-18 - 2018-07-18. (LA-UR-18-30187)

Urban, N. M., D. Pasqualini and J. C. Rowland. Coastal infrastructure adaptation: High-fidelity endogenous modeling of coastal energy-water infrastructure adaptation. Presented at *National Renewable Energy Laboratory LDRD collaborative meeting*, Golden, Colorado, United States, 2018-10-04 - 2018-10-04. (LA-UR-18-30331)

J. Wolfram, P. J. Coastal modeling using MPAS-O and E3SM. . (LA-UR-18-29530)

J. Wolfram, P. J. Coastal modeling through novel ocean developments in E3SM. Presented at *DOE Earth and Environmental System Modeling (EESM) PI Meeting*, Poto, Maryland, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30635)

J. Wolfram, P. J. Modeling the land-water interface in the Energy Exascale Earth System Model. Presented at *Toledo Lab Day*, Toledo, Ohio, United States, 2019-10-10 - 2019-10-10. (LA-UR-19-30209)

J. Wolfram, P. J. Multiscale Exascale Earth System Modeling (E3SM): gaining clarity on earth system evolution through mixing across scales in global to coastal ocean modeling. . (LA-UR-19-31491)

J. Wolfram, P. J. Understanding coastal flooding by hurricanes and drought-induced water quality degradation for coastal power and water networks. . (LA-UR-20-22017)

J. Wolfram, P. J., S. R. Brus, M. R. Petersen, Z. Cao, D. Engwirda, X. S. Asay-Davis, M. E. Maltrud, J. D. Wolfe, A. F. Roberts, T. Zhou, G. Bisht, Z. Tan and R. Leung. Global to coastal ocean modeling in the Energy Exascale Earth System Model. Presented at *The 18th International workshop on Multi-scale (Un)-structured mesh numerical Modeling for coastal, shelf, and global ocean dynamics (IMUM 2019)*, Santa Fe, New Mexico, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-29580)

J. Wolfram, P. J., S. R. Brus and Z. Cao. Coastal modeling for the Delaware using MPAS-O / E3SM for hurricane and decadal simulation. Presented at *FFMP Workgroup and Salinity group*, Trenton, New Jersey, United States, 2019-04-11 - 2019-04-11. (LA-UR-19-23344)

J. Wolfram, P. J., T. Zhou, G. Bisht, Z. Cao, Z. Tan, H. Li, C. Liao, L. Zhai, A. F. Roberts, J. D. Wolfe, M. R. Petersen, B. Arbic, D. Engwirda, S. R. Brus, M. E. Maltrud, X. S. Asay-Davis, R. Leung and I. Kraucunas. Global to coastal multiscale modeling in the Energy Exascale Earth System Model. Presented at *E3SM Nov Project Meeting*, Washington, District Of Columbia, United States, 2019-11-19 - 2019-11-21. (LA-UR-19-31392)

Xu, C. Improved representation of vegetation dynamics in Earth System Models. Presented at *Invited department seminar at Department of Civil and Environmental Engineering*, Houston, Texas, United States, 2019-04-05 - 2019-04-05. (LA-UR-19-23209)

Xu, C., L. Zhai, J. C. Rowland and D. Pasqualini. Assessing the vulnerability of coastal vegetation climate change using a dynamic vegetation model. Presented at *2019 AGU*, San Francisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-32408)

Posters

Bent, R. W., B. Li, H. Nagarajan, R. Jiang and J. Mathieu. Decomposition and Cutting-Plane Based Algorithm for Stochastic Climate Adaptation Problem Using Special Order Sets. . (LA-UR-18-27129)

Pasqualini, D., N. M. Urban, J. C. Rowland, P. J. J. Wolfram, J. D. Moulton, C. Xu, R. W. Bent, H. Nagarajan, B. A. Tasseff, D. W. Goodsman and D. C. Francom. Co-evolution of Coastal Natural and Human-Engineered Systems: Making Decisions under Uncertainty. Presented at *ECM15*, Seattle, Washington, United States, 2018-06-25 - 2018-06-28. (LA-UR-18-30410)

Rowland, J. C. and N. M. Urban. Coastal adaptation planning through coastal dynamics modeling, end-to-end uncertainty fusion, and probabilistic design optimization. . (LA-UR-18-22742)

J. Wolfram, P. J., S. R. Brus, Z. Cao, M. R. Petersen, M. E. Maltrud, L. Van Roekel, J. C. Rowland, D. Pasqualini, N. M. Urban, Z. Yang, J. D. Moulton, D. Svyatsky, C. Xu, R. W. Bent, B. Li, B. A. Tasseff and D. C. Francom. Coastal modeling through novel ocean developments in E3SM. Presented at *DOE EESM PI meeting*, Potomac, Maryland, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30478)

Zhang, Y. Wetland hydrologic resilience to climate variability: a case study at a coastal wetland of North Carolina, USA. Presented at *American Geophysical Union*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-15. (LA-UR-18-31331)

Zhang, Y. Assessing the hydrologic resilience of coastal wetlands at the Southeastern US under climate disturbances: the critical role of regional-scale hydrologic interaction. Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32008)

BioManufacturing with Intelligent Adaptive Control: BioManIAC

Babetta Marrone
20190001DR

Project Description

Plastics made from petroleum are a mainstay in our daily lives, but the environmental problems they create are driving an urgent search for bio-based alternatives. Currently, over 300 million-metric-tons of plastic are produced worldwide, yet only a fraction is derived from bio-based feedstocks. The biopolymer field suffers from lack of deep understanding of what makes a good bioplastic. Bio-derived molecules have more diverse chemical functionalities than those found in petroleum-based molecules and therefore offer a rich resource for discovering new monomers for synthesis of novel biopolymers for conversion into plastic materials with performance advantages. Microalgae are an attractive bio-feedstock for industrial applications because of their rapid growth and higher productivity-per-unit-land-area than any plant system. We will identify new molecular precursors for bioplastics using microalgae as the feedstock, and develop machine learning (ML) tools to optimize chemical discovery and design. ML will accelerate the development of new biopolymers from algae by efficiently matching large data sets of chemical structures to specific sets of properties and desired functionalities. We will build a chemical knowledge base that will provide the foundation to advance the development of novel biopolymers for the manufacture of plastics for a wide range of applications and optimal end-of-life degradation

Publications

Journal Articles

Pilania, G., B. L. Marrone and C. N. Iverson. Machine-Learning-Based Predictive Modeling of Glass Transition Temperatures: A Case of Polyhydroxyalkanoate Homopolymers and Copolymers. 2019. *Journal of Chemical Information and Modeling*. (LA-UR-19-28291 DOI: 10.1021/acs.jcim.9b00807)

Books/Chapters

Pilania, G., P. Balachandra, J. E. Gubernatis and T. Lookman. Data-Based Methods for Materials Design and Discovery Basic Ideas and General Methods. (LA-UR-19-31822)

Presentation Slides

Bejagam, K. K., C. N. Iverson, B. L. Marrone and G. Pilania. Structure-Property Mappings for Bio-Advantaged Polyhydroxyalkanoate (PHA)-based Polymers. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22031)

Jha, R. K. Synthetic Biology for a Better World.. Presented at *CFO Connect*, Los Alamos, New Mexico, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24201)

Marrone, B. L. Sustainability through Biofuels and Bioproducts. Presented at *National Lab Day*, Toledo, Ohio, United States, 2019-10-09 - 2019-11-09. (LA-UR-19-30151)

Uberuaga, B. P. Highlights performed on LANL IC on the project w19_matprops. . (LA-UR-20-22424)

Posters

Gonzalez Esquer, C. R., G. Pilania, N. M. Sudasinghe Appuhamilage, B. A. Parsons, C. R. Steadman, K. Lee, K. Campbell, R. K. Jha, C. N. Iverson, T. Lookman, S. R. Starkenburg, T. T. Dale and B. L. Marrone. Biomanufacturing with Intelligent Adaptive Control. Presented at *13th Workshop on Cyanobacteria*, Boulder, Colorado, United States, 2019-04-06 - 2019-04-09. (LA-UR-19-23867)

Lakis, I. M., P. K. Dighe, C. R. Gonzalez Esquer and B. L. Marrone. Multifactorial Optimization of Cyanobacterial Polymer Production Platforms. Presented at *2019 UGS LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27571)

Obrey, S. J., G. F. Levine and K. Erickson. Modifying Carboxylate-Alumoxane Surfaces with Click Chemistry. Presented at *LANL Annual Student Symposium*, los alamos, New Mexico, United States, 2019-08-06 - 2019-08-08. (LA-UR-19-27227)

Salts in Hot Water – Developing a Scientific Basis for Supercritical Desalination, Strategic Metal Recovery, and Industrial Water Treatment

Robert Currier
20190057DR

Project Description

Fresh water will undoubtedly become an increasingly important aspect of international stability. Fresh water production by thermal desalination with simultaneous recovery of strategic elements offers a route to affordable water and a secure supply of key metals. Deep aquifer brines contain many valuable metals. With China manipulating rare earth element supply and prices, it is important to secure domestic sources of all strategic metals. The co-production of metals with desalination can provide a means of doing so. An integrated process to accomplish these objectives will be developed using inexpensive thermal energy (heat). The process can also impact energy production. Current practice of off-site transport of water co-produces with oil/gas followed by deep well re-injection is costly and can induce earthquakes. Also, sequestration of carbon dioxide in aquifers requires removal of equal volumes of brine to avoid seismicity. Treatment/use of extracted brine would alleviate these concerns and costs. Water also facilitates the migration of heavy metals including actinides and post-detonation fission products. This effort will provide insights into their environmental transport and nuclear material fate during rare, but usually consequential, nuclear accidents. New methods for stabilizing and disposing of hazardous waste streams, and for metal recovery/recycling, are expected.

Publications

Journal Articles

Middleton, R. S., J. M. Bielicki, B. Chen, A. F. Clarens, R. P. Currier, K. M. Ellett, D. R. Harp, B. A. Hoover, R. M. Kammer, D. N. McFarlane, J. D. Ogland- Hand, R. J. Pawar, P. H. Stauffer, H. S. Viswanathan and S. P. Yaw. Great SCO2T! Rapid tool for carbon sequestration science, engineering, and economics. Submitted to *Applied Energy*. (LA-UR-19-31754)

Strzelecki, A. C., A. Migdissov, H. Boukhalfa, K. B. Sauer, K. G. McIntosh, R. P. Currier and A. E. Williams-Jones. Fluocerite: The phantom precursor for REE fractionation in natural ore-forming systems. Submitted to *Nature Geoscience*. (LA-UR-19-31633)

Yoon, T. J., L. A. Patel, M. J. Vigil, K. A. Maerzke, A. T. Findikoglu and R. P. Currier. Electrical conductivity, ion pairing, and ion self-diffusion in aqueous NaCl solutions at elevated temperatures and pressures. 2019. *Journal of Chemical Physics*. **151** (22): 224504. (LA-UR-19-27151 DOI: 10.1063/1.5128671)

Yoon, T., K. A. Maerzke, A. T. Findikoglu, R. P. Singh, L. R. Pratt, A. C. Strzelecki, L. A. Patel, D. T. Gomez, R. S. Middleton, C. D. Alcorn, M. J. Vigil, E. Judge, J. D. Riglin, K. A. Velizhanin, R. S. Reid, H. D. Nisbet, A. Migdissov and R. P. Currier. Supercritical Desalination: Opportunities and Challenges. Submitted to *Desalination*. (LA-UR-19-32498)

Yoon, T., M. J. Vigil, E. Y. Raby, R. P. Singh, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Dielectric relaxation of neodymium chloride in water and in methanol. Submitted to *Journal of Molecular Liquids*. (LA-UR-19-32739)

Presentation Slides

Currier, R. P. and A. Migdissov. Salts in Hot Water – Developing a Scientific Basis for Supercritical Desalination, Strategic Metal Recovery, and Industrial Water Treatment. . (LA-UR-20-21500)

Findikoglu, A. T., T. Yoon, M. J. Vigil and P. Sharan. Impedance/ Dielectric Spectroscopy and Theory/Engineering Implications. . (LA-UR-20-21743)

Maerzke, K. A. Monte Carlo Simulations of Phase Equilibria and Vapor-Phase Aggregation. . (LA-UR-20-21627)

Maerzke, K. A., L. A. Patel and T. Yoon. Salts in Hot Water: Developing a Scientific Basis for Supercritical Desalination and Strategic Metal Recovery. . (LA-UR-20-21963)

Migdissov, A., A. C. Strzelecki, H. Boukhalfa, K. B. Sauer, H. D. Nisbet, K. A. Velizhanin and R. P. Currier. Selective hydrothermal extraction of lanthanides: mimicking natural ore-forming processes. . (LA-UR-20-21659)

Singh, R. P. Advanced materials and technologies for FEWS. Presented at *Regional academic collaborations initiative (ReACt) Workshop on Food Energy Water Systems*, Las Cruces, New Mexico, United States, 2019-08-13 - 2019-08-14. (LA-UR-19-28119)

Velizhanin, K. A., C. D. Alcorn, A. Migdissov and R. P. Currier. Non-Ideal Solubility of Chlorides in Steam. Presented at *LDRD 20190057DR MidTerm Appraisal*, Los Alamos, New Mexico, United States, 2020-02-24 - 2020-02-24. (LA-UR-20-21646)

Yoon, T., L. A. Patel, M. J. Vigil, A. T. Findikoglu, K. A. Maerzke and R. P. Currier. Molecular dynamics study of specific conductance in sub- and supercritical brine. . (LA-UR-20-21740)

Posters

Patel, L. A. and K. A. Maerzke. NaCl Aggregation in Supercritical Water: Comparison of Classical Force Fields.. . (LA-UR-20-21629)

Riglin, J. D., P. Sharan, T. Yoon, A. T. Findikoglu and R. P. Currier. Process Design & Engineering. . (LA-UR-20-21744)

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.

Technical Outcomes

We have developed the methodology to probe fault physics at all times during the slip cycle, and to predict failure times, and in some cases earthquake magnitudes. Future work will include applications to large earthquakes.

Publications

Journal Articles

Delorey, A. A., P. A. Johnson and I. W. McBrearty. Tidal triggering of earthquakes in Oklahoma foreshadows increasing seismic hazard. Submitted to *Science*. (LA-UR-17-28778)

*Dorostkar, O., R. A. Guyer, P. A. Johnson, C. Marone and J. Carmeliet. Cohesion-Induced Stabilization in Stick-Slip Dynamics of Weakly Wet, Sheared Granular Fault Gouge. 2018. *Journal of Geophysical Research: Solid Earth*. **123** (3): 2115-2126. (LA-UR-17-30001 DOI: 10.1002/2017JB015171)

*Dorostkar, O., R. A. Guyer, P. A. Johnson, C. Marone and J. Carmeliet. On the micromechanics of slip events in sheared, fluid-saturated fault gouge. 2017. *Geophysical Research Letters*. **44** (12): 6101-6108. (LA-UR-17-25964 DOI: 10.1002/2017GL073768)

*Gao, K., B. J. Euser, E. Rougier, R. A. Guyer, Z. Lei, E. E. Knight, J. Carmeliet and P. A. Johnson. Modeling of Stick-Slip Behavior in Sheared Granular Fault Gouge Using the Combined Finite-Discrete Element Method. 2018. *Journal of Geophysical Research: Solid Earth*. **123** (7): 5774-5792. (LA-UR-18-20365 DOI: 10.1029/2018JB015668)

*Gao, K., E. Rougier, R. A. Guyer, Z. Lei and P. A. Johnson. Simulation of crack induced nonlinear elasticity using the combined finite-discrete element method. 2019. *Ultrasonics*. **98**: 51-61. (LA-UR-18-30701 DOI: 10.1016/j.ultras.2019.06.003)

Gao, K., N. Bozorgzadeh and J. P. Harrison. The Equivalence of Three Shear-Normal Stress Forms of the Hoek-Brown Criterion. Submitted to *Rock Mechanics and Rock Engineering*. (LA-UR-19-21598)

Gao, K., R. A. Guyer, E. Rougier, C. X. Ren and P. A. Johnson. From Stress Chains to Acoustic Emission. Submitted to *Physical Review Letters*. (LA-UR-19-21038)

Gao, K., R. A. Guyer, E. Rougier and P. A. Johnson. Plate motion in sheared granular fault system. Submitted to *Earth and Planetary Science Letters*. (LA-UR-19-29473)

Hulbert, C. L. Estimating the Physical State of a Laboratory Slow Slipping Fault from Seismic Signals. Submitted to *Nature Geoscience, ArXiv*. (LA-UR-18-20487)

Hulbert, C. L. A Silent Build-up in Seismic Energy Precedes Slow Slip Failure in the Cascadia Subduction Zone. Submitted to *Science*. (LA-UR-19-29445)

Hulbert, C. L., B. P. G. Rouet-Leduc, C. X. Ren, J. Riviere, c. Bolton, C. Marone and P. A. Johnson. Estimating the Physical State of a Laboratory slow slipping fault from seismic signals. Submitted to *Archive ArXiv:1801.07806*. (LA-UR-18-29848)

Hulbert, C. L., B. P. G. Rouet-Leduc, R. Jolivet and P. A. Johnson. An Exponential Build-up in Seismic Energy Suggests a Months-Long Nucleation of Slow Slip in Cascadia. Submitted to *Nature Communications*. (LA-UR-20-22489)

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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.

Technical Outcomes

This LDRD-DR project has established both experimental and theoretical capabilities at LANL applicable to the development of Redox Flow Batteries (RFBs). Iron and nickel based complexes that support multi-electron redox have been designed and synthesized. Anion exchange membranes (AEMs) based on quaternized poly arylene ether benzonitrile with very low cross over were also developed in this project and successfully demonstrated in an aqueous flow battery system

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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.

Technical Outcomes

We have addressed several critical problems currently hindering progress in predicting harmful Geomagnetically-Induced Currents in power grids. We now have a coupled end-to-end model that is capable of simulating harmful effects in power distribution systems all the way back to solar wind inputs for extreme events. This model is fully capable of ingesting observational data in a data-assimilative mode and we have demonstrated the first ever results of ensemble model runs for uncertainty quantification.

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Reports

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Henderson, M. G. The relationship between streamers, torches, omega bands and pseudo-breakups. Presented at *Teleconference Talk for American Geophysical Union*, Los Alamos, New Mexico, United States, 2017-07-31 - 2017-07-31. (LA-UR-17-26311)

Henderson, M. G. Ground Magnetic Perturbations Associated with Substorms, Pseudo-Breakups, Streamers and Omega Bands. Presented at *Fundamental Physical Processes in Solar-Terrestrial Research and Their Relevance to Planetary Physics 2018*, Kona, Hawaii, United States, 2018-01-08 - 2018-01-13. (LA-UR-18-20123)

Henderson, M. G. Impacts of Extreme Space Weather Events on Power Grid Infrastructure: Physics-Based Modeling of Carrington-Class Storm Events. . (LA-UR-18-23495)

Henderson, M. G. Carrington/GIC LDRD/DR Project Overview. . (LA-UR-18-26871)

M. Jeffery, C. A. Task 3: Propagation of Currents to Ground using LANL GeoRad. . (LA-UR-18-20474)

Jordanova, V. K. Modeling of Cross-Energy Coupling in the Inner Magnetosphere. Presented at *The Magnetosphere: New Tools, New Thinking, New Results*, Puerto Varas, Chile, 2017-11-12 - 2017-11-17. (LA-UR-17-28654)

Jordanova, V. K. SHIELDS/RAM-SCB and Opportunities for Partnership with CCMC. Presented at *9th CCMC Workshop*, College Park, Maryland, United States, 2018-04-23 - 2018-04-27. (LA-UR-18-23997)

Jordanova, V. K. Geomagnetic Storms: New Insights from Multi-Spacecraft Observations and Self-Consistent Simulations. Presented at *Center for International Collaborative Research (CICR) Colloquium Series*, Nagoya, Japan, 2019-04-04 - 2019-04-04. (LA-UR-19-22763)

Jordanova, V. K. Introduction to Space Weather: Observations, Theory & Modeling. . (LA-UR-19-26250)

Jordanova, V. K., M. A. Engel, M. G. Henderson, S. K. Morley, Y. Miyoshi, Y. Yu, Y. Zheng and L. M. Kistler. Inner Magnetosphere Multiscale Modeling and Validation. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-27776)

Jordanova, V. K., M. A. Engel, M. G. Henderson, Y. Miyoshi, Y. Yu, K. Hosokawa, W. Li, X. Shen, L. Capannolo, B. Ni, E. Spanswick, S. Y. Wang, Y. Kazama, S. Kasahara, S. Yokota, T. Mitani, T. Takashima, A. Matsuoka, I. Shinohara, Y. Kasahara, S. Matsuda, A. Kumamoto, F. Tsuchiya and A. Matsuoka. RAM-SCBE Simulations of the March 2017 CIR-Driven Storm Period. Presented at *American Geophysical Union Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-27882)

Jordanova, V. K., M. A. Engel, X. Fu, M. Cowee, M. G. Henderson and Y. Yu. The Role of Wave-Particle Interactions in the Dynamics of Energetic Particles in the Inner Magnetosphere. Presented at *AOGS 15th Annual Meeting*, Honolulu, Hawaii, United States, 2018-06-03 - 2018-06-08. (LA-UR-18-20584)

Jordanova, V. K., M. G. Henderson, M. A. Engel, S. K. Morley, J. R. Woodroffe, G. D. Reeves and C. Kletzing. Inner Magnetosphere Dynamics: Simulations and Comparisons with Multi-Spacecraft Observations. Presented at *42nd COSPAR Scientific Assembly*, Pasadena, California, United States, 2018-07-14 - 2018-07-22. (LA-UR-18-21525)

Jordanova, V. K., S. K. Morley, E. H. Lay, R. A. Haaser and K. Yakymenko. Investigations of Magnetosphere-Ionosphere Coupling with RAM-SCBE. Presented at *Living With a Star FST Kick-off Meeting*, Santa Fe, New Mexico, United States, 2019-06-28 - 2019-06-29. (LA-UR-19-26251)

Jordanova, V. K., X. Fu, M. G. Henderson, S. K. Morley, D. Welling and Y. Yu. Investigating EMIC Wave Dynamics with RAM-SCB-E. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-27454)

Jordanova, V. K., Y. Chen, S. K. Morley, M. Cowee and M. G. Henderson. Cross-Energy Coupling in the Inner Magnetosphere: Simulations and Comparisons with Van Allen Probe Observations. Presented at *2nd URSI Atlantic Radio Science Conference*, Gran Canaria, Spain, 2018-05-28 - 2018-06-01. (LA-UR-18-20204)

Martinez, K. My Big Fat Data Research Project @ LANL. Presented at *A-1 Group Meeting*, Los Alamos, New Mexico, United States, 2019-08-19 - 2019-08-19. (LA-UR-19-28331)

Morley, S. K. Ensemble Modeling of Driven Systems. Presented at *Ensemble Forecasts in Space Weather: Science and Operations*, Leiden, Netherlands, 2019-09-02 - 2019-09-06. (LA-UR-19-29116)

Morley, S. K., D. T. Welling, J. R. Woodroffe, M. A. Engel and M. G. Henderson. Uncertainties in space weather forecasting using coupled physics models. Presented at *Chapman Conference on Scientific Challenges Pertaining to Space Weather Forecasting Including Extremes*, Pasadena, California, United States, 2019-02-12 - 2019-02-15. (LA-UR-19-21525)

Morley, S. K., D. T. Welling, J. T. Steinberg, J. D. Haiducek, E. Hassan and B. P. Weaver. Perturbed-input ensemble modeling of magnetospheric dynamics. Presented at *2017 AGU Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-11. (LA-UR-17-31116)

Morley, S. K., D. T. Welling, M. A. Engel, M. K. Rivera, M. G. Henderson, J. Woodroffe and A. Panaitescu. Ensemble modeling to predict space weather impacts on the North American power grid. Presented at *Fall AGU meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-32233)

Morley, S. K., J. D. Haiducek and D. T. Welling. Probabilistic Prediction of Substorm Onset. Presented at *14th International Conference on Substorms*, Tromso, Norway, 2019-09-30 - 2019-10-04. (LA-UR-19-29850)

Morley, S. K., J. Haiducek and D. Welling. Forecasting substorm activity with global MHD and the Minimal Substorm Model. Presented at *Advancing Plasma Physics from the Sun to the Earth*, Breckenridge, Colorado, United States, 2017-05-22 - 2017-05-26. (LA-UR-17-24183)

Morley, S. K. and D. Welling. Quanitfying Model Performance for Space Weather. Presented at *42nd COSPAR Scientific Assembly*, Pasa, California, United States, 2018-07-16 - 2018-07-16. (LA-UR-18-26538)

Rivera, M. K. The Impacts of Coronal Mass Ejection(CME) on Power Systems. Presented at *Region 6 Critical Infrastructure Working Group: Long-term Power Outage Workshop*, Seattle, Washington, United States, 2019-05-23 - 2019-05-23. (LA-UR-19-24695)

Rivera, M. K. and R. W. Bent. GMD Coupling to Power Systems and Disturbance Mitigation. . (LA-UR-18-20499)

Woodroffe, J. R., S. K. Morley, M. G. Henderson, V. K. Jordanova and M. Cowee. Ground Zero for Geomagnetic Hazards. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2016-12-12 - 2016-12-16. (LA-UR-16-29310)

Posters

Engel, M. A., M. G. Henderson, V. K. Jordanova and S. K. Morley. Hurdles to Overcome to Model Carrington Class Events. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31341)

Hassan, E., S. K. Morley, D. T. Welling and J. T. Steinberg. Forecasting the Geomagnetic Disturbances using a Solar Wind Ensemble. Presented at *Geospace Environment Workshop*, Santa Fe, New Mexico, United States, 2019-06-24 - 2019-06-24. (LA-UR-19-25469)

Henderson, M. G., S. K. Morley, V. K. Jordanova, G. S. Cunningham, J. R. Woodroffe, B. A. Larsen, G. D. Reeves, R. H. W. Friedel, R. M. Kippen and J. P. Sullivan. Space Weather Data Products and Modeling Capabilities at Los Alamos National Laboratory. Presented at *Space Weather Enterprise Forum*, Washington, District Of Columbia, United States, 2017-06-27 - 2017-06-27. (LA-UR-17-25065)

Hickmann, K. S., H. C. Godinez Vazquez, M. K. Rivera and M. G. Henderson. Physics Informed Emulation of Magnetometer Data During Large Space-Weather Events. Presented at *AGU Annual*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31060)

Liemohn, M. W., J. McCollough, V. K. Jordanova, C. Ngwira, S. K. Morley, C. Cid, W. K. Tobiska, P. Wintoft, N. Y. Ganushkina, D. T. Welling, S. Bingham, M. Balikhin, H. Opgenoorth, M. A. Engel, R. Weigel, H. J. Singer, D. Buresova, S. L. Bruinsma, I. S. Zhelavskaya, Y. Y. Shprits and R. Vasile. Model evaluation guidelines for geomagnetic index predictions. Presented at *Chapman Conference on Scientific Challenges Pertaining to Space Weather Forecasting Including Extremes*, Pasadena, California, United States, 2019-02-11 - 2019-02-15. (LA-UR-19-21527)

Woodroffe, J. R., S. K. Morley and J. B. Dann. Geomagnetic Disturbances and Auroral Boundaries. Presented at *American Geophysical Union (AGU) Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-11. (LA-UR-17-31157)

Woodroffe, J. R. and M. G. Henderson. A Global Perspective on Geomagnetic Disturbances. Presented at *Space Weather Workshop*, Westminster, Colorado, United States, 2018-04-16 - 2018-04-20. (LA-UR-18-23386)

Maximizing Food Security Under Environmental Stress

Sanna Sevanto
20190003DR

Project Description

Use of plant probiotics has been suggested as a potential solution for improving plant performance and stress tolerance to match future demands for food and biofuel production. Plants and their associated microbiota are nutritionally interdependent, and constantly communicating with each other for resource requirements. Therefore, microbes can profoundly improve plant performance. Progress in optimizing plant-microbiomes, however, has been hindered by the extreme complexity of the plant-microbiome system. To overcome this challenge we propose to test the feasibility of plant-directed microbiome evolution to generate microbial consortia that improve plant performance. Directed evolution is used in protein production and enzyme engineering, but is has not been applied to plant-microbiome systems. This method has potential to revolutionize our ability to control plant and microbiome systems. If feasible, it can be used to control a myriad of plant traits such as drought tolerance, nitrogen or water use efficiency, performance under saline conditions, chemical composition, uptake of materials of interest or production of physiological signals in response to environmental stimuli. These traits are of interest to improved food and biofuel security, carbon sequestration, bioremediation and use of plants as biosensors, for example, for proliferation detection or production monitoring.

Technical Outcomes

In this project we demonstrated that 1) corn productivity under mild drought can be increased by manipulating the plant to keep stomata open under a more severe drought than it could sustain before, and 2) stomatal closure point can be altered by altering environmental conditions such as soil water retention capacity that is influenced by the root-zone microbiome. We also developed methods to analyze soil drought tolerance in corn, and propagate soil microbial inoculants.

Publications

Presentation Slides

Sevanto, S. A. Is phloem transport limited under drought and does it matter for plant survival?. Presented at *12th North American Forest Ecology Workshop*, Flagstaff, Arizona, United States, 2019-06-24 - 2019-06-27. (LA-UR-19-25826)

Posters

Sevanto, S. A., J. P. Heneghan, D. Musa, J. M. Dunbar, E. R. Lathrop, B. D. Newman, S. N. Twary, C. M. Yeager and L. Comas. Effects of life stage and oil water retention capacity on stomatal closure point of corn (Zea mays). Presented at *LANL student symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27724)

Radiation Belt Remediation: A Complex Engineered System (RBR-ACES)

Gian Delzanno
20190064DR

Project Description

A high-altitude nuclear explosion (HANE) at low latitudes (such as in North Korean nuclear test) creates a high-intensity, long-lasting artificial radiation belt of relativistic electrons that would damage all low-Earth-orbit satellites not specifically designed against a nuclear event and would cripple US national security capabilities for years. This project will develop a simplified, end-to-end modeling framework to estimate the feasibility of a space-based radiation belt remediation system based on the injection of electromagnetic plasma waves and aimed at returning the post-HANE environment to levels that are safe for our space infrastructure within less than a month.

Technical Outcomes

In this one-year project we have developed a simplified, end-to-end modeling framework for a radiation belt remediation space-based system based on the injection of electromagnetic waves. Despite its simplifications, a preliminary application of RBR-ACES to study the remediation of a Starfish-class high altitude nuclear explosion yields encouraging results on the feasibility of remediation, suggesting that power requirements might not be prohibitive for such a system and emphasizing the need for further modeling developments.

Publications

Journal Articles

Olshevsky, V., Y. V. Khotyaintsev, A. Divin, G. L. Delzanno, S. Anderzen, P. Herman, S. Chien, L. Avanov and S. Markidis. Automated classification of plasma regions using 3D particle energy distribution.. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-19-30657)

Presentation Slides

Cunningham, G. S. Drift-averaged Pitch-angle Diffusion Coefficients in Non-dipolar Magnetic Fields. Presented at *The Plasma Physics of the Magnetosphere*, Bra-Pollenzo, Italy, 2019-06-02 - 2019-06-07. (LA-UR-19-24946)

Cunningham, G. S. Project update for P185 Study of the effects of whistler-mode waves in the near Earth radiation environment. Presented at *2019 General/ Working Meeting for the International Agreement on Fundamental Science*, Bordeaux, France, 2019-06-05 - 2019-06-07. (LA-UR-19-25146)

Delzanno, G. L., Q. R. Marksteiner, G. D. Reeves, B. E. Carlsten, P. L. Colestock, M. Cowee, G. S. Cunningham, S. Dorfman, L. D. Duffy, C. A. M. Jeffery, O. Koshkarov, V. Roytershteyn, K. Yakymenko, N. Yampolsky, J. McCollough and J. M. Albert. Recent progress towards a radiation belt remediation strategy based on artificial injection of plasma waves. Presented at *URSI meeting*, Boulder, Colorado, United States, 2019-01-09 - 2019-01-09. (LA-UR-19-20131)

Marksteiner, Q. R., B. E. Carlsten, P. L. Colestock, G. S. Cunningham, G. L. Delzanno, L. D. Duffy, M. A. Holloway, J. W. I. Lewellen, D. C. Nguyen, G. D. Reeves, K. A. Shipman, K. Yakymenko and N. Yampolsky. Accelerators in Space. Presented at *The 2019 Conference on Applications of Nuclear Techniques*, Rithymna Beach, Greece, 2019-06-09 - 2019-06-14. (LA-UR-19-25280)

Posters

Shipman, K. A., P. L. Colestock and B. E. Carlsten. Characterization of On-Orbit VLF Wave Generation in the Inner Plasmasphere. Presented at *APS-DPP*, Portland, New Mexico, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30556)

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 to 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

Journal Articles

*Jung, J., W. Nishima, M. Daniels, G. Bascom, C. Kobayashi, A. Adedoyin, M. Wall, A. Lappala, D. Phillips, W. Fischer, C. Tung, T. Schlick, Y. Sugita and K. Y. Sanbonmatsu. Scaling molecular dynamics beyond 100,000 processor cores for large-scale biophysical simulations. 2019. *Journal of Computational Chemistry*. **40** (21): 1919-1930. (LA-UR-18-31413 DOI: 10.1002/jcc.25840)

Kim, D. N., N. W. Moriarty, S. Kirmizialtin, P. V. Afonine, B. Poon, O. V. Sobolev, P. D. Adams and K. Y. Sanbonmatsu. Cryo_fit: Democratization of flexible fitting for cryo-EM. Submitted to *Journal of Structural Biology*. (LA-UR-19-31082)

Kim, D. N. and K. Y. Sanbonmatsu. Tools for the cryo-EM gold rush: going from the cryo-EM map to the atomistic model. Submitted to *Bioscience Reports*. (LA-UR-19-31083)

Posters

Lappala, A. Self-organization and compaction in biological and soft matter systems. Presented at *CNLS external review*, Los Alamos, New Mexico, United States, 2018-05-03 - 2018-05-03. (LA-UR-18-23790)

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

Journal Articles

Bakhshian, S., M. Murakami, S. A. Hosseini and Q. Kang. Scaling of Imbibition Front Dynaimcs in Heterogeneous Porous Media. Submitted to *Geophysical Research Letters*. (LA-UR-20-22139)

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Inertial Effects During the Process of Supercritical CO2 Displacing Brine in a Sandstone: Lattice Boltzmann Simulations Based on the Continuum-Surface-Force and Geometrical Wetting Models. 2019. *Water Resources Research*. (LA-UR-19-23236 DOI: 10.1029/2019WR025746)

Gong, Y., M. Z. S. Mehana, I. El-monier and H. S. Viswanathan. Proppant Placement in Complex Fracture Geometries: A Computational Fluid Dynamics. Submitted to *Scientific Reports*. (LA-UR-19-29884)

S. Mehana, M. Z., S. Hosseini, T. A. Meckel and H. S. Viswanathan. Modelling the Carbon Dioxide Plume Using Modified-Invasion-Percolation Simulation. Submitted to *Transport in Porous Media*. (LA-UR-19-26910)

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)

Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, D. Derome and J. Carmeliet. Lattice Boltzmann modeling of heat conduction enhancement by colloidal nanoparticle deposition in micro-porous structures. Submitted to *Physical Review E*. (LA-UR-20-22138)

Ryan, D. P., Y. Chen, T. P. Nguyen, P. M. Goodwin, J. W. Carey, Q. Kang, J. H. Werner and H. S. Viswanathan. Go with the flow: 3D tracking and particle transport within complex fractured networks. Submitted to *Lab on A Chip*. (LA-UR-19-30100)

Presentation Slides

Chen, Y. code performance chart. . (LA-UR-19-21169)

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Pore-scale Simulation of Residual Trapping of Supercritical CO2 via Cyclic Injections. Presented at *Interpore 10th Annual Meeting*, New Orleans, Louisiana, United States, 2018-05-14 - 2018-05-17. (LA-UR-18-24118)

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Video Clips of Pore-scale Multiphase Flow Simulations in Porous Media. . (LA-UR-18-24814)

Chen, Y., H. S. Viswanathan and Q. Kang. Images of pore-scale LBM simulations. . (LA-UR-18-30193)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. animations that accompany my AGU poster. Presented at *2019 AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32164)

Kang, Q., Y. Chen and A. J. Valocchi. Final Report of Institutional Computing Project w19_porescale: Figures. . (LA-UR-20-21775)

Ryan, D. P., J. H. Werner, H. S. Viswanathan, P. M. Goodwin, J. W. Carey, T. P. Nguyen, Y. Chen and Q. Kang. Particle Transport in Fractured Networks:3D Tracking for Observing Surface-particle and Fluid-particle Interactions. Presented at *2019 American Geophysical Union Annual Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32522)

Viswanathan, H. S. dfnWorks Applications: Hydraulic Fracturing, Nuclear Waste Disposal and Nuclear Nonproliferation. Presented at *dfnWorks Workshoip*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29441)

Viswanathan, H. S., D. P. Ryan, Y. Chen, Q. Kang, T. P. Nguyen and J. H. Werner. Microfluidics Experiments and Lattice Boltzmann Simulations to Characterize Multi-phase Flow and Particle Transport in Fracture Networks. Presented at

Interpore, Valencia, Spain, 2019-05-06 - 2019-05-10. (LA-UR-19-24072)

Viswanathan, H. S. and J. W. Carey. Mechanistic Approach to Analyzing and Improving Unconventional Hydrocarbon Production. . (LA-UR-19-22101)

Posters

Chen, Y., A. J. Valocchi, Q. Kang and H. S. Viswanathan. Direct Numerical Simulation of Supercritical CO2 Displacing Brine in a Sandstone: the Importance of Inertial Effects. . (LA-UR-19-28527)

Chen, Y., Q. Kang, A. J. Valocchi and H. S. Viswanathan. Inertial Effects during the Process of scCO2 Displacing Brine in a Sandstone. Presented at *2019 AGU fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32161)

Ryan, D. P., J. H. Werner, T. P. Nguyen, Y. Chen, H. S. Viswanathan, Q. Kang and J. W. Carey. 3D Proppant Tracking through Fracture Networks. Presented at *CINT Triannual Review*, Los Alamos, New Mexico, United States, 2019-05-13 - 2019-05-13. (LA-UR-19-24206)

Ryan, D. P., T. P. Nguyen, Q. Kang, J. W. Carey, H. S. Viswanathan and J. H. Werner. 3D Tracking of Proppants through Fractured Microchannel Networks. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28840)

Ryan, D. P., Y. Chen, T. P. Nguyen, Q. Kang, J. W. Carey, P. M. Goodwin, H. S. Viswanathan and J. H. Werner. Particle Transport in Fractured Networks. Presented at *Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28610)

Geophysical Signatures of Changing Water Resources

Carene Larmat
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 Department of Energy Office of Energy Policy and Systems Analysis (EPSA) and Biological and Environmental Research (BER) programs.

Publications

Presentation Slides

Delorey, A. A., H. Goldberg, S. Son, C. N. L. Gammans and E. M. Syracuse. Monitoring Changes in Groundwater Storage with Gravity, Ground Displacement, and Seismic Observations. Presented at *American Geophysical Union*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31458)

Goldberg, H. Determining the cause and nature of anomalous Rayleigh wave H/V ratio measurements in southern California. Presented at *IRIS Virtual Meeting*, Los Alamos, New Mexico, United States, 2018-07-13 - 2018-07-13. (LA-UR-18-26221)

Syracuse, E. M. Seismic signatures of changing water resources. . (LA-UR-18-22629)

Syracuse, E. M., A. A. Delorey, H. Goldberg, J. A. Kintner, C. Larmat, K. Gao and J. Muir. Probing temporal changes in the subsurface using ambient seismic noise (and, life at a national lab). . (LA-UR-20-22005)

Syracuse, E. M., A. A. Delorey, H. Goldberg and J. B. Muir. Probing groundwater using Rayleigh wave ellipticity measurements in southern California. Presented at *American Geophysical Union Fall Meeting*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31586)

Posters

Goldberg, H. Determining the cause and nature of anomalous Rayleigh wave H/V ratio measurements in southern California. Presented at *Los Alamos National Lab Student Symposium*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-26184)

Syracuse, E. M., A. A. Delorey, H. Goldberg and J. B. Muir. Using Ambient-Noise Based Ellipticity and Delay Times to Probe Groundwater Changes in Southern California. Presented at *Seismological Society of America annual meeting*, Seattle, Washington, United States, 2019-04-24 - 2019-04-24. (LA-UR-19-23585)

Syracuse, E. M., A. A. Delorey and J. Muir. Seismic Signatures of Changing Water Resources. Presented at *Seismological Society of America Annual Meeting*, Miami, Florida, United States, 2018-05-15 - 2018-05-17. (LA-UR-18-24137)

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.

Publications

Journal Articles

Janish, M. T., M. M. Schneider, E. F. Holby, A. W. Richards, R. K. Schulze and T. G. Holesinger. Hydride mapping in uranium using MLLS fitting of electron energy-loss spectra. Submitted to *Journal of Metals*. (LA-UR-19-32305)

Presentation Slides

Holby, E. F. w18_uhydride Scientific Highlight. . (LA-UR-19-21896)

Holby, E. F., M. A. Hill, T. G. Holesinger, M. T. Janish, S. K. Lawrence, A. W. Richards, M. M. Schneider, R. K. Schulze and E. L. Tegtmeier. Uranium Hydride Corrosion: Atomistic Modeling. Presented at *DOE Technical Meeting*, Los Alamos, New Mexico, United States, 2019-06-03 - 2019-06-03. (LA-UR-19-24795)

Holesinger, T. G., M. M. Schneider, M. T. Janish, E. F. Holby, E. L. Tegtmeier, R. K. Schulze and A. W. Richards. New Insights into Early Stage Uranium Hydride Growth. Presented at *MS&T 2019*, Portland, Oregon, United States, 2019-09-29 - 2019-10-03. (LA-UR-19-29767)

Holesinger, T. G., M. M. Schneider, M. T. Janish, E. F. Holby, R. K. Schulze, M. A. Hill, E. L. Tegtmeier, S. K. Lawrence and A. W. Richards. Uranium Hydride Corrosion: Microscopy & in situ Experiments. Presented at *DOE Technical Meeting*, Los Alamos, New Mexico, United States, 2019-06-03 - 2019-06-03. (LA-UR-19-24751)

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, M. A. Hill, E. L. Tegtmeier, S. K. Lawrence, R. K. Schulze and A. W. Richards. Early Stage Uranium Hydride Development in Cast U238. Presented at *Presentation to external agency*, Reading, United Kingdom, 2020-02-12 - 2020-02-14. (LA-UR-20-20934)

Schneider, M. M. Electron Microscopy of Hydride Actinides. . (LA-UR-19-21935)

Posters

Holesinger, T. G., M. T. Janish, M. M. Schneider, E. F. Holby, R. K. Schulze, E. L. Tegtmeier and A. W. Richards. Towards Understanding the Atomistic to Mesoscopic Processes in Uranium Hydride Nucleation and Growth. Presented at *Pu Futures - The Science 2018*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28414)

Janish, M. T., M. M. Schneider, T. G. Holesinger, A. W. Richards, E. F. Holby and R. K. Schulze. Mapping Uranium Hydride Corrosion with Electron Energy-Loss Spectroscopy. Presented at *University Workshop on Damage, Shock, and Characterization*, Los Alamos, New Mexico, United States, 2019-07-30 - 2019-08-01. (LA-UR-19-27367)

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

Journal Articles

*Deodato, C. R., S. B. Barlow, B. T. Hovde and R. A. Cattolico. Naked Chrysochromulina (Haptophyta) isolates from lake and river ecosystems: An electron microscopic comparison including new observations on the type species of this taxon. 2019. *Algal Research*. **40**: 101492. (LA-UR-19-20025 DOI: 10.1016/j.algal.2019.101492)

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 reveals - acting effects influencing species-dependent essential genes. 2019. *Genome Research*. **29** (3): 396-406. (LA-UR-19-20026 DOI: 10.1101/gr.232330.117)

Presentation Slides

Hovde, B. Bioenergy Research @ Los Alamos National Lab. . (LA-UR-20-22337)

Posters

Hovde, B. Genome sequencing and analysis of two geographically distinct freshwater isolates of the genus Chrysochromulina: insights into haptophyte evolution. Presented at *The 8th International Conference on Algal Biomass, Biofuels and Bioproducts*, Seattle, Washington, United States, 2018-06-11 - 2018-06-13. (LA-UR-18-24953)

Hovde, B., M. M. A. Baysinger, J. A. Ohan and P. Nath. Generating gel microdroplets using microfluidics. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27823)

Mettler, J. G., T. Britton, S. Negi and B. Hovde. CRISPR-Directed Editing of Photoreceptor Genes to Improve Biomass Accumulation in Microalgae. Presented at *LANL Student Symposium*, Los alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-27135)

Mettler, J. G., T. Britton, S. Negi and B. T. Hovde. CRISPR-Directed Editing of Photoreceptor Genes to Improve Biomass Accumulation in Microalgae. Presented at *Algae Biomass Organization Symposium*, Houston, Texas, United States, 2018-10-14 - 2018-10-17. (LA-UR-18-29318)

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.

Publications

Journal Articles

Albert, J. M., R. S. Selesnick, S. K. Morley, M. G. Henderson and A. C. Kellerman. Calculation of Last Closed Drift Shells for the 2013 GEM Radiation Belt Challenge Events. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-19-30975)

Jaynes, A. N., A. F. Ali, S. R. Elkington, D. M. Malaspina, D. N. Baker, X. Li, S. G. Kanekal, M. G. Henderson, C. A. Kletzing and J. R. Wygant. Fast Diffusion of Ultrarelativistic Electrons in the OuterRadiation Belt: 17 March 2015 Storm Event. Submitted to *Geophysical Research Letters*. (LA-UR-19-30974)

Ripoll, J. F., T. Farges, D. Malaspina, G. S. Cunningham, E. H. Lay, G. Hospdarsky, C. A. Kletzing and J. R. Wygant. Analysis of electric and magnetic lightning-generated wave amplitudes measured by the Van Allen Probes. Submitted to *Geophysical Research Letters*. (LA-UR-19-31568)

Presentation Slides

Cunningham, G. S. Trapped Electrons in the Near-Earth Space Environment: a Golden Age for Radiation-Belt Physics. . (LA-UR-18-30486)

Godinez Vazquez, H. C. and M. G. Henderson. Data Assimilation for the Radiation Belt Environment. Presented at *SIAM Annual Meeting*, Portland, Oregon, United States, 2018-07-09 - 2018-07-13. (LA-UR-18-26293)

Godinez Vazquez, H. C. and M. G. Henderson. Data Assimilation for the Radiation Belt Environment using the Four-Dimensional Variational Method. Presented at *AGU Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32342)

Posters

Godinez Vazquez, H. C. and M. G. Henderson. Estimating Diffusion Coefficients using Variational Methods. Presented at *Geospace Environment Modeling (GEM) 2018 Summer Workshop*, Santa Fe, New Mexico, United States, 2018-06-18 - 2018-06-22. (LA-UR-18-25420)

Godinez Vazquez, H. C. and M. G. Henderson. Variational Data Assimilation for 1-D Radiation Belt Model. Presented at *The Geospace Environment Modeling workshop 2019*, Santa Fe, New Mexico, United States, 2019-06-24 - 2019-06-28. (LA-UR-19-26120)

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.

Publications

Journal Articles

Lasserre, J. B. and T. Weisser. DISTRIBUTIONALLY ROBUST POLYNOMIAL CHANCE-CONSTRAINTS UNDER MIXTURE AMBIGUITY SETS. Submitted to *Mathematical Programming*. (LA-UR-19-29307)

Luchnikov, I., D. M. R. Metivier, H. Ouerdane and M. Chertkov. Super-relaxation of loads ensembles energy consumption in discrete phase space. Submitted to *arxiv, Energy Conversion and Management*. (LA-UR-19-27341)

Marx, S., T. Weisser, D. Henrion and J. B. Lasserre. A moment approach for entropy solutions to nonlinear hyperbolic PDEs. 2019. *Mathematical Control & Related Fields*. (LA-UR-19-21398 DOI: 10.3934/mcrf.2019032)

R. Metivier, D. M., M. D. Vuffray and S. Misra. Efficient Polynomial Chaos Expansion for Uncertainty Quantification in Power Systems. Submitted to *Electric Power Systems Research*. (LA-UR-19-30262)

Roald, L. A., K. Sundar, A. V. Zlotnik, S. Misra and G. Andersson. An Uncertainty Management Framework for Integrated Gas-Electric Energy Systems. Submitted to *Proceedings of the IEEE*. (LA-UR-20-20818)

Conference Papers

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)

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)

Presentation Slides

Marx, S., T. Weisser, D. Henrion and J. B. Lasserre. A moment approach to approximating functional solutions. Presented at *IPAM: Workshop on Operator Theoretic Methods in Dynamic Data Analysis and Control*, Los Angeles, California, United States, 2019-02-11 - 2019-02-11. (LA-UR-19-21339)

Misra, S. Learning for optimization. Presented at *Grid science winter school*, Santa Fe, New Mexico, United States, 2019-01-06 - 2019-01-06. (LA-UR-19-21079)

Weisser, T. Relaxations and Uncertainty Quantification for the Power Grid. . (LA-UR-19-26045)

Weisser, T. Tighter bounds for AC-OPF through rank-one convexification. Presented at *SIAM AG 2019*, Bern, Switzerland, 2019-07-09 - 2019-07-09. (LA-UR-19-26092)

Weisser, T. and B. Legat. MomentOpt.jl. Presented at *JuliaCon 2019*, Baltimore, Maryland, United States, 2019-07-23 - 2019-07-23. (LA-UR-19-27744)

Weisser, T. and B. Legat. MomentOpt.jl. Presented at *ICCOPT 2019*, Berlin, Germany, 2019-08-05 - 2019-08-05. (LA-UR-19-27727)

Weisser, T. and C. J. Coffrin. JuliaMoments/JuMPMoments. Presented at *JuMP-dev Workshop 2019*, Santiago, Chile, 2019-03-12 - 2019-03-12. (LA-UR-19-22390)

Chemistry of a New Oxidation State for the Early Transuranic Elements

Andrew Gaunt
20190091ER

Project Description

Extremely rare and specialized radiological capabilities at Los Alamos National Laboratory will be utilized to synthesize compounds in the unusually low +2 oxidation state to conduct fundamental chemical syntheses of the highly radioactive elements of neptunium, plutonium and americium. Chemical control through oxidation state chemistry is a central tenant of actinide separation processes in the nuclear fuel cycle and waste remediation strategies (energy security) - advancement of such control can only be achieved rationally through elucidation of the electronic structure in actinide compounds and understanding the factors that favor particular oxidation states. This fundamental science will be published in top journals, be internationally recognized as world leading and of direct benefit to Department of Energy Office of Science programs to solve basic research needs in their Heavy Element Chemistry program (the 'f-electron' grand challenge). 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

Journal Articles

*P. Goodwin, C. A., J. Su, T. E. Albrecht-Schmitt, A. V. Blake, E. R. Batista, S. R. Daly, S. Dehnen, W. J. Evans, A. J. Gaunt, S. A. Kozimor, N. Lichtenberger, B. L. Scott and P. Yang. [Am(C Me H)]: An Organometallic Americium Complex. 2019. *Angewandte Chemie International Edition*. **58** (34): 11695-11699. (LA-UR-19-25159 DOI: 10.1002/anie.201905225)

Reports

P. Goodwin, C. A., J. Su, L. M. Stevens, F. D. J. White, M. T. Janicke, I. May, C. J. Windorff, J. M. Sperling, A. N. Gaiser, J. N. Cross, T. E. Albrecht-Schmitt, T. F. Jenkins, E. R. Batista, W. J. Evans, A. J. Gaunt, S. A. Kozimor, B. L. Scott and P. Yang. Bonding and Electronic Structure in a Crystallographically Authenticated Organocalifornium Complex. Unpublished report. (LA-UR-19-32441)

Presentation Slides

P. Goodwin, C. A. Np and Cf(III) Cp organometallic complexes. . (LA-UR-19-20947)

P. Goodwin, C. A. Cyclic voltammetry data (C23) on [Pu(tBuPyNO)4], a Pu(IV) coordination complex with a nitroxide ligand. . (LA-UR-19-21962)

P. Goodwin, C. A. f-element Chemistry: Oxidation States, Bonding, and Electronic Structures. . (LA-UR-19-20861)

Posters

Stevens, L. M., C. A. P. Goodwin, W. J. Evans, S. A. Kozimor and A. J. Gaunt. Probing Electronic Structure of Organometallic Transuranic Complexes. . (LA-UR-19-28587)

Understanding and Predicting Hydrocarbon Behaviors in Nanopores of Tight Reservoirs

Qinjun Kang
20190153ER

Project Description

Energy security and national security are inherently linked. National security can be either strengthened or weakened through energy security. That is why energy security is a central issue of interest to the Laboratory, Department of Energy(DOE)/National Nuclear Security Administration(NNSA), and the nation. This research directly supports DOE/NNSA's energy security/independence goal by addressing the fundamental problems underlying the low recovery rates of tight oil/gas productions. The knowledge and fundamental understanding gained from this research may provide important insights for designing better production strategies to maximize recovery rates from the reservoir matrix, paving the way towards U.S. independence of foreign petroleum resources in the foreseeable future while minimizing the environmental impact. The advanced experimental and modeling capabilities to be developed in this project will also be applicable to other mission-critical areas such as carbon dioxide (CO2) sequestration and enhanced geothermal systems.

Publications

Journal Articles

Bakhshian, S., M. Murakami, S. A. Hosseini and Q. Kang. Scaling of Imbibition Front Dynaimcs in Heterogeneous Porous Media. Submitted to *Geophysical Research Letters*. (LA-UR-20-22139)

Fang, C., Q. Kang and R. Qiao. The Role of Disjoining Pressure and Thermal Activation in the Invasion of Droplets into Nanopores. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-20142)

*Feifei, Q., A. Mazloomi Moqaddam, L. Del Carro, K. Qinjun, T. Brunschwiler, D. Derome and J. Carmeliet. Tricoupled hybrid lattice Boltzmann model for nonisothermal drying of colloidal suspensions in micropore structures. 2019. *Physical Review E*. **99** (5): 053306. (LA-UR-19-22956 DOI: 10.1103/PhysRevE.99.053306)

Gong, Y., M. Z. S. Mehana, I. El-monier and H. S. Viswanathan. Proppant Placement in Complex Fracture Geometries: A Computational Fluid Dynamics. Submitted to *Scientific Reports*. (LA-UR-19-29884)

Lee, S., H. Xu, J. Wempner, H. Xu and J. Wen. Gold nanoparticles in Marcellus Shale. Submitted to *Nature Communications*. (LA-UR-19-26399)

S. Mehana, M. Z., S. Hosseini, T. A. Meckel and H. S. Viswanathan. Modelling the Carbon Dioxide Plume Using Modified-Invasion-Percolation Simulation. Submitted to *Transport in Porous Media*. (LA-UR-19-26910)

S. Mehana, M. Z. and J. Callard. Complex Fracture Depletion Model for Reserves Estimations in Shale. Submitted to *journal of energy resources technology*. (LA-UR-20-21346)

S. Mehana, M. Z. and M. Fahes. The Impact of the Geochemical Interactions on the Fate of Fracturing Fluid and Well Performance in Shale Reservoirs.. Submitted to *Petroleum*. (LA-UR-20-20809)

Mohamed, T., M. Z. S. Mehana and Z. Reza. Coalbed methane Review and Outlook. Submitted to *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*. (LA-UR-20-21924)

Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, D. Derome and J. Carmeliet. Lattice Boltzmann modeling of heat conduction enhancement by colloidal nanoparticle deposition in micro-porous structures. Submitted to *Physical Review E*. (LA-UR-20-22138)

Qin, F., M. Su, J. Zhao, A. Mazloomi Moqaddam, L. Del Carro, T. Brunschwiler, Q. Kang, Y. Song, D. Derome and J. Carmeliet. Design of 3D colloidal nanoparticle deposition in thin micro-porous architectures. Submitted to *ACS Applied Materials & Interfaces*. (LA-UR-19-31518)

Wang, H., L. Chen, Z. Qu, Y. Yin, Q. Kang, B. Yu and W. Q. Tao. Modeling of multi-scale transport phenomena in shale gas production — A critical perspective. Submitted to *Applied Energy*. (LA-UR-19-27980)

*Zhao, B., C. W. MacMinn, B. K. Primkulov, Y. Chen, A. J. Valocchi, J. Zhao, Q. Kang, K. Bruning, J. E. McClure, C. T. Miller, A. Fakhari, D. Bolster, T. Hiller, M. Brinkmann, L. Cueto-Felgueroso, D. A. Cogswell, R. Verma, M. Prodanovic, J. Maes, S. Geiger, M. Vassvik, A. Hansen, E.

Segre, R. Holtzman, Z. Yang, C. Yuan, B. Chareyre and R. Juanes. Comprehensive comparison of pore-scale models for multiphase flow in porous media. 2019. *Proceedings of the National Academy of Sciences*. **116** (28): 13799-13806. (LA-UR-19-21742 DOI: 10.1073/pnas.1901619116)

Zhao, J., F. Qin, D. Derome, Q. Kang and J. Carmeliet. Improved Pore Network Models to Simulate Single-phase Flow in Porous Media by Coupling with Lattice Boltzmann Method. Submitted to *Water Resources Research*. (LA-UR-20-21321)

Zhao, J., Q. Kang, Y. Wang, J. Yao, L. Zhang and Y. Yang. Viscous Dissipation and Apparent Permeability of Gas Flow in Tight Porous Media. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-19-30105)

Presentation Slides

Chen, Y., Q. Kang, H. S. Viswanathan and A. J. Valocchi. Investigation of the inertial effects during the drainage process in a real rock. Presented at *InterPore 11th Annunal Meeting*, Valencia, Spain, 2019-05-06 - 2019-05-10. (LA-UR-19-24097)

Kang, Q. Pore-Scale Direct Numerical Simulation of Transport and Interfacial Phenomena. . (LA-UR-18-29213)

Kang, Q. 2018 Annual Report of Institutional Computing Project w17_porescale: Figures. . (LA-UR-19-21741)

Kang, Q., M. Z. S. Mehana, H. Xu and T. P. Nguyen. Understanding and Predicting Hydrocarbon Behaviors in Nanopores of Tight Reservoirs. Presented at *TAMU visit*, college station, Texas, United States, 2019-11-25 - 2019-11-26. (LA-UR-19-31750)

Nguyen, T. P. Using Methane Isotope Signatures to Evaluate and Improve the Shale Production Curve. Presented at *CSES Symposium*, Los Alamos, New Mexico, United States, 2019-08-15 - 2019-08-15. (LA-UR-19-30282)

Posters

S. Mehana, M. Z., Q. Kang and H. S. Viswanathan. Molecular Modeling of the Fluid Behavior in shale Nanopores. Presented at *Postdoc Research Symposium*, Los alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28653)

Using Solar Energetic Protons to Monitor the Outer Magnetosphere

Steven Morley
20190262ER

Project Description

This project targets understanding and modeling of the outer reaches of Earth's magnetic field, with a specific goal of specifying and predicting the access of solar energetic particles within Earth's magnetic field. This magnetic field plays a critical role in protecting assets such as the International Space Station, satellites, and aircraft from harmful radiation. As this part of Earth's magnetic field is sparsely measured we expect to develop new understanding of how the Sun drives space weather, as well as underpinning a new capability that can improve satellite and aviation safety during space weather events with predictive capabailites.

Publications

Journal Articles

Chakraborty, S. and S. K. Morley. Probabilistic Prediction of Geomagnetic Storms and the Kp index. Submitted to *Journal of Space Weather and Space Climate*. (LA-UR-20-20109)

Chen, Y., S. K. Morley and M. R. Carver. Global Prompt Proton Sensor Network: Monitoring Solar Energetic Protons based on GPS Satellite Constellation. Submitted to *Journal of Geophysical Research: Space Physics*. (LA-UR-19-31569)

Morley, S. K. Challenges in magnetospheric space weather prediction. Submitted to *Space Weather*. (LA-UR-19-26681)

*Qin, M., M. Hudson, B. Kress, R. Selesnick, M. Engel, Z. Li and X. Shen. Investigation of Solar Proton Access Into the Inner Magnetosphere on 11 September 2017. 2019. *Journal of Geophysical Research: Space Physics*. **124** (5): 3402-3409. (LA-UR-18-31475 DOI: 10.1029/2018JA026380)

Reports

Thompson, R. L. and S. K. Morley. Pro-L*: probabilistic hourly L* values, with associated McIlwain Lm, magnetic field intensity B, and Cartesian coordinates for 7 global magnetic field models in the Northern Hemisphere in the period 2006-2016. Unpublished report. (LA-UR-19-29115)

Presentation Slides

Morley, S. K. Statistical Modeling and Machine Learning for Space Physics. Presented at *Coupling, Energetics and Dynamics of Atmospheric Regions (CEDAR) workshop*, Santa Fe, New Mexico, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25471)

Posters

Carver, M. R., Y. Chen and S. K. Morley. The GPS Constellation of Satellites as a Global Proton Sensor Netowrk. Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-20-20580)

Chakraborty, S. and S. K. Morley. Probabilistic Geomagnetic Storm Forecasting Using Machine Learning. Presented at *Coupling, Energetics and Dynamics of Atmospheric Regions (CEDAR) Workshop*, Santa Fe, New Mexico, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25470)

Morley, S. K., M. R. Carver, Y. Chen and A. L. Stricklan. GPS: A Constellation Mission Measuring Solar Energetic Protons and the Electron Radiation Belts. Presented at *American Meteorological Society 100th Annual Meeting*, Boston, Massachusetts, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20317)

Innovating Wildfire Representation in Earth System Models (ESMs)

Alexandra Jonko
20190310ER

Project Description

Changes in local and regional climate will have a significant impact on critical infrastructure and have been recognized as a national security concern, which the Department of Energy is working to address through its Energy Exascale Earth System Model (E3SM) project. Wildland fire is an important climate process which interacts with ecosystems and the atmosphere through two-way feedbacks. However, it is currently represented crudely in Earth System Models - including E3SM -, which neglect the impacts of local topography and vegetation on wildland fire behavior. These shortcomings impede our ability to accurately simulate important interactions between fire and climate remains a challenge, and ultimately limit our ability to make predictions about future climate impacts on ecosystems and critical infrastructure, as well as water, carbon, and energy budgets. Our project proposes to improve the representation of wildland fire activity within Earth System Models and to enable them to accurately capture fire-climate feedbacks. Our novel, multi-scale model-based approach will reduce uncertainty in climate projections, directly supporting decision-making for national security applications related to the environment and infrastructure.

Publications

Journal Articles

Linn, R. R. Quick Study Fluid Dynamics of Wildfire. Submitted to *Physics Today*. (LA-UR-19-30531)

Presentation Slides

Jonko, A. Using Supercomputers to Understand Wildfire Behavior. . (LA-UR-19-20192)

Jonko, A., K. E. Bennett, R. R. Linn, S. Brambilla and D. R. Livingston. Incorporating effects of small-scale topography and vegetation heterogeneity on Wildland fire in Earth System Models. Presented at *AFE Fire Congress*, Tucson, Arizona, United States, 2019-11-18 - 2019-11-22. (LA-UR-19-31623)

Jonko, A., K. Yedinak, R. R. Linn, J. L. Conley, R. Parsons and A. L. Atchley. Sensitivity of modeled fire behavior to small perturbations in initial conditions. Presented at *6th International Wildland Fore Behavior and Fuels Conference*, Albuquerque, New Mexico, United States, 2019-04-29 - 2019-05-02. (LA-UR-19-23934)

Jonko, A., R. R. Linn and K. E. Bennett. Innovating Wildfire Representation in ESMs. Presented at *Meeting with potential collaborators at NCAR*, Boulder, Colorado, United States, 2018-10-17 - 2018-10-18. (LA-UR-18-29850)

Linn, R. R. Institutional Computing Report slide for FIRETEC project. . (LA-UR-19-22597)

Illuminating Plutonium: Spectroelectrochemisty in High Temperature Molten Salts

Benjamin Stein

20190364ER

Project Description

The production of plutonium "pits" for nuclear weapons requires very high-purity (>99.9% pure) plutonium metal. The only current source of this high-purity metal is the electrorefining process, which utilizes a high-temperature (~900C) molten salt bath. While this process produces the necessary purity, the recovery of valuable plutonium needs improvement and the refining time is very long. Little is known about the behavior of plutonium in these extreme environments, making it difficult to suggest rational improvements to the electrorefining process. We will develop a capability designed to monitor the chemistry of plutonium in real time as a function of process changes using a variety of optical and X-ray based techniques. This will give us a more complete understanding of these systems, allowing us to inform our plutonium processing colleagues about potential process improvements.

Publications

Presentation Slides

Stein, B., Z. R. Jones, P. Yang, E. R. Batista, S. K. Schrell, F. Rein Rocha, N. H. Anderson and V. Mocko. Plutonium speciation in molten salts. Presented at *JOWOG 22*, Los Alamos, New Mexico, United States, 2019-07-15 - 2019-07-15. (LA-UR-19-27622)

Biogenic Uranium Isotope Fractionation for Biotechnology

Robert Williams
20190372ER

Project Description

Since the discovery of Uranium (U), it has received a great deal of attention from scientists and governments worldwide, largely due to its fissile properties. The complex biological processes that allow microorganisms to sequester and chemically alter actinides is of great importance for environmental and biosecurity applications. We will assess the practicality of microbial-based or microbial-inspired biotechnology systems for uranium isotope fractionation, by understanding how organisms process the uranium isotopes and favor the formation of insoluble uranium oxide. We will utilize the Laboratory's cross-cutting expertise in biochemistry, microbiology and actinide chemistry to elucidate the mechanism of uranium isotope fractionation that occurs during bioreduction. We will focus on the characterization of the three main aspects of uranyl bioreduction that likely control U isotope fractionation; U adsorption, sequestration, and/or uptake and its subsequent reduction; cellular processes that support the electron transport pathways and enzymatic reduction of uranium; and characterizing/ mapping of the cellular location of U reduction and precipitation. Ultimately, we will evaluate the practicality for biotechnology applications of the mechanistic driver(s) of U fractionation and the processes from the interactions between the cell and soluble U that lead to the accumulation of U mineral precipitates near or within the cell.

Publications

Journal Articles

Jemison, N. E., M. T. Bizjack, T. M. Johnson and J. L. Druhan. 238U/2356 U Ratios Record Reactive Transport Controls on Immobilization Pathways during Bioremediation of a U-contaminated Aquifer. Submitted to *Geochimica et Cosmochimica Acta*. (LA-UR-19-21464)

Jemison, N. E., P. W. Reimus, R. J. Harris, H. Boukhalfa, J. T. Clay and K. Chamberlain. Reduction and potential remediation of U(VI) by dithionite at an in-situ recovery mine: Insights gained by \xce\xb4238U. 2020. *Applied Geochemistry*. 104560. (LA-UR-19-27182 DOI: 10.1016/ j.apgeochem.2020.104560)

Lefebvre, P., V. Noel, K. V. Lau, N. E. Jemison, K. L. Weaver, K. H. Williams and K. Maher. Isotopic Fingerprint of Uranium Accumulation and Redox Cycling in Floodplains of the Upper Colorado River Basin. 2019. *Environmental Science & Technology*. acs.est.8b05593. (LA-UR-19-20457 DOI: 10.1021/acs.est.8b05593)

Presentation Slides

Guardincerri, E. Colloquium at Drexel University about Muon Radiography at the Los Alamos National Laboratory. . (LA-UR-19-20983)

Miner, J. C. Quantifying interactions of biomolecules and cosolvents - or - linking structure to solution. . (LA-UR-19-24546)

Posters

Jemison, N. E., H. Boukhalfa, R. Marti-Arbona, C. M. Yeager and N. Xu. Mechanisms of Uranium Isotope Fractionation. Presented at *Goldschmidt 2019*, Barcelona, Spain, 2019-08-18 - 2019-08-23. (LA-UR-19-27953)

Understanding Glycan Dynamics and Heterogeneity for Effective Human Immunodeficiency Virus (HIV) Vaccine Development

Kshitij Wagh
20190441ER

Project Description

Our long-term goal is to better understand the important role of protein-attached sugars ("glycans") in infectious disease, immunology, cancer, and other biological fields, 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 computational strategies required for realizing our long-term research program, and their application to understanding the role of Human Immunodeficiency Virus (HIV) glycans in successful antibody responses. If successful, this work will directly contribute to the design of effective HIV vaccines designed to elicit broad efficacious antibody responses. Furthermore, our glycan modeling strategies can be applied to different biological fields to extract basic biological data on glycans that are inaccessible to experimental measurement, or are difficult to measure, thereby facilitating high-throughput studies investigating biological importance of glycans. This research directly supports the basic science efforts of the Department of Energy 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/National Nuclear Security Administration such as plant sugars, algal biofuels, etc.

Publications

Presentation Slides

Lopez Bautista, C. A. Capability allows faster screening of HIV Env with native glycan diversity. . (LA-UR-20-21204)

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.

Technical Outcomes

The optical properties and the water uptake by biomass burning were measured over a range of conditions and fuel types to gain fundamental knowledge of processes during their transport. Field observations of large fires were used to test the Laboratory results and develop simplified treatments in models. We used our results to evaluate the first simulations of biomass burning aerosols with DOE's high-resolution Energy Exascale Earth System Model that should enable model evaluation and refinement.

Publications

Journal Articles

Bhandari, J., S. China, K. K. Chandrakar, G. Kinney, W. Cantrell, R. A. Shaw, L. R. Mazzoleni, G. Girotto, N. Sharma, K. Gorkowski, S. Gilardoni, S. Decesari, M. C. Facchini, N. Zanca, G. Pavese, F. Esposito, M. K. Dubey, A. C. Aiken, R. K. Chakrabarty, H. Moosm\xc3\xbcller, T. B. Onasch, R. A. Zaveri, B. V. Scarnato, P. Fialho and C. Mazzoleni. Extensive Soot Compaction by Cloud Processing from Laboratory and Field Observations. 2019. *Scientific Reports*. **9** (1): 11824. (LA-UR-19-28388 DOI: 10.1038/s41598-019-48143-y)

*Girotto, G., S. China, J. Bhandari, K. Gorkowski, B. V. Scarnato, T. Capek, A. Marinoni, D. P. Veghte, G. Kulkarni, A. C. Aiken, M. Dubey and C. Mazzoleni. Fractal-like Tar Ball Aggregates from Wildfire Smoke. 2018. *Environmental Science & Technology Letters*. **5** (6): 360-365. (LA-UR-19-22759 DOI: 10.1021/acs.estlett.8b00229)

*Gomez, S. L., C. M. Carrico, C. Allen, J. Lam, S. Dabli, A. P. Sullivan, A. C. Aiken, T. Rahn, D. Romonosky, P. Chylek, S. Sevanto and M. K. Dubey. Southwestern U.S. Biomass Burning Smoke Hygroscopicity: The Role of Plant Phenology, Chemical Composition, and Combustion Properties. 2018. *Journal of Geophysical Research: Atmospheres*. **123** (10): 5416-5432. (LA-UR-18-20787 DOI: 10.1029/2017JD028162)

*Romonosky, D. E., S. L. Gomez, J. Lam, C. M. Carrico, A. C. Aiken, P. Chylek and M. K. Dubey. Optical Properties of Laboratory and Ambient Biomass Burning Aerosols: Elucidating Black, Brown, and Organic Carbon Components and Mixing Regimes. 2019. *Journal of Geophysical Research: Atmospheres*. **124** (9): 5088-5105. (LA-UR-18-30035 DOI: 10.1029/2018JD029892)

Presentation Slides

Aiken, A. C., M. K. Dubey, A. Zelenyuk, R. Zaveri, J. Shilling and C. Mazzoleni. Absorption Enhancement and Optical Properties – Aging Diesel Emissions with Alpha-Pinene Coatings. Presented at *American Association for Aerosol Research Annual Conference*, Raleigh, North Carolina, United States, 2017-10-16 - 2017-10-16. (LA-UR-17-29470)

Bixler, S. L. Aerosol Hygroscopic Properties from the Combustion of Southwestern U.S. Biomass. Presented at *2017 Student Symposium*, Los Alamos, New Mexico, United States, 2017-08-09 - 2017-08-09. (LA-UR-17-26709)

Dubey, M. K. Smoke-Human-Climate System Science to Safeguard Human Health and Resources in the 21st Century. Presented at *AGU meeting*, New Orleans, Louisiana, United States, 2017-12-12 - 2017-12-15. (LA-UR-17-31164)

Dubey, M. K. Materials Applications in Geos. Presented at *LANL hosted ReACT Workshop*, Provo, Utah, United States, 2018-08-10 - 2018-08-10. (LA-UR-18-27616)

Dubey, M. K., S. L. Bixler, D. Romonosky, J. Lam, C. Carrico and A. C. Aiken. Laboratory Studies of Water Uptake by Biomass Burning Smoke: Role of Fuel Inorganic Content, Combustion Phase and Aging. Presented at *American Geophysical Union Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31095)

Lam, J. T. Aerosol Optical Properties of Biomass Smoke from Southwestern U.S. Fuels. Presented at *2017 Student Symposium*, Los Alamos, New Mexico, United States, 2017-08-09 - 2017-08-09. (LA-UR-17-26708)

Lee, J. E., M. K. Dubey, A. C. Aiken, P. Chylek and C. Carrico. Optical and chemical analysis of absorption enhancement by mixed carbonaceous aerosols in the 2019 Woodbury, AZ fire plume. Presented at *American Geophysical Union Fall Meeting 2019*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32199)

Romonosky, D., C. Carrico, J. T. Lam, M. K. Dubey, A. C. Aiken, P. Chylek and S. Gomez. Optical Properties of Biomass Burning Carbonaceous Aerosol from Controlled Laboratory Burns and Ambient Wildfires. Presented at *International Aerosol Conference*, St. Louis, Missouri, United States, 2018-09-03 - 2018-09-07. (LA-UR-18-28363)

Posters

Aiken, A. C., M. K. Dubey, J. E. Lee, F. Gallo, P. Chylek, C. Carrico, T. Watson and P. Zuidema. Aged Biomass Burning during LASIC: Understanding BC-dominated Absorbing Aerosol. Presented at *2019 Joint ARM User Facility and ASR PI Meeting*, Rockville, Maryland, United States, 2019-06-10 - 2019-06-14. (LA-UR-19-25103)

Dubey, M. K., J. T. Lam, T. Capek, C. Carrico, C. Mazzoleni, A. C. Aiken, T. Onasch and A. Freedman. A Novel Humidity-Controlled Single Scatter Albedo Monitor to Quantify the Effects of Water on Light Absorption by Black and Brown Carbon. Presented at *AGU Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-09 - 2018-12-14. (LA-UR-18-31294)

Dubey, M. K., J. T. Lam, T. Capek, C. Carrico, C. Mazzoleni, A. C. Aiken, T. Onasch and A. Freedman. A Novel Humidity-Controlled Single Scatter Albedo Monitor to Quantify the Effects of Water on Light Absorption by Black and Brown Carbon. Presented at *ARM/ASR Science Team Meeting*, Bethesda, Maryland, United States, 2019-06-10 - 2019-06-14. (LA-UR-19-25202)

Gulick, S., J. M. Karacaoglu, C. Carrico, J. E. Lee, A. C. Aiken and M. K. Dubey. Biomass Combustion Aerosols and Their Surrogates: Characterizing Key Optical Properties Using Advanced Techniques. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26995)

Romonosky, D., S. Gomez, J. T. Lam, C. Carrico, A. C. Aiken, P. Chylek and M. K. Dubey. Optical Properties of Biomass Burning Carbonaceous Aerosol from Controlled Laboratory Burns and Ambient Wildfires. Presented at *LANL Post-Doc Symposium*, Los Alamos, New Mexico, United States, 2018-08-28 - 2018-08-28. (LA-UR-18-28064)

Schlosser, J. S., D. Romonosky, J. T. Lam, C. Carrico, W. Tang, A. Arellano, A. C. Aiken, A. Sarooshian and M. K. Dubey. Predicting the Optical Absorption Properties of Biomass Burning using Absorption Angstrom Exponent (AAE). Presented at *AGU Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31354)

Mapping Cotranscriptional Assembly of the Small 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 staphylococcos aureus (MRSA), and provide defense against bio-threats such as anthrax and plague.

Technical Outcomes

Outcomes of this project include: (i) development of high-throughput methods to monitor the transcription of single RNA fragments under conditions similar to those that would be encountered in vivo; (ii) development of high-throughput methods to monitor cotranscriptional folding of single RNA fragments using SHAPE (selective 2'-hydroxyl acylation by primer extension) probing; and (iii) development of computational models of ribosomal RNA folding.

Publications

Posters

Nemashkalo, A., S. P. Hennelly, Y. A. Kunde, K. Y. Sanbonmatsu, S. R. Starkenburg and P. M. Goodwin. Watching co-transcriptional biomolecular machine assembly one molecule at a time. Presented at *Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28273)

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.

Technical Outcomes

We developed a new family of spectral-based numerical methods that can be effectively used to solve high-dimensional Boltzmann-like/kinetics equations by combining sparsification techniques and the dynamical adaptation of spectral modes. Our proof of concept is the MPI/OpenMP parallel implementation code SpectralPlasmaSolver (SPS) that allowed us to study turbulence phenomena in the solar wind.

Publications

Journal Articles

*Fatone, L., D. Funaro and G. Manzini. Arbitrary-order time-accurate semi-Lagrangian spectral approximations of the Vlasov–Poisson system. 2019. *Journal of Computational Physics*. **384**: 349-375. (LA-UR-18-22660 DOI: 10.1016/j.jcp.2019.01.020)

*Manzini, G., D. Funaro and G. L. Delzanno. Convergence of Spectral Discretizations of the Vlasov--Poisson System. 2017. *SIAM Journal on Numerical Analysis*. **55** (5): 2312-2335. (LA-UR-16-22601 DOI: 10.1137/16M1076848)

Manzini, G., L. Fatone and D. Funaro. A Semi-Lagrangian Spectral Method for the Vlasov–Poisson System Based on Fourier, Legendre and Hermite Polynomials. 2019. *Communications on Applied Mathematics and Computation*. **1** (3): 333-360. (LA-UR-18-25332 DOI: 10.1007/s42967-019-00027-8)

*Roytershteyn, V., S. Boldyrev, G. L. Delzanno, C. H. K. Chen, D. Gro\xc5\xa1elj and N. F. Loureiro. Numerical Study of Inertial Kinetic-Alfv\xc3\xa9n Turbulence. 2019. *The Astrophysical Journal*. **870** (2): 103. (LA-UR-18-28710 DOI: 10.3847/1538-4357/aaf288)

Roytershteyn, V. and G. L. Delzanno. Spectral Approach to Plasma Kinetic Simulations Based on Hermite Decomposition in the Velocity Space. 2018. *Frontiers in Astronomy and Space Sciences*. **5**. (LA-UR-18-23813 DOI: 10.3389/fspas.2018.00027)

Conference Papers

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)

Reports

Delzanno, G. L., G. Manzini, C. Pagliantini and S. Markidis. Physics-based adaptivity of a spectral method for the Vlasov-Poisson equations based on the asymmetrically-weighted Hermite expansion in velocity space. Unpublished report. (LA-UR-19-29686)

Koshkarov, O., G. Manzini, C. Pagliantini, G. L. Delzanno and V. Roytershteyn. Conservation properties of the multi-dimensional Runge-Kutta Hermite-dG method for the Vlasov-Maxwell equations. Unpublished report. (LA-UR-19-29579)

Koshkarov, O., G. Manzini, G. L. Delzanno, C. Pagliantini and V. Roytershteyn. The multi-dimensional Hermite-discontinuous Galerkin method for the Vlasov-Maxwell equations. Unpublished report. (LA-UR-19-29578)

Manzini, G., G. L. Delzanno and D. Funaro. Stability and conservation properties of Hermite-based approximations of the Vlasov-Poisson system. Unpublished report. (LA-UR-19-29687)

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., O. Koshkarov and G. L. Delzanno. The Legendre-discontinuous Galerkin discretization of the 1D-1V Vlasov-Poisson system. Unpublished report. (LA-UR-19-29576)

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)

Presentation Slides

Delzanno, G. L. Spectral methods for multiscale plasma-physics simulations. . (LA-UR-17-23328)

Delzanno, G. L. Spectral Methods for Multiscale Plasma Physics Simulations. Presented at *VII International Conference on Coupled Problems in Science and Engineering*, Rhodes Island, Greece, 2017-06-12 - 2017-06-12. (LA-UR-17-25062)

Delzanno, G. L., V. Roytershteyn, O. Koshkarov, G. Manzini and C. Pagliantini. A framework for microscopic/macroscopic simulations of magnetized plasmas. Presented at *URSI*, Boulder, Colorado, United States, 2019-01-09 - 2019-01-09. (LA-UR-19-20093)

Koshkarov, O., G. L. Delzanno, V. Roytershteyn and G. Manzini. A framework for microscopic/macroscopic simulations of magnetized plasmas. Presented at *ASTRONUM-2018, the 13th International Conference on Numerical Modeling of Space Plasma Flows*, Panama City Beach, Florida, United States, 2018-06-25 - 2018-06-29. (LA-UR-18-23538)

Koshkarov, O., V. Roytershteyn and G. L. Delzanno. Reversing reconnection with spectral plasma solver. . (LA-UR-19-27871)

Koshkarov, O., V. S. Roytershteyn, G. L. Delzanno and G. Manzini. Spectral/Discontinuous Galerkin approach to fully kinetic simulations of plasma turbulence with reduced velocity space. Presented at *NCSA Blue Water Symposium for Petascale Science and Beyond*, Sunriver, Oregon, United States, 2019-06-03 - 2019-06-03. (LA-UR-19-25179)

Posters

Weichman, K. J., V. Roytershteyn, G. L. Delzanno and N. Pogorelov. Instabilities and Turbulence Generation by Pick-Up Ion Distributions In the Outer Heliosheath. Presented at *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31090)

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 Department of Energy(DOE)/National Nuclear Security Administration(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.

Technical Outcomes

A new theoretical capability to treat excited electronic states was developed and applied to several ultracold reactions. The control of ultracold molecular collisions via quantum interference was explicitly demonstrated for the hydrogen exchange reactions. Signatures of chaos were discovered in the K + KRb reaction and quantum interference effects in photodissociation were uncovered. A new quantum annealer eigensolver algorithm was developed and applied to compute molecular vibrational spectra on Los Alamos' D-Wave machine.

Publications

Journal Articles

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*. **8**: 15897. (LA-UR-17-20822 DOI: 10.1038/ncomms15897)

*E. Croft, J. F., J. Hazra, N. Balakrishnan and B. K. Kendrick. Symmetry and the geometric phase in ultracold hydrogen-exchange reactions. 2017. *The Journal of Chemical Physics*. **147** (7): 74302. (LA-UR-17-23377 DOI: 10.1063/1.4998226)

*E. Croft, J. F., N. Balakrishnan and B. K. Kendrick. Long-lived complexes and signatures of chaos in ultracold K2+Rb collisions. 2017. *Physical Review A*. **96** (6): 062707. (LA-UR-17-29347 DOI: 10.1103/PhysRevA.96.062707)

*Kendrick, B. K. Non-adiabatic quantum reactive scattering in hyperspherical coordinates. 2018. *The Journal of Chemical Physics*. **148** (4): 044116. (LA-UR-17-30356 DOI: 10.1063/1.5014989)

*Kendrick, B. K. Non-adiabatic quantum reactive scattering calculations for the ultracold hydrogen exchange reaction: H\xe2\x80\xaf+\xe2\x80\xafH2( ) H\xe2\x80\xaf+ \xe2\x80\xafH2( ). 2018. *Chemical Physics*. **515**: 387-399. (LA-UR-18-23192 DOI: 10.1016/j.chemphys.2018.07.001)

Kendrick, B. K. Non-adiabatic ultracold quantum reactive scattering of hydrogen with vibrationally excited HD(v=5-9). Submitted to *The Journal of Physical Chemistry*. (LA-UR-19-27618)

*Kendrick, B. K. and N. Balakrishnan. Geometric Phase Effects in Ultracold Chemical Reactions. 2019. *Atoms*. **7** (3): 65. (LA-UR-19-23245 DOI: 10.3390/atoms7030065)

*Teplukhin, A., B. K. Kendrick and D. Babikov. Calculation of Molecular Vibrational Spectra on a Quantum Annealer. 2019. *Journal of Chemical Theory and Computation*. **15** (8): 4555-4563. (LA-UR-18-29586 DOI: 10.1021/acs.jctc.9b00402)

*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*. **13** (5): 1902-1910. (LA-UR-17-20533 DOI: 10.1021/acs.jctc.7b00124)

Posters

Kendrick, B. K., M. Li, H. Li, S. Kotochigova, J. Croft and N. Balakrishnan. Non-adiabatic quantum dynamics of the ultracold Li+LiNa -> Li2 + Na chemical reaction. Presented at *International Conference on Photonic, Electronic, and Atomic Collisions*, Deauville, France, 2019-07-23 - 2019-07-23. (LA-UR-19-26866)

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 Department of Defense and Department of Energy.

Technical Outcomes

This project has designed, built and tested multimodal laser-scanning nonlinear-optical microscopy system for imaging biological and non-biological samples. We demonstrated imaging of in-sample quasi-DC electric field distributions using molecular vibrations and nonlinear frequency mixing in the sample. We developed novel nonlinear imaging contrast mechanisms based on third-order sum-frequency generation and four-wave mixing involving resonant molecular excitations. The project also established neuronal cell culturing protocols for cell growth and subsequent imaging using our developed imaging methods.

Publications

Conference Papers

Perillo, E., M. E. Phipps, J. S. Martinez and A. V. Efimov. Electric \xef\xac\x81eld imaging with vibrationally-resonant electric \xef\xac\x81eld-induced sum-frequency generation. Presented at *SPIE Photonics West*. (San Francisco, California, United States, 2020-02-01 - 2020-02-01). (LA-UR-20-20351)

Perillo, E., M. E. Phipps, J. S. martinez and A. V. Efimov. Femtosecond third-order sum frequency and four-wave mixing imaging. Presented at *SPIE Photonics West*. (San Francisco, California, United States, 2020-02-01 - 2020-02-01). (LA-UR-20-20350)

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 Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions in warfighter and civilian protection from biological attacks, as well as helping with national needs in preventing the spread of infectious disease.

Technical Outcomes

This project developed a simple microfluidics system capable of performing serial manipulations on single cells. It explored the response of human immune cells to the earliest stages of bacterial infection and engaged leading external experts in helping to understand immune gene response.

Publications

Journal Articles

Catanach, T., H. Vo, B. Munsky and J. H. Werner. Bayesian Inference of stochastic reaction networks using multifidelity sequentil tempered markov chain monte carlo. Submitted to *International Journal for Uncertainty Quantification*. (LA-UR-19-32525)

*Kalb, D. M., S. H. Adikari, E. Hong-Geller and J. H. Werner. Single-cell correlations of mRNA and protein content in a human monocytic cell line after LPS stimulation. 2019. *PLOS ONE*. **14** (4): e0215602. (LA-UR-19-20143 DOI: 10.1371/journal.pone.0215602)

Werner, J. H., S. N. Micheva-Viteva, E. Hong-Geller, J. Gao and S. H. Adikari. Increased Mortality in Mice following Immunoprophylaxis Therapy with High Dosage of Nicotinamide in Burkholderia Persistent Infections. Submitted to *Infection and Immunity*. (LA-UR-19-29708)

Books/Chapters

Werner, J. H., D. M. Kalb, P. M. Goodwin, D. P. Morales and D. P. Ryan. Three-Dimensional Single-Molecule Tracking in Live Cells. (LA-UR-19-29186)

Presentation Slides

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Probing Ionosphere and Magnetosphere Connections with an Electron Gun

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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.

Technical Outcomes

This project has been successful and provides the first experimental demonstration of the physics of ion emission from a plasma contactor. This is a critical step to use the contactor technology to mitigate spacecraft charging induced by high-power electron beams in low-density environments in space. This project might open up a new era of active experiments in space based on electron-beam technology.

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Reports

Dors, E. E., E. MacDonald, L. Kepko, J. E. Borovsky, G. D. Reeves, G. L. Delzanno, M. F. Thomsen, E. R. Sanchez, M. G. Henderson, D. C. Nguyen, M. Argall, H. Vaith, B. E. Gilchrist, E. Donovan, E. Spanswick, R. A. Marshall, B. A. Larsen, J. Dorelli, J. Neilson, B. E. Carlsten, G. Miars and R. H. W. Friedel. CONNection EXplorer (CONNEX): An Active Space Experiment to Probe Magnetosphere-Ionosphere Coupling. Unpublished report. (LA-UR-19-21988)

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Delzanno, G. L. Plane geometry: Introduction. . (LA-UR-17-20613)

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Delzanno, G. L., B. E. Wohlberg, H. C. Godinez Vazquez, D. Svyatsky, K. Yakymenko and M. Denton. Spacecraft charging of the Van Allen Probes: theory and simulations. Presented at *American Geophysical Union Fall meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-11. (LA-UR-17-31118)

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Delzanno, G. L. and V. Roytershteyn. On the coupling between a magnetized plasma and an electron beam. Presented at *Advancing Plasma Physics from the Sun to the Earth*, Breckenridge, Colorado, United States, 2017-05-22 - 2017-05-22. (LA-UR-17-24322)

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Aromatic Actinide Metallacycles

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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.

Technical Outcomes

The first 2-metallabiphenylene systems were synthesized through thorium- and uranium-mediated reductive coupling of 1,2-bis(phenylethynyl)benzene to simultaneously fabricate an antiaromatic cyclobutadiene ring fused between an aromatic benzene ring and a metallacyclopentadiene. This represents new chemistry for the periodic table and provides a powerful C–C coupling reaction enabled by actinide 5f-orbitals to form antiaromatic cyclobutadiene rings. The uranium complex revealed delocalization of the 5f-electrons, suggestive appreciable covalency and multiple bond character in the uranium-carbon bonds.

Publications

Journal Articles

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Posters

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ERIS: Electrolysis Rocket Ignition System

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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.

Technical Outcomes

Solid rockets provide high thrust and good performance while being relatively simple, safe, scalable, low cost, and compatible with long storage durations. However, solid rockets are traditionally limited to a single burn per motor. ERIS developed a re-usable non-pyrotechnic rocket ignition system and a novel extinguishing aerospike nozzle. These combined with Los Alamos' existing segmented solid fuel solid oxidizer propellant enabled development and demonstration of a single solid rocket motor capable of multiple independent impulses.

Publications

Presentation Slides

Dallmann, N., K. Chintam, M. P. Coblentz, D. K. Hemsing, J. P. Lichthardt, I. A. J. Shelburne, B. C. Tappan and M. S. Wilson. ERIS: Enabling Small Satellites with Solid Rockets Repeatable electrolytic ignition and decompressive extinguishing. Presented at *SmallSat*, Logan, Utah, United States, 2018-08-06 - 2018-08-09. (LA-UR-18-27450)

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Posters

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J. Shelburne, I. A., N. Dallmann, B. C. Tappan, J. P. Lichthardt, M. S. Wilson, K. Chintam and D. K. Hemsing. ERIS: A Safe Segmented Solid-Fuel Solid-Oxidizer Propulsion System with Electrolyzer Ignition System. Presented at *Small Sat 2019*, Logan, Utah, United States, 2019-08-07 - 2019-08-07. (LA-UR-19-27907)

Constrained Minimization Approach for Spacecraft-charging Calculations

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Project Description

Spacecraft (satellite) charging is a major application of space-weather research since charging can lead to spacecraft anomalies. The latter can range from inconsequential to catastrophic (damage to sensitive electronics and total loss of the spacecraft). Unfortunately, current direct spacecraft-charging calculations are extremely limited due to unknown space environment and material properties (material decay during the spacecraft mission). To address this problem, we will develop for the first time an inverse approach to use available spacecraft-charging data to infer important information regarding the space environment around the spacecraft and material degradation. Our long-term goals are to (1) learn critical information about the space environment (in particular the low-energy particles, a key component of space weather research), (2) understand how materials age in space (with important national-security applications), and (3) assist operators in the resolution of spacecraft anomalies.

Technical Outcomes

In this study, we initially applied an optimization method to a simplified model of spacecraft charging. The results show convergence and the ability of the method to recover the correct solution in a series of synthetic observation experiments. The results of a synthetic experiment where optimization is coupled to a first-principle spacecraft-charging code show slow convergence and the need for more sophisticated optimization techniques to demonstrate the feasibility of the technique in this case.

Publications

Presentation Slides

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Diagnosing Near-Future Changes in Arctic Sea Ice and Ocean Conditions

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20190608ER

Project Description

Arctic warming is affecting US national interests in the Arctic, including defense operations, resource management, trade routes, and energy infrastructure. Transitions occurring in Arctic sea ice cover are unprecedented in the last 1450 years, and expanding Arctic Ocean sovereign claims complicate the US response to sea ice and ocean hydrographic changes, which affect surface and submarine operations by the US, allies and potential adversaries. Quantifying spatial and temporal distributions of future Arctic conditions and seasonal sea ice coverage is necessary to enhance the US national security and economic posture in the Arctic. With a long history of Arctic research, Los Alamos has expertise in ocean, sea-ice, and atmospheric physics and uncertainty quantification, global and regional modeling, and a wealth of Earth system simulations available for analysis. The goal of this project is to use those simulations to characterize physical properties and uncertainties in the Arctic relevant to ocean acoustics, hazardous weather conditions, and navigable shipping corridors. In addition to producing a peer-reviewed publication describing our results, we will assess the quality of Department of Energy (DOE) simulations for national security use. In addition, this research will provide a baseline to articulate future model development needs for DOE Office of Science.

Technical Outcomes

We apply novel statistical techniques to simultaneously characterize multiple physical properties and uncertainties relevant for Arctic shipping, to understand the likelihood of encountering high wind and low ice conditions along potential transportation routes through the Arctic Ocean. We find that the Arctic system is highly variable, but its large-scale patterns are captured by models including DOE's new modeling system (E3SM). An initialization procedure that increases predictability could be beneficial for E3SM.

Publications

Reports

Hunke, E. C., A. F. Roberts, G. D'Angelo, T. Verma, M. Chen, J. B. Dann, J. R. Urrego Blanco, C. J. Wilson, N. M. Urban and M. E. Maltrud. LDRD 20190608ER: DIAGNOSING NEAR-FUTURE CHANGES IN ARCTIC SEA ICE AND OCEAN CONDITIONS. Unpublished report. (LA-UR-19-29886)

Posters

Hunke, E. C., A. F. Roberts, T. Verma, C. J. Wilson, J. B. Dann, J. R. Urrego Blanco, G. D'Angelo, N. M. Urban and M. E. Maltrud. Diagnosing Near-Future Changes in Arctic Sea Ice and Ocean Conditions. Presented at *8th Symposium on the Impacts of an Ice-Diminishing Arctic on Naval and Maritime Operations*, Washington, District Of Columbia, United States, 2019-07-17 - 2019-07-18. (LA-UR-19-26603)

Neutron Radiography for the Determination of Molten Chloride Viscosity, Density, and Homogeneity

Jay Jackson
20190633ER

Project Description

The technical goal of this project is to demonstrate that dynamic neutron radiography can be used to accurately measure thermophysical properties of actinide bearing molten salt solutions. Achievement of this goal will advance the state of the art by providing high fidelity results where little or no data is reported. This research will further the Nuclear Energy (NE) portfolio of the laboratory. However, the benefits of developing this technology and expertise extend beyond NE. In Nuclear Security, results from this proposal will provide foundational knowledge to enable advancements in both nonproliferation and safeguards. Additionally, molten salt technology is critical to providing both plutonium and uranium metal for defense programs. Therefore, advancements in this area will comprise a major contribution towards the 30+ pits per year manufacturing mission at Los Alamos National Laboratory, and contribute to the uranium pyrochemical process development activities at Y-12.

Technical Outcomes

A prototype viscosity test apparatus was designed, built, and tested in a neutron beamline at the Los Alamos Neutron Science Center. Benchmarking measurements of the density and viscosity of a well-characterized, inert fluid were in close agreement with published data. The density as a function of temperature of UCl_3, NaCl+70wt%UCl_3, and NaCl+16.5wt%UCl_3 was measured from melt point to 1150 °C. The viscosity of NaCl+16.5wt%UCl_3 was measured at 825 °C in an inert (argon) environment.

Publications

Reports

Vogel, S. C., A. M. Long, E. B. Watkins and E. N. Caspi. Summary report for “Neutron Phase Contrast Imaging for <1micrometer Feature Detection in Bulk Materials”. Unpublished report. (LA-UR-19-30103)

Presentation Slides

Jackson, J. M. Pyrochemical Processing of Actinides: Uranium and Plutonium Purification. Presented at *LANL Nuclear Forensics Workshop*, Los Alamos, New Mexico, United States, 2020-02-05 - 2020-02-07. (LA-UR-20-21332)

Jackson, J. M., M. J. Monreal, S. S. Parker, A. M. Long, S. C. Vogel and B. Winkler. Neutron Radiography for the Determination of Molten Chloride Viscosity, Density, and Homogeneity. Presented at *2019 AIChE*, Orlando, Florida, United States, 2019-11-10 - 2019-11-15. (LA-UR-19-31334)

Jackson, J. M. and M. J. Monreal. Preparation and Characterization of Molten Salt Systems. Presented at *TerraPower Site Visit*, Seattle, Washington, United States, 2019-08-19 - 2019-08-21. (LA-UR-19-28236)

Stochastic Viral Dynamic Models for Rational Design of Therapeutics to Achieve a Functional Human Immunodeficiency Virus Cure

Ruian Ke
20190634ER

Project Description

We propose to develop novel stochastic models that integrate HIV infection dynamics and the immune response to aid the rational design of immuno-therapeutics and clinical trials to achieve a functional HIV cure, i.e. HIV remission in the absence of treatment – an outcome that can save millions of lives. This work will address the national security challenge by providing a predictive model of the interactions between virus infections and the immune response that can be used for developing effective therapeutic interventions, thus preparing us for virus outbreaks such as HIV and other viruses. We will employ a large deviation theory to analyze rare events (i.e. viral rebound) from the stochastic model and derive probability distributions of the mean HIV remission time. We will fit the model to clinical data. The expected outcome of the work will be to provide a quantitative understanding of the role of the immune system on suppressing virus infection during HIV remission, a critical knowledge needed for achieving a functional cure. This work will serve a foundation for projects involving predicting/quantifying the risk of rare events from data, for example in areas such as epidemics, drug resistance and disease prediction from electronic medical records.

Technical Outcomes

We developed mathematical models that integrate HIV dynamics and the immune response to aid the design of immuno-therapeutics to achieve a functional HIV cure. The work strengthened Los Alamos National Laboratory's world-leading role in viral dynamics modeling, enhances Los Alamos National Laboratory's capability in ‘big data analytics’.

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.

Publications

Journal Articles

Garanaik, A., R. Robey, L. Van Roekel and Q. Li. A Mass Flux Vertical Mixing Parameterization for the Ocean Surface Boundary Layer. Submitted to *Journal of Advances in Modeling Earth Systems*. (LA-UR-19-31170)

Li, Q. and L. Van Roekel. Towards Multiscale Modeling of Ocean Surface Turbulent Mixing Using Coupled MPAS-Ocean and PALM. Submitted to *Geoscientific Model Development*. (LA-UR-20-20427)

Posters

Li, Q. and L. Van Roekel. Towards Multiscale Modeling of Ocean Surface Turbulent Mixing Using Coupled MPAS-Ocean and PALM. Presented at *Ocean Sciences Meeting*, San Diego, California, United States, 2020-02-16 - 2020-02-21. (LA-UR-20-21454)

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 tests in an evolving epidemic.

Publications

Journal Articles

*Bulla, I., I. H. Spickanll, D. Gromov and E. O. Romero-Severson. Sensitivity of joint contagiousness and susceptibility-based dynamic optimal control strategies for HIV prevention. 2018. *PLOS ONE*. **13** (10). (LA-UR-18-30123 DOI: 10.1371/journal.pone.0204741)

Ezeonwumellu, I., I. Bartolo, F. Martin, A. Abecasis, T. Campos, E. Romero-Severson, T. K. Leitner and N. Taveira. Accidental father-to-son HIV-1 transmission during the seroconversion period. Submitted to *AIDS Research and Human Retroviruses*. (LA-UR-19-25850)

Giardina, F., E. Romero-Severson, M. Axelsson, V. Svedhem, T. K. Leitner, T. Britton and J. Albert. Getting more from heterogeneous HIV-1 surveillance data in a high immigration country: estimation of incidence and undiagnosed population size using multiple biomarkers. 2019. *International Journal of Epidemiology*. (LA-UR-19-25855 DOI: 10.1093/ije/dyz100)

*Goyal, A. and E. O. Romero-Severson. Screening for hepatitis D and PEG-Interferon over Tenofovir enhance general hepatitis control efforts in Brazil. 2018. *PLOS ONE*. **13** (9). (LA-UR-18-28686 DOI: 10.1371/journal.pone.0203831)

Gromov, D., I. Bulla, S. Serea and E. Romero-Severson. Numerical optimal control for HIV prevention with dynamic budget allocation.. Submitted to *Mathematical Medicine and Biology: A Journal of the IMA*. (LA-UR-19-30214)

*Gromov, D., I. Bulla and E. O. Romero-Severson. Systematic evaluation of the population-level effects of alternative treatment strategies on the basic reproduction number. 2019. *Journal of Theoretical Biology*. **462**: 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.. Submitted to *Nature Microbiology*. (LA-UR-19-30216)

*Leitner, T. and E. Romero-Severson. Phylogenetic patterns recover known HIV epidemiological relationships and reveal common transmission of multiple variants. 2018. *Nature Microbiology*. **3** (9): 983-988. (LA-UR-18-28043 DOI: 10.1038/s41564-018-0204-9)

Romero-Severson, E., F. Giardina, T. K. Leitner, M. Axelsson, V. Svedhem and J. Albert. Getting more from heterogeneous HIV-1 surveillance data in a high immigration country: estimation of incidence and undiagnosed population size using multiple biomarkers. 2019. *International Journal of Epidemiology*. **48** (6): 1795-1803. (LA-UR-19-30213 DOI: 10.1093/ije/dyz100)

Romero-Severson, E., R. M. Ribeiro and M. Castro. Noise Is Not Error: Detecting Parametric Heterogeneity Between Epidemiologic Time Series. Submitted to *Frontiers in Microbiology*. (LA-UR-19-30215)

*Song, H., E. E. Giorgi, V. V. Ganusov, F. Cai, G. Athreya, H. Yoon, O. Carja, B. Hora, P. Hraber, E. Romero-Severson, C. Jiang, X. Li, S. Wang, H. Li, J. F. Salazar-Gonzalez, M. G. Salazar, N. Goonetilleke, B. F. Keele, D. C. Montefiori, M. S. Cohen, G. M. Shaw, B. H. Hahn, A. J. McMichael, B. F. Haynes, B. Korber, T. Bhattacharya and F. Gao. Tracking HIV-1 recombination to resolve its contribution to HIV-1 evolution in natural infection. 2018. *Nature Communications*. **9** (1): 1928. (LA-UR-19-30217 DOI: 10.1038/s41467-018-04217-5)

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

Journal Articles

Bennett, K. E., J. Cherry, B. Balk and S. Lindsey. Using MODIS estimates of fractional snow cover area to improve streamflow forecasts in interior Alaska. 2019. *Hydrology and Earth System Sciences*. **23** (5): 2439-2459. (LA-UR-18-21603 DOI: 10.5194/hess-23-2439-2019)

Bennett, K. E., V. C. Tidwell, D. Llewellyn, S. Behery, L. Barrett, M. Stansbury and R. S. Middleton. Threats to a Colorado river provisioning basin under coupled future climate and societal scenarios. 2019. *Environmental Research Communications*. **1** (9): 95001. (LA-UR-18-30685 DOI: 10.1088/2515-7620/ab4028)

Presentation Slides

Hornbein, B. Infrastructure Capabilities. . (LA-UR-20-21360)

Illuminating the Subsurface with Nonlinear Behavior

Andrew Delorey
20190552ECR

Project Description

The country's energy and environmental security depends on effective use of the subsurface because most of our energy comes from the subsurface and most of our waste material such as nuclear, brine (produced during oil and gas extraction) and CO2, is or will be stored in the subsurface. Despite this importance, we have very little timely information on subsurface conditions that affect the performance of these systems while avoiding hazards such as induced earthquakes and leakage of waste materials. Fractures at all scales are important to the performance of subsurface systems because they form the pathways for fluid migration and because their coalescence leads to earthquakes and containment failures. We are developing a new way to measure and monitor fractures in the subsurface using background seismic noise. As seismic waves travel through fractured materials, their travel times are perturbed by how weak or strong the contacts are across the fractures. Weak fracture contacts typically indicate that permeability is increasing and decreasing material strength, while stronger contacts typically indicate decreasing permeability and increasing material strength. These relationships have been observed in laboratory samples of rocks. Observing these relationships in the Earth will substantially contribute to our effective use of the subsurface.

Publications

Presentation Slides

Delorey, A. A. Nonlinear Elastic Behavior from Laboratory to Earth Scale. . (LA-UR-19-31933)

Accurate Model for Predicting Mosquito Population Response to Weather and Water Management

Carrie Manore
20190581ECR

Project Description

Food security, health, and political stability are linked to coupled natural, climate, and human-engineered systems. This project will focus on mosquito-borne diseases that cause millions of deaths and hundreds of millions of illnesses globally every year. Accurately modeling mosquito populations and how they respond to weather, water management, and interventions is critical to quantifying risk, controlling outbreaks, and prevention of future outbreaks. Also, the United States has seen a 300% increase in cases of diseases spread by mosquitoes and ticks in the past decade. Since local and national government organizations are driven by minimizing risk and optimizing control, providing accurate mosquito forecasts will provide critical planning information. This project will develop an accurate model for predicting mosquito populations within-season using weather, water management, and demographic information. Models that couple water management and climate with mosquito habitat and populations will be critical to developing models coupling climate, weather, and mosquito dynamics to forecast mosquito-borne diseases, which are important to warfighter health, and to U.S. and global public health, with the potential to revolutionize prediction and planning for vector-borne disease risk now and in the future.

Publications

Journal Articles

Manore, C. A., K. C. Kempfert, K. Martinez, A. S. Siraj, J. R. Conrad, L. A. Castro, D. A. Osthus, E. N. A. Generous, N. K. Parikh, G. Fairchild, A. Ziemann and S. Y. Del Valle. Heterogeneous Data Fusion of Time Series to Nowcast Dengue at the State Level in Brazil. Submitted to *ArXiV*. (LA-UR-20-21471)

Manore, C. A., S. Y. Del Valle, E. N. A. Generous, K. Martinez, N. K. Parikh, D. A. Osthus and D. A. Romero-Alvarez. Google Health Trends performance to reflect dengue incidence in Brazilian states. Submitted to *BMC Infectious Diseases*. (LA-UR-19-31066)

Shutt, D. A., D. Goodsman, Z. J. L. Hemez, J. R. Conrad, C. Xu, D. A. Osthus, C. Russell, J. M. Hyman and C. A. Manore. A Process-Based Model with Temperature and Water Data Improve Predictions of Daily Mosquito Density. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-20732)

Presentation Slides

Fenimore, P. W., J. R. Mourant, J. R. Conrad, J. C. Miner, C. A. Manore, N. W. Hengartner, A. L. Atchley and B. H. Mcmahon. Project Review of EpiGrid: Comprehensive and Operational Model. . (LA-UR-19-20358)

Manore, C. A. Modeling Mosquitoes. Presented at *CMPD5*, Ft Lauderdale, Florida, United States, 2019-05-20 - 2019-05-22. (LA-UR-19-24635)

Manore, C. A., S. Y. Del Valle and D. A. Romero-Alvarez. Google Health Trends accuracy to reflect dengue incidence at the Brazilian states. Presented at *Meeting and conference*, Quito, Ecuador, 2019-07-22 - 2019-07-24. (LA-UR-19-26940)

Manore, C. A. and S. E. Michalak. Mathematics and Los Alamos National Laboratory: Advances and Collaboration. Presented at *ICIAM/SIAM*, Valencia, Spain, 2019-07-14 - 2019-07-19. (LA-UR-19-26713)

Shutt, D. A., S. Pankavich and A. Porter. Embedded ODE Model for the 2014 Ebola Outbreak in West Africa; An analysis of Guinea, Liberia & Sierra Leone. Presented at *2019 Annual Meeting Society for Mathematical Biology*, Montreal, Canada, 2019-07-22 - 2019-07-22. (LA-UR-19-22954)

Posters

Coronado, I. D. Mosquito-Borne Disease: A Worldwide Epidemic. . (LA-UR-19-28086)

Shutt, D. A., C. A. Manore, D. W. Goodsman, Z. J. L. Hemez, J. R. Conrad, C. Xu, J. M. Hyman and C. Russel. Heterogeneous Data Streams for Predicting Mosquito Density. Presented at *GS Symposium*, Los Alamos, New Mexico, United States, 2019-11-13 - 2019-11-13. (LA-UR-19-31203)

Spencer, J. A. and H. J. Wearing. Fitness Differences between Drug Resistant and Sensitive Strains of Mycobacterium tuberculosis. Presented at *Society for Mathematical*

Biology Annual Meeting, Montreal, Canada, 2019-07-21 - 2019-07-26. (LA-UR-19-27013)

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 Department of Energy 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.

Technical Outcomes

We identified the enzymes responsible for xyloglucanase activity in A. protothecoides, paving the way for novel plant wall breakdown strategies. In addition, we discovered that an industrially-relevant saltwater strain has increased biomass productivity and total lipid increases with plant substrate addition. Lastly, we examined algae growth on plant substrates to identify the best parameters for deployment. We have communicated our results to industry collaborators for future projects, reaffirming LANL as a leader in this field.

Publications

Journal Articles

*Vogler, B. W., S. R. Starkenburg, N. Sudasinghe, J. Y. Schambach, J. A. Rollin, S. Pattathil and A. N. Barry. Characterization of plant carbon substrate utilization by Auxenochlorella protothecoides. 2018. *Algal Research*. **34**: 37-48. (LA-UR-18-21621 DOI: 10.1016/j.algal.2018.07.001)

Reports

Barry, A. N. Proposal for LDRD ECR: Boosting Algae Biomass for Biofuels with Plant Substrate Utilization. Unpublished report. (LA-UR-18-28460)

Presentation Slides

Barry, A. N. Boosting algae biomass: Examining plant substrate degradation and utilization by algae. . (LA-UR-17-28012)

Barry, A. N. Characterization of plant carbon substrate utilization by Auxenochlorella protothecoides. Presented at *Algal Biomass, Biofuels and Bioproducts*, Seattle, Washington, United States, 2018-06-10 - 2018-06-10. (LA-UR-18-24856)

Barry, A. N. Characterization of Plant Carbon Substrate Utilization by Two Microalgae. Presented at *Algae Biomass Organization Summit*, Houston, Texas, United States, 2018-10-14 - 2018-10-17. (LA-UR-18-29649)

Barry, A. N., S. R. Starkenburg, B. W. Vogler, J. Rollin, A. Villalba, S. Pattathil and N. M. Sudasinghe Appuhamilage. Degradation and utilization of plant substrates by microalgae. Presented at *Western Photosynthesis*, Oracle, Arizona, United States, 2018-01-03 - 2018-01-07. (LA-UR-17-31419)

Barry, A. N., S. R. Starkenburg and S. Pattathil. Boosting algae biomass for biofuels with plant substrate utilization. Presented at *Algal Biomass, Biofuel and Bioproducts*, Miami, Florida, United States, 2017-06-18 - 2017-06-21. (LA-UR-17-24903)

Schambach, J. Y. The World of Algae. Presented at *Fall 2018 STEM Santa Fe Expanding Your Horizons Conference*, Santa Fe, New Mexico, United States, 2018-10-13 - 2018-10-13. (LA-UR-18-29736)

Schambach, J. Y. Exploring mixotrophic growth of Nannochloropsis using plant carbon substrate. Presented at *Algal Biomass Summit 2019*, Orlando, Florida, United States, 2019-09-16 - 2019-09-19. (LA-UR-19-28937)

Posters

Finck, A. M., A. N. Barry and J. Y. Schambach. Improving the Biomass Productivity of a Biofuel Production Strain, Nannochloropsis gaditana. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-27155)

Lamcaj, S., J. Y. Schambach and A. N. Barry. Investigating the Lignocellulosic Degradation Activity of Auxenochlorella protothecoides. Presented at *2018 LANL student symposium*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-27070)

Vogler, B. W., A. N. Barry, J. E. Raab, A. Villalba, S. R. Starkenburg and W. Shin. Boosting algae biomass: Examining plant substrate degradation and utilization by algae. Presented at *LANL 2017 Student Symposium*, Los Alamos, New Mexico, United States, 2017-08-09 - 2017-08-09. (LA-UR-17-26892)

Impacts of Climate and Land Use on Global River Dynamics

Jonathan Schwenk
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

Journal Articles

*Gran, K. B., C. Dolph, A. Baker, M. Bevis, S. J. Cho, J. A. Czuba, B. Dalzell, M. Danesh-Yazdi, A. T. Hansen, S. Kelly, Z. Lang, J. Schwenk, P. Belmont, J. C. Finlay, P. Kumar, S. Rabotyagov, G. Roehrig, P. Wilcock and E. Foufoula-Georgiou. The Power of Environmental Observatories for Advancing Multidisciplinary Research, Outreach, and Decision Support: The Case of the Minnesota River Basin. 2019. *Water Resources Research*. **55** (4): 3576-3592. (LA-UR-18-29803 DOI: 10.1029/2018WR024211)

Schwenk, J. P., A. Piliouras and J. C. Rowland. Determining flow directions in river channel networks using planform morphology and topology. 2020. *Remote Sensing of Environment*. **8** (1): 87-102. (LA-UR-19-22689 DOI: 10.5194/esurf-8-87-2020)

Presentation Slides

Schwenk, J. P., A. Piliouras, Y. Zhang, M. M. Fratkin, J. C. Rowland, M. M. Douglas, A. Chadwick and M. P. Lamb. Permafrost control on river migration along the Koyukuk River, AK. Presented at *American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32556)

Posters

Schwenk, J. P., J. C. Rowland, A. Piliouras, A. Tejedor and E. Foufoula-Georgiou. Automatic Extraction of Channel Network Topology. Presented at *American Geophysical Union*, Washington, D.C., District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31483)

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

Anand Kumar
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.

Technical Outcomes

We have successfully integrated a combination of techniques, including microfluidics, culturing, flow sorting, isolation and sequencing, to develop a ‘High-Throughput Microbiome Screening’ (HTMS) platform. We have utilized this developed HTMS platform to identify therapeutic bacterial species from a healthy human skin microbiome that naturally inhibit methicillin-resistant Staphylococcus aureus, MRSA.

Publications

Presentation Slides

Kumar, A. Targeting Emerging Pathogen Infections with Next Generation Therapeutic Probiotics. Presented at *MICROBIOME & PROBIOTICS SERIES: USA*, San Diego, California, United States, 2019-10-29 - 2019-10-30. (LA-UR-19-31051)

Posters

Kumar, A., K. Martinez, M. R. Kron, J. M. Kelliher, B. M. Butler, J. L. Aslin, S. E. Pasqualoni, A. E. K. Dichosa and P. S. G. Chain. Combating antibiotic-resistant pathogens by microbiome-based therapeutics. Presented at *2019 Chemical and Biological Defense Science & Technology (CBD S&T) Conference*, Cinncinati, Ohio, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-31339)

Forecasting Failure

Bertrand Rouet-Leduc
20170673PRD2

Project Description

A large earthquake in Cascadia or California would devastate the regional and potentially national economies. The primary national security challenge this 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 Midwest. 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

Journal Articles

G. Rouet-Leduc, B. P., C. L. Hulbert and P. A. Johnson. Breaking Cascadia's Silence: Machine Learning Reveals the Constant Chatter of the Megathrust. Submitted to *Arxiv; Nature*. (LA-UR-18-24744)

*Rouet-Leduc, B., C. Hulbert, D. C. Bolton, C. X. Ren, J. Riviere, C. Marone, R. A. Guyer and P. A. Johnson. Estimating Fault Friction From Seismic Signals in the Laboratory. 2018. *Geophysical Research Letters*. **45** (3): 1321-1329. (LA-UR-17-29312 DOI: 10.1002/2017GL076708)

Posters

Johnson, P. A., A. A. Delorey, K. M. Barros, N. E. Lubbers, B. P. G. Rouet-Leduc and C. L. Hulbert. Machine Learning algorithm predicts time to failure of laboratory earthquake machine. . (LA-UR-17-23157)

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

Journal Articles

Aguirre Castiblanco, N. F., J. C. A. O. Jung and P. Yang. Unraveling the structural stability and the electronic structure of ThO 2 clusters. Submitted to *Chemical Science*. (LA-UR-18-29967)

A. O. Jung, J. C., M. A. Islam, V. L. Pecoraro, T. Mallah, C. Berthon and H. Bolvin. Derivation of Lanthanide Series Crystal Field Parameters From First Principles. 2019. *Chemistry – A European Journal*. **25** (66): 15112-15122. (LA-UR-19-23436 DOI: 10.1002/chem.201903141)

A. O. Jung, J. C., S. Loffler, K. Meyer, F. W. Heinemann, E. Bill, G. Bistoni, M. Atanasov and F. Neese. Dispersion Forces Drive the Formation of Uranium-Alkane Adducts. Submitted to *Journal of the American Chemical Society*. (LA-UR-19-22994)

Presentation Slides

A. O. Jung, J. C. Understanding Actinide Bonding with High Accuracy. . (LA-UR-18-24995)

A. O. Jung, J. C. Using effective models to “translate” ab initio energies and wave functions\xe2\x80\xa8 into physics and chemistry. . (LA-UR-19-31270)

A. O. Jung, J. C., H. Bolvin, M. A. Islam and C. Berthon. Ab initio Derivation of Crystal Field Parameters in Lanthanide Series. Presented at *European Conference on Molecular Magnetism*, Florence, Italy, 2019-09-15 - 2019-09-18. (LA-UR-19-28551)

A. O. Jung, J. C., P. Yang and E. R. Batista. First principle simulation of the EPR g-values in actinide complexes (to support chemical bonding analysis). Presented at *4th International Workshop on Advanced Techniques in Actinide Spectroscopy*, NICE, France, 2018-11-06 - 2018-11-09. (LA-UR-18-30275)

Posters

A. O. Jung, J. C. Understanding metal-ligand bonding in actinide complexes with high accuracy. . (LA-UR-18-24861)

A. O. Jung, J. C. Bacteria-inspired Energy Production: Insight from Quantum Chemistry. . (LA-UR-19-28508)

A. O. Jung, J. C., P. Yang, E. R. Batista and S. A. Kozimor. Computational Chemistry: \xe2\x80\xa8A Powerful Tool to Analyze Actinide Molecules !. . (LA-UR-18-28017)

A. O. Jung, J. C., P. Yang, E. R. Batista and S. A. Kozimor. Computational Chemistry: \xe2\x80\xa8A Powerful Tool to Analyze Actinide Molecules !. . (LA-UR-18-28127)

A. O. Jung, J. C., P. Yang and E. R. Batista. Electronic Structure and Optical Spectroscopy of Actinide Complexes Using Correlated Multi-Reference Calculations. Presented at *2018 Conference on Excited States Processes*, SANTA FE, New Mexico, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-24807)

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).

Technical Outcomes

We successfully cultivated a harmful algae bloom (HAB) species in vitro and recapitulated its bloom phenotype. These laboratory cultivation capabilities were established in conjunction with high throughput assessments of cellular functions and characteristics, including assays for measuring epigenetic regulation of algae genomes. DNA methylation assessment revealed that epigenetic mechanisms control microalgae behavior and phenotype. By harnessing these capabilities and manipulating the epigenome, we can develop novel strategies to manage HABs for biosecurity purposes.

Publications

Journal Articles

*S. Tyler, C. R., J. J. W. Smoake, E. R. Solomon, E. Villicana, K. K. Caldwell and A. M. Allan. Sex-Dependent Effects of the Histone Deacetylase Inhibitor, Sodium Valproate, on Reversal Learning After Developmental Arsenic Exposure. 2018. *Frontiers in Genetics*. **9**. (LA-UR-18-20125 DOI: 10.3389/fgene.2018.00200)

*Tyler, C. R., S. Noor, T. L. Young, V. Rivero, B. Sanchez, S. Lucas, K. K. Caldwell, E. D. Milligan and M. J. Campen. Aging Exacerbates Neuroinflammatory Outcomes Induced by Acute Ozone Exposure. 2018. *Toxicological Sciences*. **163** (1): 123-139. (LA-UR-18-20155 DOI: 10.1093/toxsci/kfy014)

Zychowski, K. E., C. R. Steadman, B. Sanchez, M. Harmon, J. Liu, H. Irshad, J. McDonald, B. Bleske and M. J. Campen. Vehicular Particulate Matter (PM) Characteristics Impact Vascular Outcomes Following Inhalation. Submitted to *Toxicology and Applied Pharmacology*. (LA-UR-19-22500)

*Zychowski, K. E., V. Kodali, M. Harmon, C. R. Tyler, B. Sanchez, Y. Ordonez Suarez, G. Herbert, A. Wheeler, S. Avasarala, J. M. Cerrato, N. K. Kunda, P. Muttil, C. Shuey, A. Brearley, A. Ali, Y. Lin, M. Shoeb, A. Erdely and M. J. Campen. Respirable Uranyl-Vanadate-Containing Particulate Matter Derived From a Legacy Uranium Mine Site Exhibits Potentiated Cardiopulmonary Toxicity. 2018. *Toxicological Sciences*. **164** (1): 101-114. (LA-UR-18-21620 DOI: 10.1093/toxsci/kfy064)

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.

Publications

Journal Articles

*Kong, Q., D. T. Trugman, Z. E. Ross, M. J. Bianco, B. J. Meade and P. Gerstoft. Machine Learning in Seismology: Turning Data into Insights. 2019. *Seismological Research Letters*. **90** (1): 3-14. (LA-UR-18-28089 DOI: 10.1785/0220180259)

*Koper, K. D., K. L. Pankow, J. C. Pechmann, J. M. Hale, R. Burlacu, W. L. Yeck, H. M. Benz, R. B. Herrmann, D. T. Trugman and P. M. Shearer. Afterslip Enhanced Aftershock Activity During the 2017 Earthquake Sequence Near Sulphur Peak, Idaho. 2018. *Geophysical Research Letters*. **45** (11): 5352-5361. (LA-UR-18-22721 DOI: 10.1029/2018GL078196)

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 an Improved Stress Map. 2019. *Journal of Geophysical Research: Solid Earth*. (LA-UR-18-27043 DOI: 10.1029/2019JB018377)

*Ross, Z. E., D. T. Trugman, E. Hauksson and P. M. Shearer. Searching for hidden earthquakes in Southern California. 2019. *Science*. **364** (6442): 767-771. (LA-UR-19-20273 DOI: 10.1126/science.aaw6888)

Ross, Z. E., D. T. Trugman, K. Azizzadenesheli and A. Anandkumar. Directivity Modes of Earthquake Populations with Unsupervised Learning. 2020. *Journal of Geophysical Research: Solid Earth*. **125** (2): e2019JB018299. (LA-UR-19-26206 DOI: 10.1029/2019JB018299)

*Shearer, P. M., R. E. Abercrombie, D. T. Trugman and W. Wang. Comparing EGF Methods for Estimating Corner Frequency and Stress Drop From Wave Spectra. 2019. *Journal of Geophysical Research: Solid Earth*. **124** (4): 3966-3986. (LA-UR-18-30681 DOI: 10.1029/2018JB016957)

Trugman, D. T. Stress Drop and Source Scaling of the 2019 Ridgecrest, California Earthquake Sequence. Submitted to *Bulletin of the Seismological Society of America*. (LA-UR-20-20288)

Trugman, D. T., G. C. Beroza and P. A. Johnson. Machine Learning in Geoscience: Riding a Wave of Progress. 2019. *Eos*. **100**. (LA-UR-19-22852 DOI: 10.1029/2019EO122671)

*Trugman, D. T., M. T. Page, S. E. Minson and E. S. Cochran. Peak Ground Displacement Saturates Exactly When Expected: Implications for Earthquake Early Warning. 2019. *Journal of Geophysical Research: Solid Earth*. 2018JB017093. (LA-UR-18-30809 DOI: 10.1029/2018JB017093)

Trugman, D. T., Z. E. Ross and P. A. Johnson. Imaging Stress and Faulting Complexity Through Earthquake Waveform Similarity. 2020. *Geophysical Research Letters*. **47** (1): e2019GL085888. (LA-UR-19-30627 DOI: 10.1029/2019GL085888)

Trugman, D. T. and P. M. Shearer. Strong Correlation between Stress Drop and Peak Ground Acceleration for Recent M \xc2\xa01–4 Earthquakes in the San Francisco Bay Area. 2018. *Bulletin of the Seismological Society of America*. (LA-UR-18-20708 DOI: 10.1785/0120170245)

*Trugman, D. T. and Z. E. Ross. Pervasive Foreshock Activity Across Southern California. 2019. *Geophysical Research Letters*. **46** (15): 8772-8781. (LA-UR-19-23605 DOI: 10.1029/2019GL083725)

Presentation Slides

Trugman, D. T. Machine Learning Applications to Earthquake Source Characterization and Hazard Analysis. . (LA-UR-18-24892)

Trugman, D. T. Do large and small earthquakes start alike? Rupture determinism and earthquake early warning. . (LA-UR-19-20107)

Trugman, D. T. Unsupervised Learning : A Gentle Introduction. Clustering the ComCat Earthquake Catalog using Python's Scikit-Learn Package.. Presented at *Seismological Society of America*, Seattle, Washington, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23604)

Trugman, D. T. Big Data, Small Earthquakes. . (LA-UR-19-24388)

Trugman, D. T. Earthquake Nucleation: Observations and Applications From Megaquakes in Japan to Microforeshocks in California. . (LA-UR-19-27171)

Trugman, D. T. New Perspectives on Earthquake Nucleation from Megaquakes in Japan and Microforeshocks in California. . (LA-UR-19-29868)

Posters

Trugman, D. T., Z. E. Ross and P. A. Johnson. Anti-similar aftershocks in the Ridgecrest, California earthquake sequence. Presented at *Southern California Earthquake Center Annual Meeting*, Palm Springs, California, United States, 2019-09-09 - 2019-09-09. (LA-UR-19-28255)

Unusual Oxidation States and Covalency-Tuning in Transuranic Molecules

Conrad Goodwin
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

Journal Articles

I. Brewster, J. T., D. N. Mangel, D. P. Saunders, H. Zafar, A. J. Gaunt, V. M. Lynch, M. A. Boreen, M. E. Garner, C. A. P. Goodwin, N. Settineri, J. Arnold and J. L. Sessler. In-plane Thorium(IV), Uranium(IV), and Neptunium(IV) Expanded Porphyrin Complexes. Submitted to *Nature Chemistry*. (LA-UR-19-28070)

P. Goodwin, C. A., D. Reta and F. Ortu. Experimental and Theoretical Collaborative Work in the Field of Molecular Magnetism. Submitted to *International Journal of Quantum Chemistry*. (LA-UR-19-28416)

P. Goodwin, C. A., F. Ortu and D. Reta. Strangely Attractive: Collaboration and Feedback in the Field of Molecular Magnetism. Submitted to *International Journal of Quantum Chemistry*. (LA-UR-20-22240)

*P. Goodwin, C. A., J. Su, T. E. Albrecht-Schmitt, A. V. Blake, E. R. Batista, S. R. Daly, S. Dehnen, W. J. Evans, A. J. Gaunt, S. A. Kozimor, N. Lichtenberger, B. L. Scott and P. Yang. [Am(C Me H)]: An Organometallic Americium Complex. 2019. *Angewandte Chemie International Edition*. **58** (34): 11695-11699. (LA-UR-19-25159 DOI: 10.1002/anie.201905225)

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)

Reports

P. Goodwin, C. A., J. Su, L. M. Stevens, F. D. J. White, M. T. Janicke, I. May, C. J. Windorff, J. M. Sperling, A. N. Gaiser, J. N. Cross, T. E. Albrecht-Schmitt, T. F. Jenkins, E. R. Batista, W. J. Evans, A. J. Gaunt, S. A. Kozimor, B. L. Scott and P. Yang. Bonding and Electronic Structure in a Crystallographically Authenticated Organocalifornium Complex. Unpublished report. (LA-UR-19-32441)

Presentation Slides

P. Goodwin, C. A. Am(III) and Ce(III) CpMe4 organometallic complexes. . (LA-UR-18-31034)

P. Goodwin, C. A. Np and Cf(III) Cp organometallic complexes. . (LA-UR-19-20947)

P. Goodwin, C. A. Cyclic voltammetry data (C23) on [Pu(tBuPyNO)4], a Pu(IV) coordination complex with a nitroxide ligand. . (LA-UR-19-21962)

P. Goodwin, C. A. [Np(DPAM)(OTMS)2] – A Np(IV) expanded porphyrin complex. . (LA-UR-19-22240)

P. Goodwin, C. A. Trans-uranic organometallic chemistry: Oxidation states, bonding and electronic. Presented at *ACS National Meeting and Expo 2019*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22542)

P. Goodwin, C. A. Pictures of drybox in 48-0001-426 to assist with repairs. . (LA-UR-19-22514)

P. Goodwin, C. A. NMR study of transition metal metallocene monoanions. . (LA-UR-19-30154)

P. Goodwin, C. A. Cyclic voltammetry data (K164) on [Np(tBuPyNO)4], a Np(IV) coordination complex with a nitroxide ligand. . (LA-UR-19-20540)

P. Goodwin, C. A. f-element Chemistry: Oxidation States, Bonding, and Electronic Structures. . (LA-UR-19-20861)

P. Goodwin, C. A. Photographs of Conrad Goodwin (Z# 328031) taken by the media office. . (LA-UR-20-21767)

P. Goodwin, C. A., A. J. Gaunt and S. T. Liddle. A Np(IV)-bridged azide complex. . (LA-UR-19-29826)

P. Goodwin, C. A., M. T. Janicke, L. M. Stevens, F. D. J. White and A. J. Gaunt. F-block Seleno-imidodiphosphinate Complexes. . (LA-UR-19-32130)

P. Goodwin, C. A., S. Ciccone, W. J. Evans and A. J. Gaunt. Actinide cryptate complexes. . (LA-UR-19-30805)

P. Goodwin, C. A. and A. J. Gaunt. Voltammetry data (C35) on [Np(TrenTIPS)(Cl)], a Np(IV) coordination complex with a triamidoamine ligand. . (LA-UR-19-27163)

Staun, S. L., L. M. Stevens, C. A. P. Goodwin, A. J. Gaunt and B. L. Scott. Np cyclometallation chemistry. . (LA-UR-19-30153)

Windorff, C. J. and C. A. P. Goodwin. Actinyl phosphineoxide complexes. . (LA-UR-19-30804)

Posters

P. Goodwin, C. A., S. A. Kozimor and A. J. Gaunt. Transuranium organometallic and redox chemistry. . (LA-UR-19-25165)

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.

Publications

Journal Articles

Batrice, R. J., J. N. Wacker, E. N. Glass, S. Z. Jilani, Y. J. Tong, M. Nyman and K. E. Knope. Template-Free Cyclic Hexavanadate: Synthesis, Characterization, Solid-State Structure, and Solution-State Dynamics. Submitted to *Polyhedron*. (LA-UR-19-23747)

Presentation Slides

Batrice, R. J., P. Dub and J. C. Gordon. Outer-Sphere Ruthenium Catalysts for the Generation of Value Added Chemicals. . (LA-UR-19-31309)

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.

Publications

Journal Articles

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)

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 B\xe2\x89\xa1B 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 \xce\xb4 Back-Donation in AnIV Metallacycles. Submitted to *Nature Communications*. (LA-UR-19-21182)

*Liu, C., I. A. Popov, Z. Chen, A. I. Boldyrev and Z. Sun. Aromaticity and Antiaromaticity in Zintl Clusters. 2018. *Chemistry - A European Journal*. **24** (55): 14583-14597. (LA-UR-18-23061 DOI: 10.1002/chem.201801715)

*Popov, I. A., B. L. Davis, R. Mukundan, E. R. Batista and P. Yang. Catalyst-Inspired Charge Carriers for High Energy Density Redox Flow Batteries. 2019. *Frontiers in Physics*. **6**. (LA-UR-18-28568 DOI: 10.3389/fphy.2018.00141)

*Popov, I. A., N. Mehio, T. Chu, B. L. Davis, R. Mukundan, P. Yang and E. R. Batista. Impact of Ligand Substitutions on Multielectron Redox Properties of Fe Complexes Supported by Nitrogenous Chelates. 2018. *ACS Omega*. **3** (11): 14766-14778. (LA-UR-18-22442 DOI: 10.1021/acsomega.8b01921)

Rice, N. T., I. A. Popov, D. R. Russo, T. P. Gompa, A. Ramanathan, J. Bacsa, E. R. Batista, P. Yang and H. S. La Pierre. Comparison of tetravalent cerium and terbium ions in a conserved, homoleptic imidophosphorane ligand field. Submitted to *Chemical Science*. (LA-UR-20-22218)

*Zhang, X., I. A. Popov, K. A. Lundell, H. Wang, C. Mu, W. Wang, H. Schn\xc3\xb6ckel, A. I. Boldyrev and K. H. Bowen. Realization of an Al\xe2\x89\xa1Al Triple Bond in the Gas-Phase Na Al Cluster via Double Electronic Transmutation. 2018. *Angewandte Chemie International Edition*. **57** (43): 14060-14064. (LA-UR-18-22726 DOI: 10.1002/anie.201806917)

Presentation Slides

Popov, I. A. Ligand Effects on the Multi-Electron Redox Properties of Fe Complexes. Presented at *256th ACS National Meeting*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-28005)

Popov, I. A., M. P. Kelley, E. R. Batista and P. Yang. Importance of the unprecedented \xce\xb4 back-donation in AnIV metallacycles. Presented at *256th ACS National Meeting*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-27949)

Popov, I. A., M. P. Kelley, E. R. Batista and P. Yang. \xce\xb4 Back-Donation in AnIV Metallacycles (An=Th, Pa, U, Np, Pu). Presented at *Plutonium Futures 2018*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28566)

Posters

Popov, I. A., T. Chu, G. A. Andrade, S. Maurya, B. L. Scott, B. L. Davis, R. Mukundan, E. R. Batista and P. Yang. Theoretical Modeling of Charge Carriers for High Energy Density Redox Flow Batteries. Presented at *Workshop on Non-Aqueous Flow Batteries*, Santa Fe, New Mexico, United States, 2019-01-30 - 2019-01-31. (LA-UR-19-20645)

Principles for Optimal Establishment and Resilience of Microbial Communities

Michaeline Albright
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.

Publications

Journal Articles

N. Albright, M. B., S. A. Sevanto and J. M. Dunbar. Principles for engineering microbial composition and ecosystem functioning. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-19-27879)

Presentation Slides

N. Albright, M. B. and J. M. Dunbar. Principles for Engineering Microbial Composition and Ecosystem Functioning. Presented at *Applied and Environmental Microbiology Gordon Research Conference*, South Hadley, Massachusetts, United States, 2019-07-13 - 2019-07-19. (LA-UR-19-26384)

Posters

N. Albright, M. B., L. A. Gallegos-Graves, J. C. Thompson, R. Johansen, D. Ulrich, K. L. Avery, B. Timalsina, K. K. Stringfield, A. C. Runde, D. L. Lopez, T. M. Yoshida, M. Shakya, S. A. Sevanto and J. M. Dunbar. Principles for Microbiome Engineering. . (LA-UR-19-28938)

Investigating Actinide-Based Molecular Magnetism with Electron Paramagnetic Resonance

Benjamin Stein
20180759PRD4

Project Description

Beyond their fundamentally interesting chemistry, actinides are an essential aspect of the nuclear weapons enterprise and nuclear energy. Understanding of the detailed relationship between chemical properties and the atomic structure of actinides is important to challenges as diverse as plutonium aging, actinide separations for reprocessing efforts, and plutonium electrorefining. This project seeks to apply modern, advanced magnetic techniques to both improve the understanding of actinides as a whole, and advance the research needs of the field of molecular magnetism. The latter has impacts on areas such as quantum computing and molecular information storage, both areas with significant recent interest (including in areas of national security).

Publications

Posters

Greer, S. M., R. Meyer, K. E. Aldrich, J. Marbey, K. Kundu, L. M. Lilley, S. Hill, S. A. Kozimor and B. Stein. Applications of Advanced Electron Paramagnetic Resonance Techniques to Actinide-Based Coordination Complexes. Presented at *Molecular Magnetism in North America*, St Simon Island, Georgia, United States, 2020-02-21 - 2020-02-24. (LA-UR-20-21656)

Enabling Artificial Selection Programs through Characterizing the Lifecycle of Green Algae

Shawn Starkenburg
20190616PRD1

Project Description

Characterizing the life cycle of Scenedesmus obliquus, a candidate feedstock for biofuel production, would enable artificial selection programs for desired algal traits. Artificial selection programs have the potential to dramatically increase the productivity of algal-based renewable energy feedstocks. This new area of research complements the existing bioenergy portfolio of Los Alamos National Laboratory (LANL) and directly aligns with LANL mission to provide energy independence and security solutions for the nation.

Publications

Journal Articles

Hanschen, E. R., B. Hovde and S. R. Starkenburg. Evaluating the quality of algal genome assemblies. Submitted to *Algal Research*. (LA-UR-20-22201)

Presentation Slides

Hanschen, E. R., S. R. Starkenburg, K. K. Hixson, M. Costa, S. Moinuddin, K. Engbrecht, T. Fillmore, R. Sayre, M. S. Lipton, D. T. Hanson, O. Monje, J. Richards, L. Davin and N. Lewis. Patterns of gene expression in Arabidopsis thaliana in response to microgravitational environment. Presented at *American Society for Gravitational and Space Research*, Denver, Colorado, United States, 2019-11-20 - 2019-11-23. (LA-UR-19-31557)

Posters

N. Abbott, A. R., E. R. Hanschen and S. R. Starkenburg. Environmental conditions causing mating of green alga Scenedesmus. Presented at *Student Symposium 2019*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27334)

Hanschen, E. R., J. E. W. Polle, J. Umen and S. R. Starkenburg. Sexual reproduction and mating in the green alga Scenedesmus obliquus. Presented at *Sequencing, Finishing, and Analysis in the Future*, Sante Fe, New Mexico, United States, 2019-05-21 - 2019-05-23. (LA-UR-19-24631)

Multiscale Quantitative Description of Drug Resistance Mechanisms in Bacterial Systems

Sandrasegaram Gnanakaran
20190644PRD3

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 systems-level understanding of the operating principles governing how antibiotics are transported out of bacterial membranes by efflux pumps, dominant mechanism of drug resistance in many potential bioterrorism pathogens. The combined approach of multi-scale mathematical models and big data from large-scale simulations and high-throughput experiments proposed in this project is not limited to biological system, but rather can be applied to understand other multi-scale problems of interest to the Department of Energy(DOE)/National Nuclear Security Administration(NNSA). It has the potential to connect the statistical physics based multi-scale models to high performance computing help solidify DOE's exascale computing initiatives, thereby strengthening the key NNSA goal of stockpile stewardship.

Toward a Universal Description for Aqueous Solutions

Alp Findikoglu
20190653PRD4

Project Description

Meeting humanity's growing demand for fresh water is a major challenge. In particular, affordable methods to desalinate Earth's vast saline water resources remain elusive. One promising approach to meeting this challenge is supercritical water desalination, which is based on using high temperatures and pressures to manipulate water's properties and hence its ability to precipitate salts. Supercritical desalination is very well-suited for integration into other industrial processes; however, a number of both fundamental and practical issues exist. The proposed work combines both theoretical and experimental studies to make significant advances in our understanding of how salt ions and water behave in supercritical water. The knowledge generated by this work should have direct relevance for the development of the supercritical water desalination processes.

Publications

Journal Articles

Yoon, T., M. J. Vigil, E. Y. Raby, R. P. Singh, K. A. Maerzke, R. P. Currier and A. T. Findikoglu. Dielectric relaxation of neodymium chloride in water and in methanol. Submitted to *Journal of Molecular Liquids*. (LA-UR-19-32739)

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.

Technical Outcomes

As planned, we performed simulations exploring more advanced (kinetic) simulations of space and laboratory plasmas. These simulations demonstrated a marked improvement over simpler fluid models for matching details of data collected in inertial fusion experiments at laboratory laser facilities as well as observations gathered by NASA spacecraft in the Earth's magnetosphere.

Publications

Journal Articles

*Chen, L. -., S. Wang, L. B. I. Wilson, S. Schwartz, N. Bessho, T. Moore, D. Gershman, B. Giles, D. Malaspina, F. D. Wilder, R. E. Ergun, M. Hesse, H. Lai, C. Russell, R. Strangeway, R. B. Torbert, A. F. -. Vinas, J. Burch, S. Lee, C. Pollock, J. Dorelli, W. Paterson, N. Ahmadi, K. Goodrich, B. Lavraud, O. Le Contel, Y. V. Khotyaintsev, P. -. Lindqvist, S. Boardsen, H. Wei, A. Le and L. Avanov. Electron Bulk Acceleration and Thermalization at Earth's Quasiperpendicular Bow Shock. 2018. *Physical Review Letters*. **120** (22): 225101. (LA-UR-18-26991 DOI: 10.1103/PhysRevLett.120.225101)

*Egedal, J., A. Le, W. Daughton, B. Wetherton, P. A. Cassak, L. -. Chen, B. Lavraud, R. B. Torbert, J. Dorelli, D. J. Gershman and L. A. Avanov. Spacecraft Observations and Analytic Theory of Crescent-Shaped Electron Distributions in Asymmetric Magnetic Reconnection. 2016. *Physical Review Letters*. **117** (18): 185101. (LA-UR-17-27741 DOI: 10.1103/PhysRevLett.117.185101)

*Egedal, J., B. Wetherton, W. Daughton and A. Le. Processes setting the structure of the electron distribution function within the exhausts of anti-parallel reconnection. 2016. *Physics of Plasmas*. **23** (12): 122904. (LA-UR-17-27438 DOI: 10.1063/1.4972135)

*Hong, S., L. Chikang, C. E. Parker, B. Lahmann, A. Le, S. Atzeni and R. D. Petrasso. Fuel-ion diffusion in shock-driven inertial confinement fusion implosions. 2019. *Matter and Radiation at Extremes*. **4** (5): 055401. (LA-UR-19-24138 DOI: 10.1063/1.5090783)

*Le, A., 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*. **23** (10): 102705. (LA-UR-16-24469 DOI: 10.1063/1.4965913)

*Le, A., V. Roytershteyn, H. Karimabadi, A. Stanier, L. Chacon and K. Schneider. Wavelet methods for studying the onset of strong plasma turbulence. 2018. *Physics of Plasmas*. **25** (12): 122310. (LA-UR-18-29103 DOI: 10.1063/1.5062853)

*Le, A., W. Daughton, L. -. 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)

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*Liu, Y., M. Hesse, T. C. Li, M. Kuznetsova and A. Le. Orientation and Stability of Asymmetric Magnetic Reconnection X Line. 2018. *Journal of Geophysical Research: Space Physics*. **123** (6): 4908-4920. (LA-UR-18-26828 DOI: 10.1029/2018JA025410)

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ion effects, and ion-electron equilibration rates in Inertial Confinement Fusion plasmas at OMEGA (invited). 2016. *Review of Scientific Instruments*. **87** (11): 11D701. (LA-UR-17-27853 DOI: 10.1063/1.4961552)

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Reports

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)

Presentation Slides

Le, A. Y. Recent LSP Modeling of Omega Experiments. Presented at *LLNL Kinetic Effects Workshop*, Livermore, California, United States, 2016-04-05 - 2016-04-05. (LA-UR-16-22243)

Le, A. Y. Results from kinetic plasma simulation on Grizzly--IC Project: w17_eclosure.. . (LA-UR-19-21763)

Le, A. Y., W. S. Daughton, L. Chen and J. Egedal. Enhanced Electron Heating and Mixing in a 3D Kinetic Simulation for MMS Magnetopause Crossings with Weak Guide Fields. Presented at *APS Division of Plasma Physics Annual Meeting*, San Jose, California, United States, 2016-10-31 - 2016-10-31. (LA-UR-16-28154)

Le, A. Y., W. S. Daughton, O. Ohia, L. Chen and Y. Liu. Energization and Transport in 3D Kinetic Simulations of MMS Magnetopause Reconnection Site Encounters with Varying Guide Fields. Presented at *AGU Fall Meeting 2017*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-11. (LA-UR-17-31079)

Le, A. Y. and W. S. Daughton. Enhanced Electron Heating and Mixing in a 3D Kinetic Simulation for MMS Magnetopause Crossings with Weak Guide Fields. Presented at *Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2017-03-06 - 2017-03-06. (LA-UR-17-21937)

Posters

T. Kwan, T. J., A. Y. Le, M. J. Schmitt and H. W. Herrmann. Kinetic simulation of hydrodynamic equivalent capsule implosions. Presented at *58th Annual Meeting of APS Division of Plasma Physics*, San Jose, California, United States, 2016-10-31 - 2016-11-04. (LA-UR-16-28101)

Le, A. Y., V. S. Roytershteyn, H. Karimabadi, A. J. Stanier, L. Chacon and K. Schneider. An iterative wavelet method for diagnosing the onset of turbulence in magnetized plasma. Presented at *APS DPP*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30032)

Le, A. Y., W. S. Daughton, O. Ohia, L. Chen and Y. Liu. Plasma Transport at the Magnetopause in 3D Kinetic Simulations of MMS Reconnection Site Encounters with Varying Guide Fields. Presented at *APS DPP*, Milwaukee, Wisconsin, United States, 2017-10-23 - 2017-10-23. (LA-UR-17-29338)

Regulation of Intercellular Signaling

Christopher Neale
20160676PRD4

Project Description

G-protein coupling receptors (GPCR) are a large familiy 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 projects employs high performance computational tools to simulate the dynamics of GPCRs in environments that mimic the cell surface. The simulations are validated with experimental ata 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.

Technical Outcomes

Much of the work in our cells is accomplished by proteins, whose misfunction is due to mutation, infection, or bio/chemical agents that can lead to disease. We have developed new computational methods to accelerate our functional understanding of cellular signaling proteins and have used the resulting knowledge to rationally designed small molecules to influence the behavior of these proteins. This project is related to chem/bio defense and national heath interests.

Publications

Journal Articles

*Ye, L., C. Neale, A. Sljoka, B. Lyda, D. Pichugin, N. Tsuchimura, S. T. Larda, R. Pomes, A. E. Garcia, O. P. Ernst, R. K. Sunahara and R. S. Prosser. Mechanistic insights into allosteric regulation of the A2A adenosine G protein-coupled receptor by physiological cations. 2018. *Nature Communications*. **9** (1): 1372. (LA-UR-18-20653 DOI: 10.1038/s41467-018-03314-9)

Presentation Slides

Garcia, A. E. and C. A. Neale. Uncovering the dynamics of a Molecular Switch: Atomistic Simulations of the interaction of KRas with membranes. Presented at *Wesleyan University Molecular Biophysics and Biological Chemistry Program Retreat*, Middletown, Connecticut, United States, 2018-09-27 - 2018-09-28. (LA-UR-18-29124)

Neale, C. A. Molecules to be suggested to the National Cancer Institute for their experimental quantification of ability to reduce growth driven by oncogenic Ras mutants. . (LA-UR-18-20654)

Ye, L., C. A. Neale, A. Sljoka, B. Lyda, D. Pichugin, N. Tsuchimura, S. T. Larda, R. Pomes, A. E. Garcia, O. P. Ernst, R. K. Sunahara and S. R. Prosser. Mechanistic insights into allosteric regulation of the A2A adenosine G protein-coupled receptor by physiological cations. . (LA-UR-18-23370)

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.

Technical Outcomes

The project collected more than 5 microseconds of simulation of a massive HIV-1 vesicle in water and have drafted preliminary analysis codes. Extensive work has been completed on critical and fundamental open source codes: SciPy, NumPy, and MDAnalysis.

Publications

Journal Articles

Chavent, M., A. L. Duncan, P. Rassam, O. Birkholz, J. Helie, T. J. E. Reddy, D. Beliaev, B. Hambly, J. Piehler, C. Kleanthous and M. S. Sansom. How nanoscale protein interactions determine the mesoscale dynamic organisation of bacterial outer membrane proteins. 2018. *Nature Communications*. **9** (1): 2846. (LA-UR-19-29545 DOI: 10.1038/s41467-018-05255-9)

Chavent, M., A. L. Duncan, P. Rassam, O. Birkholz, J. Helie, T. J. E. Reddy, D. Beliaev, B. Hambly, J. Piehler, C. Kleanthous and M. S. Sansom. How nanoscale protein interactions determine the mesoscale dynamic organisation of bacterial outer membrane proteins. 2018. *Nature Communications*. **9** (1): 2846. (LA-UR-19-29545 DOI: 10.1038/s41467-018-05255-9)

Virtanen, P., R. Gommers, T. E. Oliphant, M. Haberland, T. J. E. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, J. Millman, N. Mayorov, A. R. Nelson, E. Jones, R. Kern, E. Larson, C. Carey, I. Polat, Y. Feng, E. W. Moore, J. VanderPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt and S. 1. Contributors. SciPy 1.0—Fundamental Algorithms for Scientific Computing in Python. Submitted to *Nature Methods*. (LA-UR-19-29085)

Virtanen, P., R. Gommers, T. E. Oliphant, M. Haberland, T. J. E. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, J. Millman, N. Mayorov, A. R. Nelson, E. Jones, R. Kern, E. Larson, C. Carey, I. Polat, Y. Feng, E. W. Moore, J. VanderPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt and S. 1. Contributors. SciPy 1.0—Fundamental Algorithms for Scientific Computing in Python. Submitted to *Nature Methods*. (LA-UR-19-29085)

Conference Papers

Gowers, R. J., M. Linke, J. Barnoud, T. J. E. Reddy, M. N. Melo, S. L. Seyler, J. Domanski, D. L. Dotson, S. Buchoux, I. M. Kenney and O. Beckstein. MDAnalysis: A Python Package for the Rapid Analysis of Molecular Dynamics Simulations. Presented at *PROC. OF THE 15th PYTHON IN SCIENCE CONF. (SCIPY 2016)*. (Austin, Texas, United States, 2016-07-11 - 2016-07-11). (LA-UR-19-29136)

Gowers, R. J., M. Linke, J. Barnoud, T. J. E. Reddy, M. N. Melo, S. L. Seyler, J. Domanski, D. L. Dotson, S. Buchoux, I.

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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.

Technical Outcomes

This project focused on evaluating the nature of chemical bonding for actinide elements. This represents one of the most important and long-standing problems in actinide science. We developed novel compounds, established methods for safely containing the radioactive samples for characterization, and recovered the precious isotopes for future study. Additionally, orbital mixing in many compounds were quantified using X-ray absorption spectroscopy and relativistic density functional theory.

Publications

Journal Articles

*Cary, S. K., J. Su, S. S. Galley, T. E. Albrecht-Schmitt, E. R. Batista, M. G. Ferrier, S. A. Kozimor, V. Mocko, B. L. Scott, C. E. Van Alstine, F. D. White and P. Yang. A series of dithiocarbamates for americium, curium, and californium. 2018. *Dalton Transactions*. **47** (41): 14452-14461. (LA-UR-18-22699 DOI: 10.1039/C8DT02658K)

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*Choi, H., W. Zhu, S. K. Cary, L. E. Winter, Z. Huang, R. D. McDonald, V. Mocko, B. L. Scott, P. H. Tobash, J. D. Thompson, S. A. Kozimor, E. D. Bauer, J. Zhu and F. Ronning. Experimental and theoretical study of topology and electronic correlations in PuB4. 2018. *Physical Review B*. **97** (20): 201114. (LA-UR-18-21188 DOI: 10.1103/PhysRevB.97.201114)

Cross, J. N., J. Su, E. R. Batista, S. K. Cary, W. J. Evans, S. A. Kozimor, V. Mocko, B. L. Scott, B. W. Stein, C. J. Windorff and P. Yang. Covalency in Americium(III) Hexachloride. 2017. *Journal of the American Chemical Society*. **139** (25): 8667-8677. (LA-UR-17-22510 DOI: 10.1021/jacs.7b03755)

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)

*Ferrier, M. G., B. Stein, S. E. Bone, S. K. Cary, A. S. Ditter, S. A. Kozimor, J. S. Lezama Pacheco, V. Mocko and G. T. Seidler. The coordination chemistry of Cm , Am , and Ac in nitrate solutions: an actinide L -edge EXAFS study. 2018. *Chemical Science*. **9** (35): 7078-7090. (LA-UR-18-22688 DOI: 10.1039/C8SC02270D)

*Stein, B. W., S. K. Cary, J. M. Berg, E. R. Birnbaum, S. A. Kozimor, V. Mocko and B. L. Scott. A series of F-Element chelators; diaza crown ethers functionalized with catecholate binding substituents. 2018. *Journal of Organometallic Chemistry*. **857**: 170-179. (LA-UR-17-28162 DOI: 10.1016/j.jorganchem.2017.11.026)

Books/Chapters

Schrell, S. K., A. R. Chavez, D. M. Lopez, S. A. Kozimor, A. D. Montoya and V. Mocko. Tender X-ray Absorption Measurements. (LA-UR-18-24809)

Presentation Slides

Schrell, S. K. \xc2\xa0Exploring the Actinide Series from Periodic Trends to Electronic Structure and Bonding. . (LA-UR-18-29767)

Schrell, S. K. and S. A. Kozimor. Improving The Understanding Of Actinides Through Spectroscopy. Presented at *the 65th Annual American Vacuum Society (AVS) International Symposium and Exhibition*, Long Beach, California, United States, 2018-10-22 - 2018-10-26. (LA-UR-18-29527)

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.

Technical Outcomes

Through the use of novel catalysts and ingenuity of this team, we have developed a number of new catalysts for the dehydrogenation of formic acid under relevant conditions. While our attempts to achieve tandem olefin hydrogenation were foiled by the vastly different rates of the two processes, we were able to develop a secondary polymerization catalyst system that was capable of providing the heat required to drive the gas generator without a power source.

Publications

Journal Articles

*Anderson, N. H., J. M. Boncella and A. M. Tondreau. Reactivity of Silanes with (tbuPONOP)Ruthenium Dichloride: Facile Synthesis of Chloro-Silyl Ruthenium Compounds and Formic Acid Decomposition. 2017. *Chemistry - A European Journal*. **23** (55): 13617-13622. (LA-UR-17-25821 DOI: 10.1002/chem.201703722)

*Anderson, N. H., J. M. Boncella and A. M. Tondreau. Investigation of Nitrile Hydration Chemistry by Two Transition Metal Hydroxide Complexes: Mn–OH and Ni–OH Nitrile Insertion Chemistry. 2018. *Organometallics*. **37** (24): 4675-4684. (LA-UR-18-28930 DOI: 10.1021/acs.organomet.8b00687)

Reports

Anderson, N. H. Tandem Dehydrogenation of Formic Acid and Olefin Hydrogenation: Steps Towards a Self-Sustaining Pressure/Volume System. Unpublished report. (LA-UR-20-20212)

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.

Technical Outcomes

Forest ecosystems including the semi arid forests of the Southwest, play key roles in regional meteorology, precipitation and hydrology. Disturbances such as wildfires, drought and land-use changes can exacerbate or dampen the vulnerability of such ecosystems. This work has provided a physics-based mechanistic framework for the investigation of the complex and nonlinear effects of multiple feed backs associated with ecosystem disturbances.

Publications

Journal Articles

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)

Banerjee, T., W. Heilman, S. Goodrick, K. Hiers and R. R. Linn. Effects of canopy midstory management and fuel moisture on wildfire behavior. Submitted to *EarthArXiv*. (LA-UR-19-23583)

Holland, T. M., T. Banerjee, K. C. Solander, M. J. Holmes and R. R. Linn. Identifying Characteristics of Wildfire "Towers and Troughs". Submitted to *Fire*. (LA-UR-19-30049)

Presentation Slides

Banerjee, T., M. J. Holmes and R. R. Linn. Orchard on Fire, a simulation study.. Presented at *12th Fire and Forest Meteorology Symposium*, Boise, Idaho, United States, 2018-05-13 - 2018-05-18. (LA-UR-18-24258)

Linn, R. R. and T. Banerjee. Using Coupled Fire/Atmosphere Modeling to Advance Wildland Fire Science and Assist Decision Makers. Presented at *European Geosciences Union (EGU) General Assembly 2018*, Vienna, Austria, 2018-04-08 - 2018-04-13. (LA-UR-18-22909)

Posters

Banerjee, T., R. R. Linn, W. Heilman, S. Goodrick and C. Clements. Turbulence in a wildland fire – A micrometeorological perspective. Presented at *American Geophysical Union (AGU) Fall Meeting*, Washington, D.C., District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31400)

Banerjee, T. and R. R. Linn. Ecosystem disturbance modeling, a systems approach. Presented at *European Geosciences Union (EGU) General Assembly 2018*, Vienna, Austria, 2018-04-08 - 2018-04-13. (LA-UR-18-22910)

Toward a Next-Generation Pathogen Surveillance Platform: Integrating Clinical Metagenomics with Epidemiological Modeling to Characterize/Understand Disease

Patrick Chain
20190615PRD1

Project Description

Given the diversity and complexity of infectious diseases, the expected outcome of this research is the reduction of biothreats by (i) rapidly identifying the agent and (ii) integrating multiple data streams to allow for better predictions on the origins and spread of said agent. Additionally, this approach will highlight critical gaps in traditional disease surveillance systems, and facilitate strengthening of national surveillance systems.

Technical Outcomes

In this project, we applied cutting-edge sequencing and bioinformatic analysis to a key emerging pathogen (Klebsiella pneumoniae), integrated genomic data with a powerful visualization pipeline, as well as laid the groundwork for creating of a novel framework for merging genomic and traditional epidemiological modeling techniques using cholera data.

Publications

Journal Articles

Domman, D. B., C. Ruis, M. J. Dorman, M. Shakya and P. S. G. Chain. Novel Insights Into the Spread of Enteric Pathogens Using Genomics. 2019. *The Journal of Infectious Diseases*. (LA-UR-19-23908 DOI: 10.1093/infdis/jiz220)

Presentation Slides

Domman, D. B. Cholera Genomic Database. Presented at *WHO Global Taskforce for Cholera Control*, Annecy, France, 2019-04-15 - 2019-04-17. (LA-UR-19-23335)

Information Science and Technology

Enabling Predictive Scale-Bridging Simulations through Active Learning

Timothy Germann
20190005DR

Project Description

Exascale supercomputers that will arrive in the next few years offer tremendous computational power, if one can coordinate the approximately one billion different calculations that are occurring at any given time. Our project combines these exciting advances in computing architectures with similarly exciting advances in machine learning algorithms to enable computational science and engineering simulations with greater physical fidelity, combining molecular-scale simulations with continuum fluid dynamics ones. Just as understanding nanomaterial properties has been a grand challenge over the past two decades, understanding fluids in complex nanopores is the next frontier. Our computational framework for incorporating nanoscale physics will enable efficient extraction of subsurface energy (hydrocarbon and geothermal) from tight unconventional resources which have proved to be extremely challenging. Similarly, we expect to be able to efficiently and accurately account for complex atomistic effects such as non-local transport in inertial confinement fusion (ICF) simulations, providing a valuable computational tool for understanding whether ignition is ultimately achievable and, if yes, suggest practical avenues for controlling mix, instabilities, and heat loss from the hot spot. Our active learning approach will bring about transformational advances in the way nanoconfinement effects of fluids are modeled in these and other applications.

Publications

Journal Articles

Bakhshian, S., M. Murakami, S. A. Hosseini and Q. Kang. Scaling of Imbibition Front Dynaimcs in Heterogeneous Porous Media. Submitted to *Geophysical Research Letters*. (LA-UR-20-22139)

Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Ex machina determination of structural correlation functions. Submitted to *Physical Review Letters*. (LA-UR-19-32446)

Gong, Y., M. Z. S. Mehana, I. El-monier and H. S. Viswanathan. Proppant Placement in Complex Fracture Geometries: A Computational Fluid Dynamics. Submitted to *Scientific Reports*. (LA-UR-19-29884)

S. Mehana, M. Z., S. Hosseini, T. A. Meckel and H. S. Viswanathan. Modelling the Carbon Dioxide Plume Using Modified-Invasion-Percolation Simulation. Submitted to *Transport in Porous Media*. (LA-UR-19-26910)

S. Mehana, M. Z. and J. Callard. Complex Fracture Depletion Model for Reserves Estimations in Shale. Submitted to *journal of energy resources technology*. (LA-UR-20-21346)

S. Mehana, M. Z. and M. Fahes. Molecular Simulation Study of Low salinity Waterflooding Mechanisms. Submitted to *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. (LA-UR-20-20808)

S. Mehana, M. Z. and M. Fahes. The Impact of the Geochemical Interactions on the Fate of Fracturing Fluid and Well Performance in Shale Reservoirs.. Submitted to *Petroleum*. (LA-UR-20-20809)

Mohamed, T., M. Z. S. Mehana and Z. Reza. Coalbed methane Review and Outlook. Submitted to *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*. (LA-UR-20-21924)

Qin, F., J. Zhao, Q. Kang, T. Brunschwiler, D. Derome and J. Carmeliet. Lattice Boltzmann modeling of heat conduction enhancement by colloidal nanoparticle deposition in micro-porous structures. Submitted to *Physical Review E*. (LA-UR-20-22138)

Samarakoon, A. M., K. M. Barros, Y. W. Li, M. Eisenbach, Q. Zhang, F. Ye, Z. L. Dun, H. Zhou, S. A. Grigera, C. D. Batista and A. D. Tennant. Machine Learning Assisted Insight to Spin Ice Dy2Ti2O7. Submitted to *Nature Communications*. (LA-UR-19-30738)

Wu, H., W. Z. Fang, Q. Kang, W. Q. Tao and R. Qiao. Predicting Effective Diffusivity of Porous Media from Images by Deep Learning. 2019. *Scientific Reports*. **9** (1): 20387. (LA-UR-19-23183 DOI: 10.1038/s41598-019-56309-x)

Presentation Slides

Li, Y. W. Machine Learning Assisted Monte Carlo Methods for the Studies of Materials Properties. Presented at *XXXI IUPAP Conference on Computational Physics*, Hong Kong, China, 2019-07-28 - 2019-08-01. (LA-UR-19-27508)

Lubbers, N. E. Realizing Physical Principles in Atomistic Machine Learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-19 - 2019-02-21. (LA-UR-19-21277)

Lubbers, N. E. Machine Learning & Neural Networks Tutorial. Presented at *IMAC XXXVIII*, Houston, Texas, United States, 2020-02-10 - 2020-02-13. (LA-UR-20-21292)

McKerns, M. rigorous model validation and engineering design under uncertainty. Presented at *Computational Data Science Approaches for Materials Conference*, Los Alamos, New Mexico, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-32500)

McKerns, M. mystic - a brief introduction. . (LA-UR-19-22525)

Rosenberger, D. G. Learning diffusion coefficients of particles with the help of thermodynamics. Presented at *2019 ALCF Simulation, Data, and Learning Workshop*, Argonne, Illinois, United States, 2019-10-01 - 2019-10-03. (LA-UR-19-29611)

Rosenberger, D. G. Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21573)

Viswanathan, H. S. Flow and Fracture in Microstructure Accelerated by Machine Learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-20 - 2019-02-20. (LA-UR-19-21272)

Posters

S. Mehana, M. Z., Q. Kang and H. S. Viswanathan. On the Molecular Modeling of Hydrocarbon Behavior in Shale Nano-pores. Presented at *LANL postdoc Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28695)

S. Mehana, M. Z., Q. Kang and H. S. Viswanathan. Molecular Modeling of the Fluid Behavior in shale Nanopores. Presented at *Postdoc Research Symposium*, Los alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28653)

Sagert, I., J. R. Haack, A. Diaw, C. Junghans, B. Keenan, N. E. Lubbers, M. McKerns, R. S. Pavel and D. Livescu. A 3D Multi-Species Kinetic-Fluid Coupling Technique for HEDP Simulations. Presented at *International Conference on Numerical Simulations of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28767)

Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics (U)

Boian Alexandrov
20190020DR

Project Description

The world's data is the most valuable exponentially-growing resource. Terabyte scale datasets are generated every minute by massive computer simulations, large-scale experiments, and global surveillance systems. Analyses of these data are of crucial importance for global security and directly related to Department of Energy mission-critical research areas. Development of machine learning (ML) techniques for efficient and robust data analyses is of paramount importance to perform timely, accurate, and meaningful data interpretation. Our project addresses this need by developing a novel ML methodology and a unique high-performance computing toolbox to perform data analyses and extract meaningful and interpretable features from high-dimensional extra-large datasets. High-dimensional data are naturally organized in tensors (multi-dimensional arrays) and our methodology will focus on cutting-edge tensor-based ML methods utilizing novel techniques. We will target terabyte and petabyte scale datasets in this project but if this high-risk/high-reward research is successful, the developed high-performance computing tools will be able to address larger problems. The new methodology will be important for DOE, the National Nuclear Security Administration, National Security Agency, Nuclear Regulatory Commission, Enviornmental Protection Agency, National Institutes of Health, and other agencies, placing the Laboratory in a leadership position in the field of Big-Data Analytics.

Publications

Journal Articles

Ahmmed, B., M. K. Mudunuru, S. Karra, S. C. James and V. V. Vesselinov. A Comparative Study of 20 Machine Learning Models for Predicting the State of Reactive Mixing. Submitted to *Journal of Computational Physics*. (LA-UR-20-21737)

Akhter, N., G. Chennupati, K. L. Kabir, H. Djidjev and A. Shehu. Unsupervised and Supervised Learning over the Energy Landscape for Protein Decoy Selection. 2019. *Biomolecules*. **9** (10): 607. (LA-UR-19-27828 DOI: 10.3390/biom9100607)

Alexandrov, B., B. Zhu, M. L. Poeta, M. Costantini, T. Zhang, J. Shi, S. S. Sentinelli, V. Pompeo, M. Cardelli, B. Otlu, X. Hua, K. Jones, S. Brodie, J. R. Toro, M. Yeager, M. Wang, B. Hicks, L. B. Alexandrov, K. M. Brown, S. Chanock, V. M. Fazio, M. Gallucci and M. T. Landi. Intratumor heterogeneity and clonal expansion cascade in papillary renal cell carcinoma. Submitted to *Genome Biology*. (LA-UR-18-31218)

Alexandrov, B., C. A. Lopez Bautista and S. Gnanakaran. Unsupervised Machine Learning for Analysis of Coexisting Lipid Phases and Domain Growth in Biological Membranes. Submitted to *JCTC*. (LA-UR-18-29079)

Alexandrov, B., D. F. DeSantis, G. Manzini and E. W. Skau. Nonnegative Canonic Polyadic Decomposition with Rank Deficient Factors. Submitted to *SIAM Journal on Mathematics of Data Science*. (LA-UR-19-29298)

Alexandrov, B., K. O. Rasmussen, G. Weissman, G. Bel, U. Yermiyahu, A. Ben-Gal and O. Dahan. Effects of salinity and soil heterogeneity on water, nitrate and bromide flow under agricultural fields. Submitted to *Vadose Zone Journal*. (LA-UR-19-31560)

Alexandrov, B., M. Karimi, V. Petkova, J. M. Asara, M. Griffin and A. Usheva. Aberrant cardiac energy metabolism in metabolic syndrome: insight from metabolomics and a pig model. Submitted to *Scientific Reports*. (LA-UR-19-25878)

Alexandrov, B., R. Vangara, K. O. Rasmussen, D. Petsev and G. Bel. Identification of 2D Anomalous Diffusion by Unsupervised Learning Combined with Green's Function Inverse Method. Submitted to *Physical Review E*. (LA-UR-19-25879)

Carrillo Cabada, H. A., E. W. Skau, G. Chennupati, B. Alexandrov and H. N. Djidjev. An Out of Memory tSVD for Big-Data Factorization. Submitted to *IEEE Access*. (LA-UR-20-22236)

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. Distributed Non-Negative Matrix Factorization with Determination of the Number of Latent

Features. Submitted to *Journal of Supercomputing*. (LA-UR-20-20469)

DeSantis, D. F., P. J. J. Wolfram, B. Alexandrov and K. E. Bennett. Multi-resolution Cluster Analysis - Addressing Trust in Climate Classification. Submitted to *Theoretical and applied climatology*. (LA-UR-19-27331)

Nebgen, B. T., R. Vangara, M. A. Hombrados Herrera, S. Kuksova and B. Alexandrov. A Neural Network for Determination of Latent Dimensionality in NMF. Submitted to *Machine Learning: Science and Technology*. (LA-UR-20-20994)

O'Malley, D., H. N. Djidjev and B. Alexandrov. Boolean Tensor Factorization with QuantumAnnealers. Submitted to *npj Quantum Information*. (LA-UR-20-21860)

O'Malley, D., J. K. Golden and V. V. Vesselinov. Learning to regularize with a variational autoencoder for hydrologic inverse analysis. Submitted to *Water Resources Research*. (LA-UR-19-24983)

Truong, D. P., E. W. Skau, V. I. Valtchinov and B. Alexandrov. Determination of Latent Dimensionality in International Trade Flow. Submitted to *Machine Learning: Science and Technology*. (LA-UR-20-21947)

Conference Papers

Alexandrov, B., G. Manzini and E. W. Skau. Nonnegative Canonic Polyadic Decomposition for Tensors with Rank Deficient Factors. Presented at *International Conference on Machine Learning*. (Long Beach, California, United States, 2019-06-10 - 2019-06-15). (LA-UR-19-20517)

Nasrin, A., R. Vangara, G. Chennupati, B. Alexandrov, H. N. Djidjev and S. Amarda. Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures. Presented at *IEEE International Conference on Bioinformatics and Biomedicine*. (San Diego, California, United States, 2019-11-18 - 2019-11-21). (LA-UR-19-30412)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Optimizing the spin reversal transform on the D-Wave 2000Q. Presented at *ICRC 2019*. (San Mateo, California, United States, 2019-11-06 - 2019-11-08). (LA-UR-19-25307)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Peering into the Anneal Process of a Quantum Annealer. Presented at *PDCAT 2019*. (Gold Coast, Australia, 2019-12-05 - 2019-12-07). (LA-UR-19-27870)

Reports

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. distNMFk: Distributed Non-negative Matrix Factorization to Extract Optimal Number of Features. Unpublished report. (LA-UR-19-25810)

Presentation Slides

Alexandrov, B. Unsupervised Phase Mapping of X-ray Diffraction Data by Nonnegative Matrix Factorization. Presented at *Invited talk in UC Irvine University on AI and Materials*, Irvine, California, United States, 2019-11-21 - 2019-11-21. (LA-UR-19-31561)

Chennupati, G. Massively Parallel Big-Data Nonnegative Factorization. Presented at *Internal DR appraisal review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21162)

Chennupati, G., R. Vangara, E. W. Skau, H. N. Djidjev and B. Alexandrov. Distributed Non-negative Matrix Factorization with Model Determination. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Los Alamos, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29294)

Kober, E. M., M. F. Francis, R. Vangara and B. Alexandrov. Tensor Factorization Applied to the Reaction Analysis of Energetic Materials. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29243)

Marcillo, O. E. and J. K. MacCarthy. Mapping Tonal Noise in the Continental US. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29507)

Nebgen, B. T., J. K. MacCarthy and B. Alexandrov. Non-Negative Tensor Factorization for Interpretable Unsupervised Signal Discovery in Continuous Seismic Data. Presented at *Seismological Society of America National Meeting*, Seattle, Washington, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23443)

Nebgen, B. T., R. Vangara, S. Kuksova, M. A. Hombrados Herrera and B. Alexandrov. Machine Learning for Automated Feature Recognition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29238)

O'Malley, D. Tensor factorization with quantum annealing. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29405)

Skau, E. W. Nonnegative Canonical Polyadic Decomposition with Rank Deficient Factors. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29328)

Vesselinov, V. V. Physics-Informed Machine Learning Methods for Data Analytics and Model Diagnostics. Presented at *M3 DRIVE Science Center:*, Los Alamos, New Mexico, United States, 2019-05-14 - 2019-05-14. (LA-UR-19-24562)

Posters

Bhattarai, M., R. Vangara, G. Chennupati, J. M. Patchett, J. P. Ahrens and B. Alexandrov. pyDnMFk: A Python implementation of Distributed Non-Negative Matrix

Factorization with determination of Rank. Presented at *LDRD Project Review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21243)

Carrillo Cabada, H. A., E. W. Skau, G. Chennupati, H. N. Djidjev and B. Alexandrov. Out-of-Core Singular Value Decomposition for the Tensor Train Decomposition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29330)

Carrillo, H., E. W. Skau, G. Chennupati, H. N. Djidjev and B. Alexandrov. Out-of-Core Singular Value Decomposition for the Tensor Train Decomposition. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29862)

Francis, M. F., E. M. Kober, B. Alexandrov, R. Vangara and B. T. Nebgen. Machine Learning of Transient Chemical Kinetics: NMF, NN, and SVR of HMX. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29274)

Hombrados Herrera, M. A., R. Vangara, E. W. Skau and B. Alexandrov. Methods for determination of dimensionality of latent features: Principal Angles and PCAk. Presented at *AI and Tensor Factorizations for Physical, Chemical and Biological Systems.*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-19. (LA-UR-19-29467)

Kuksova, S., B. Alexandrov and K. O. Rasmussen. Nonegative Tensor Train Analysis for Feature Extraction. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29464)

M. Mallory, E. J., B. T. Nebgen, O. E. Marcillo, J. K. MacCarthy, K. O. Rasmussen and B. Alexandrov. Tensor Decomposition for Mars Seismology. Presented at *Elizabeth Mallory*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-17. (LA-UR-19-29281)

M. Mallory, E. J., T. B. Peery and M. F. Francis. Statistical Representations and Unbiased Metrics for Stable Isotope Fractionation. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32132)

Nasrin, A., R. Vangara, G. Chennupati, B. Alexandrov, H. N. Djidjev and S. Amarda. Non-Negative Matrix Factorization for Decoy Selection from Ensembles. Presented at *AI and Tensor Factorization in Physics, Chemistry and Biology*, Los Alamos, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29332)

Rasmussen, K. O., E. J. M. Mallory, B. T. Nebgen, O. E. Marcillo, J. K. MacCarthy and B. Alexandrov. Tensor Decomposition for Mars Seismology. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, SANTA FE, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29777)

Rasmussen, K. O., G. Bel, R. Vangara, D. Petsev and B. Alexandrov. Unsupervised Learning for Anomalous Diffusion Source Identification. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29256)

Rasmussen, K. O., S. Kuksova and B. Alexandrov. Nonnegative Tensor Train Analysis for Feature Extraction. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29776)

Rijal, B., B. T. Nebgen, C. A. Neale and B. Alexandrov. Tensor Factorization for Protein Conformation Identification. Presented at *AI and Tensor Factorization for Physical, Chemical and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29311)

Skau, E. W. Symmetric Tucker Rank Determination. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29329)

Truong, D., E. W. Skau and B. Alexandrov. Symmetric Tucker Rank Determination. Presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*, Santa Fe, New Mexico, United States, 2019-09-17 - 2019-09-20. (LA-UR-19-29863)

Vangara, R., E. M. Kober and B. Alexandrov. Tensor Methods for Reaction Analysis of Energetic Materials and High Explosives. Presented at *DR Midterm Review*, Los Alamos, New Mexico, United States, 2020-02-10 - 2020-02-10. (LA-UR-20-21230)

Vangara, R., G. Chennupati and B. Alexandrov. Symmetric Non-Negative Matrix Factorization with PAC for Estimating Number of Clusters. Presented at *Conference on Data Analysis (CODA 2020)*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21809)

Machine Learning for Turbulence

Daniel Livescu
20190059DR

Project Description

Machine Learning for Turbulence will develop a novel framework which will dramatically improve models used in hydrodynamic codes at Los Alamos National Laboratory and other National Laboratories of the Department of Energy. The models are significant for such mission critical applications as weapons design and simulations, modeling and predictive weather and understanding astrophysical phenomena. Our main hypothesis is that an automatic design of the hydrodynamic closures is achievable through new approach, coined Physics Informed Machine Learning, suggesting and developing smart embedding of the underlying physics into Machine Learning techniques. We will test the hypothesis by developing a theoretical and algorithmic methods guided by insight from the hydrodynamic applications of interest. We will examine the power of the new tools in bridging existing approaches. Thus, application agnostic machine learning will be augmented with the physical constraints reflecting basic hydrodynamic symmetries. Complementary, current Laboratory closure models of turbulence will be enhanced by embedding into them Neural Networks thus allowing automatic evaluation, larger time steps and faster in line computations.

Publications

Journal Articles

Andrews, S. J., C. L. Fryer, S. Jones, W. P. Even and M. Pignatari. The Nucleosynthetic Yields of Core-Collapse Supernovae, prospects for the Next Generation of Gamma-Ray Astronomy. Submitted to *Astrophysical Journal*. (LA-UR-19-30411)

Chertkov, M., M. Escobar Santoro and D. Bienstock. Learning from power system data stream: phasor - detective approach. Submitted to *Arvix*. (LA-UR-18-30924)

Chertkov, M. and Y. Maximov. Gauges, Loops & Polynomials for Partition Functions of Graphical Model. Submitted to *IEEE Transactions on Information Theory (tentative)*. (LA-UR-18-30593)

Li, B., D. Saad and A. Lokhov. Reducing Urban Traffic Congestion Due To Localized Routing Decisions. Submitted to *Physical Review Letters*. (LA-UR-20-22351)

Likhosherstov, V., Y. Maximov and M. Chertkov. Tractable Minor-free Generalization of Planar Zero-field Ising Models. Submitted to *IEEE Transactions on Information Theory*. (LA-UR-19-30102)

Maulik, R., A. T. Mohan, B. Lusch, S. Madireddy, P. Balaprakash and D. Livescu. Time-series learning of latent-space dynamics for reduced-order model closure. Submitted to *Physica D: Nonlinear Phenomena*. (LA-UR-19-28714)

Mohan, A. T., D. Daniel, M. Chertkov and D. Livescu. COMPRESSED CONVOLUTIONAL LSTM: AN EFFICIENT DEEP LEARNING FRAMEWORK TO MODEL HIGH FIDELITY 3D TURBULENCE. Submitted to *Arxiv*. (LA-UR-19-21568)

Mohan, A. T., N. E. Lubbers, D. Livescu and M. Chertkov. Embedding Hard Physical Constraints in Neural Network Coarse-Graining of 3D Turbulence. Submitted to *Physical Review Fluids*. (LA-UR-20-20560)

Portwood, G. D., B. T. Nadiga, J. A. Saenz and D. Livescu. Diagnostics and interprettability of out-performing artificial neural network residual flux models. Submitted to *Journal of Fluid Mechanics Rapids*. (LA-UR-20-20405)

Portwood, G. D., S. de Bruyn Kops, E. Rietman and D. Saunders. Unsupervised Machine Learning to Teach Fluid Dynamicists to Think in 15 Dimensions. Submitted to *Journal of Turbulence*. (LA-UR-19-27313)

Pulido, J. J., R. Dutra da Silva, D. Livescu and B. Hamann. Multiresolution Classification of Turbulence Features Through Image Processing. Submitted to *Computers & Fluids*. (LA-UR-19-31868)

Conference Papers

Mohan, A. T., D. Livescu and M. Chertkov. Wavelet-Powered Neural Networks for Turbulence. Presented at *33rd Conference on Neural Information Processing Systems (NeurIPS)*. (Vancouver, Canada, 2019-12-14 - 2019-12-14). (LA-UR-19-31274)

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)

Reports

Belyy, A., A. Sholokhov, M. R. Amini and Y. Maximov. MEMOIR: Multi-class Extreme Classification with Inexact Margin. Unpublished report. (LA-UR-19-21219)

Chertkov, M., Y. Maximov and V. LIkhosherstov. Inference and Sampling of K(3,3)-free Ising Models. Unpublished report. (LA-UR-18-31783)

Crum, J. R. LANL MELT Project. Unpublished report. (LA-UR-19-27901)

Krechetov, M., Y. Maximov, J. Marecek and M. Takac. Entropy-Penalized Semidefinite Programming. Unpublished report. (LA-UR-18-24430)

Likhosherstov, V., Y. Maximov and M. Chertkov. Inference and Sampling of K33-free Ising Models. Unpublished report. (LA-UR-19-26932)

Likhosherstov, V., Y. Maximov and M. Chertkov. A New Family of Tractable Ising Models. Unpublished report. (LA-UR-19-24712)

Presentation Slides

Aslangil, D. Denis Aslangil web-page contents (denisaslangil.com). . (LA-UR-20-20826)

Livescu, D. LDRD DR – MELT: Machine Learning for Turbulence. . (LA-UR-20-20578)

Maulik, R., A. T. Mohan, S. Madireddy, B. Lusch, P. Balaprakash and D. Livescu. MACHINE LEARNING OF SEQUENTIAL DATA FOR REDUCED ORDER MODELS. Presented at *APS DFD 2019*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31882)

Mitra, P. P. and G. D. Portwood. Improving climate sub-closures with ML. Presented at *NVIDIA GTC 2020: Deep Learning & AI Conference*, San Jose, California, United States, 2020-03-22 - 2020-03-26. (LA-UR-19-29812)

Mohan, A. T. Deep Learning for Efficient Modeling of High Dimensional Spatiotemporal Physics. Presented at *Nvidia GTC Conference 2020*, San Jose, California, United States, 2020-03-23 - 2020-03-26. (LA-UR-20-21748)

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Portwood, G. D., P. P. Mitra, M. Dias Ribeiro, T. Nguyen, B. T. Nadiga, J. A. Saenz, M. Cherkov, A. Garg, A. Anandkumar, A. Dengel, R. Baraniuk and D. Schmidt. Turbulence Forecasting via Neural ODEs. Presented at *NeurIPS 2019 Workshop on Machine Learning and the Physical Sciences*, Vancouver, Canada, 2019-12-13 - 2019-12-14. (LA-UR-19-31796)

Taming Defects in Quantum Computers

Scott Pakin

20190065DR

Project Description

Since the enactment of the Comprehensive Nuclear Test Ban Treaty, stockpile stewardship has relied heavily on computer simulations of weapons effects. Until recently, continuous improvements in supercomputing technology have made it possible to increase the physics fidelity of these simulations without unduly slowing them down. Alas, with all of the low-hanging fruit long since picked, performance improvements are becoming increasing elusive with each new generation of supercomputers. The situation existentially threatens the National Nuclear Security Administration's ability to ensure the safety, security, and effectiveness of America's nuclear stockpile. Quantum computing is a new technology that offers the potential of drastically improved computational speed—well beyond what any supercomputer in the foreseeable future is capable of. Unfortunately, early quantum computers are extremely unreliable and extremely difficult to program. Our project will address both those issues. We will develop a framework that enables NNSA computational scientists to describe a mapping of inputs to outputs and automatically converts that mapping into a quantum algorithm, and one that is customized to work around a particular quantum computer's individual shortcomings. This will enable stockpile stewardship simulations to continue their prior trajectory of ever-improving accuracy and ever-improving utility to national security.

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.

Technical Outcomes

Bayesian statistical emulation was used to quickly estimate model parameters for dynamic compression simulations and to provide uncertainties and sensitivities with those parameters. Emulation was demonstrated for two experimental datatypes, velocimetry and X-ray diffraction, showing that emulation can be a useful real-time tool to guide experimentalists. Multi-view visualization tools, accelerated workflows and optimization techniques were developed to speed up experimental data analysis. A dynamic compression data analysis workflow was deployed at a light source experiment.

Publications

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Biswas, A., J. P. Ahrens and E. C. Lawrence. High-Dimensional Data Analysis and Visualization Using High Fidelity Emulators with Uncertainty. Presented at *IEEE Vis*. (Berlin, Germany, 2018-03-31 - 2018-03-31). (LA-UR-18-22810)

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Biswas, A., K. R. Moran, J. P. Ahrens and E. C. Lawrence. Visualization of Uncertainty for Computationally Intensive Simulations Using High Fidelity Emulators. Presented at *Ieee visualization*. (berlin, Germany, 2018-10-21 - 2018-10-21). (LA-UR-18-28622)

W. Myren, S. T., E. Herrera, A. J. Shoats, E. C. Lawrence, E. M. Casleton, D. J. Luscher and S. J. Fensin. Input Estimation and Dimension Reduction for Material Models. Presented at *IMAC XXXVII*. (Orlando, Florida, United States, 2019-01-28 - 2019-01-28). (LA-UR-18-28203)

Orban, D. T., D. Keefe, A. Biswas, J. P. Ahrens and D. H. Rogers. Drag and Track: A Direct Manipulation Interface for Contextualizing Data Instances within a Continuous Parameter Space: Application to Shock Physics. Presented at *IEEE Vis*. (Berlin, Germany, 2018-10-21 - 2018-10-26). (LA-UR-18-22844)

Reports

Banesh, D., D. C. Francom, D. J. Walters, J. L. Barber, K. J. Ramos, C. A. Bolme, C. M. Biwer and J. P. Ahrens. Comparison of experimental and simulated single crystal diffraction datasets using geometric hashing. Unpublished report. (LA-UR-18-30543)

Biwer, C. M., M. McKerns, S. C. Vogel and J. P. Ahrens. Spotlight: Automation of Rietveld analyses using an ensemble of local optimizers. Unpublished report. (LA-UR-18-30288)

Hou, E. M. and E. C. Lawrence. Notes on Fast Calibration with Gaussian Mixture of Experts. Unpublished report. (LA-UR-18-29108)

Orban, D. T. Design Queries: Toward Immersive Exploration of Large Parameter Spaces using Visual Comparison and Direct Manipulation of Query Widgets. Unpublished report. (LA-UR-18-22845)

Presentation Slides

Ahrens, J. P. Supporting Knowledge-based Decision-making via Accelerated High-dimensional Analysis and Modeling of Simulation and Experimental Scientific Data. Presented at *Invited Talk for LBNL Camera Group*, Berkeley, California, United States, 2017-10-16 - 2017-10-16. (LA-UR-17-29736)

Ahrens, J. P. Supercharging the Scientific Process Via Data Science at Scale. Presented at *New York Scientific Data Summit*, New York, New York, United States, 2017-08-07 - 2017-08-09. (LA-UR-17-29754)

Ahrens, J. P. Data Science for Material Science - A Database, Data-driven Modeling and Visualization Approach. Presented at *Computational Data Science Approaches for Materials*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-25628)

Ahrens, J. P. Project Overview: Real-time Adaptive Acceleration of Dynamic Experimental Science. Presented at *LANL ICF/HED Community Seminar Series*, Los Alamos, New Mexico, United States, 2020-01-13 - 2020-01-13. (LA-UR-20-20298)

Ahrens, J. P., C. A. Bolme and R. L. Sandberg. LANL LDRD ASSIST: Progress Appraisal, Review criteria and our responses. Presented at *2nd Year LDRD-DR Project Review*, Los Alamos, New Mexico, United States, 2019-01-23 - 2019-01-23. (LA-UR-19-20505)

Ahrens, J. P., D. Banesh, J. L. Barber, D. Bingham, A. Biswas, C. M. Biwer, C. A. Bolme, M. J. Cawkwell, S. Dutta, D. C. Francom, D. A. Fredenburg, A. Krishnapriyan, E. C. Lawrence, D. J. Luscher, K. R. Moran, D. T. Orban, A. Ramanathan, K. J.

Ramos, D. H. Rogers, R. L. Sandberg, C. M. Sweeney, C. S. Tauxe, A. Tripathi, S. C. Vogel and D. J. Walters. LDRD DR Mid-project Review: Real-time Adaptive Acceleration of Dynamic Experimental Science. . (LA-UR-18-21337)

Ahrens, J. P., D. Banesh, J. L. Barber, D. Bingham, A. Biswas, C. M. Biwer, C. A. Bolme, M. J. Cawkwell, S. Dutta, D. C. Francom, D. A. Fredenburg, A. Krishnapriyan, E. C. Lawrence, D. J. Luscher, K. R. Moran, D. T. Orban, A. Ramanathan, K. J. Ramos, D. H. Rogers, R. L. Sandberg, C. M. Sweeney, C. S. Tauxe, A. Tripathi, S. C. Vogel and D. J. Walters. Real-time Adaptive Acceleration of Dynamic Experimental Science. . (LA-UR-18-24270)

Barber, J. L. An Overview of Bragg Scattering. . (LA-UR-16-29465)

Biwer, C. M. Automation of diffraction analyses and real-time data exploration. Presented at *Advancing the Development Cycle Through Intelligent Materials Design, Informatics, and Characterization Workshop*, Golden, Colorado, United States, 2018-09-06 - 2018-09-06. (LA-UR-18-28647)

Bolme, C. A. LANL in-kind contributions to HiBEF. Presented at *European XFEL Users Meeting*, Hamburg, Germany, 2020-01-28 - 2020-01-28. (LA-UR-20-20747)

Bolme, C. A., A. Biswas, C. M. Biwer, D. J. Walters, D. T. Orban, D. C. Francom, E. C. Lawrence, D. Banesh, C. S. Tauxe, K. R. Moran, R. A. Saavedra, C. M. Sweeney, R. L. Sandberg, D. J. Luscher, D. A. Fredenburg, D. H. Rogers and J. P. Ahrens. Data analytics for XFEL HED experiments. . (LA-UR-20-20193)

Bolme, C. A., D. A. Fredenburg and C. M. Sweeney. Plots from Trial 3 of Al-Al FLAG Simulations. Presented at *IEEE Visual Analytics Science and Technology*, Pheonix, Arizona, United States, 2017-10-01 - 2017-10-01. (LA-UR-17-25330)

Bolme, C. A., D. A. Fredenburg and C. M. Sweeney. Plots from Al-Al FLAG Simulations -- Trial 4. Presented at *IEEE Visual Analytics Science and Technology*, Pheonix, Arizona, United States, 2017-10-01 - 2017-10-01. (LA-UR-17-25398)

Bolme, C. A., D. T. Orban, D. Banesh, C. S. Tauxe, C. M. Biwer, A. Biswas, R. A. Saavedra, C. M. Sweeney, R. L. Sandberg, J. P. Ahrens and D. H. Rogers. Workflow and visual analysis for XFEL shock physics experiments using Cinema:Bandit. Presented at *American Physical Society - Shock Compression of Condensed Matter Topical Group Conference*, Portland, Oregon, United States, 2019-06-17 - 2019-06-21. (LA-UR-19-25598)

Cawkwell, M. J., F. L. Addessio, D. J. Luscher, J. L. Barber, C. A. Bolme, R. L. Sandberg and K. J. Ramos. Anisotropic Mechanics of Energetic Materials. Presented at *Mesoscale Modeling of Explosives Initiation*, Santa Fe, New Mexico, United States, 2017-09-26 - 2017-09-28. (LA-UR-17-28635)

Dutta, S., J. L. Woodring and J. P. Ahrens. Uncertainty, sensitivity, and error analysis and visualization of high-dimensional Input-output models. . (LA-UR-17-28481)

Francom, D. C. Statistical Emulation and Inverse Modeling. Presented at *Gap Analysis: Materials Discovery through Data Science at Advanced User Light Sources*, Santa Fe, New Mexico, United States, 2018-10-03 - 2018-10-03. (LA-UR-18-29444)

Francom, D. C. Functional Nonlinear Regression and Registration using Bayesian Adaptive Splines. Presented at *Joint Research Conference*, Santa Fe, New Mexico, United States, 2018-06-11 - 2018-06-11. (LA-UR-18-25027)

Francom, D. C., E. C. Lawrence, D. R. Bingham, D. Banesh, C. M. Biwer, J. L. Barber, D. J. Walters, D. J. Luscher, S. C. Vogel, J. D. Lazarz, C. A. Bolme, R. L. Sandberg, J. P. Ahrens, D. H. Rogers and C. M. Sweeney. Toward Real-Time Decision Making in Experimental Settings. Presented at *Defense and Aerospace Test and Analysis (DATA) Workshop*, Springfield, Virginia, United States, 2019-04-09 - 2019-04-11. (LA-UR-19-22965)

Hou, E. M. and E. C. Lawrence. Variational Methods for Posterior Estimation of Non-linear Inverse Problems. . (LA-UR-18-29254)

Lawrence, E. C. and B. P. Weaver. Model Emulation and Calibration: Uncertainty Quantification and Making Inference with Simulation. . (LA-UR-19-24650)

McKerns, M. rigorous model validation and engineering design under uncertainty. Presented at *Computational Data Science Approaches for Materials Conference*, Los Alamos, New Mexico, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-32500)

Orban, D. T. Interactive VisualQuerying of Large Parameter Spaces: Shooting the Unknown While Controlling Stress Under Pressure. . (LA-UR-17-30271)

Orban, D. T. Drag and Track Videos. Presented at *IEEE VIS 2018*, Berlin, Germany, 2018-10-21 - 2018-10-21. (LA-UR-18-28319)

Orban, D. T. Drag and Track Fast Forward Video. Presented at *IEEE VIS 2018*, Berlin, Germany, 2018-10-21 - 2018-10-21. (LA-UR-18-28320)

Orban, D. T., D. F. Keefe, A. Biswas, J. P. Ahrens and D. H. Rogers. Drag and Track: A Direct Manipulation Interface for Contextualizing Data Instances within a Continuous Parameter Space. Presented at *IEEE VIS 2018*, Berlin, Germany, 2018-10-19 - 2018-10-19. (LA-UR-18-29162)

Sandberg, R. L. Current and future detector needs for coherent imaging experiments at XFELs. Presented at *Ulitima Conference*, Lemont, Illinois, United States, 2018-09-11 - 2018-09-14. (LA-UR-18-28666)

Sandberg, R. L., C. A. Bolme, J. P. Ahrens, C. M. Sweeney, D. H. Rogers, E. C. Lawrence, A. Biswas, M. J. Cawkwell, K. J. Ramos, S. C. Vogel, D. J. Luscher, J. L. Barber, D. J. Walters, D. Banesh and C. M. Biwer. Tools for Real-time Adaptive Acceleration of Dynamic Compression Science at Light Sources. Presented at *CoDA 2018: Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2018-03-07 - 2018-03-09. (LA-UR-18-21916)

Sandberg, R. L., C. A. Bolme, J. P. Ahrens, C. M. Sweeney, D. H. Rogers, E. C. Lawrence, A. Biswas, M. J. Cawkwell, K. J. Ramos, S. C. Vogel, D. J. Luscher, J. L. Barber, D. J. Walters, D. Banesh, C. M. Biwer and D. T. Orban. Data visualization and organization tools for dynamic compression science at XFELs. Presented at *ULITIMA Conference*, Lemont, Illinois, United States, 2018-09-11 - 2018-09-13. (LA-UR-18-28676)

Sandberg, R. L., C. A. Bolme and J. P. Ahrens. Tools for Real-time Adaptive Acceleration of Dynamic Compression Science at Light Sources. Presented at *LCLS/SSRL User Meeting*, Menlo Park, California, United States, 2017-09-27 - 2017-09-29. (LA-UR-17-28807)

Stokes, S. R. and D. C. Francom. Emulating Flyer Plate Simulation Data. . (LA-UR-19-28218)

Sweeney, C. M. Light Source Application Patterns and Components for Advanced Cyberinfrastructure Platform (ACP). Presented at *Big Data and Extreme-Scale Computing 2*, Kobe, Japan, 2019-02-19 - 2019-02-21. (LA-UR-19-21322)

Sweeney, C. M. Addressing Challenges of High-Repetition and High-Throughput Data Analysis at Advanced User Light Sources. Presented at *LANL Delegation visiting Eu-XFEL*, Hamburg, Germany, 2019-04-08 - 2019-04-09. (LA-UR-19-22604)

Sweeney, C. M. Addressing Challenges of High-Repetition and High-Throughput Data Analysis at Advanced User Light Sources. . (LA-UR-19-21459)

Vogel, S. C., J. P. Ahrens, C. A. Bolme, D. J. Luscher, R. L. Sandberg, E. C. Lawrence, M. J. Cawkwell, C. M. Sweeney and D. H. Rogers. Real-Time Adaptive Acceleration of Dynamic Experimental Science. Presented at *APS User Meeting*, Argonne, Illinois, United States, 2017-05-08 - 2017-05-09. (LA-UR-17-23736)

Vogel, S. C., V. W. C. Yuan, S. Takajo, L. Lutterotti, G. T. I. Gray, C. P. Trujillo, D. W. Brown and C. A. Bolme. Dynamic Compression Characterization by the MST-8 Scattering Team. Presented at *Informal Seminar at European XFEL/DESY*, Hamburg, Germany, 2019-10-14 - 2019-10-14. (LA-UR-19-30197)

Posters

Ahrens, J. P., C. A. Bolme, R. L. Sandberg, D. Banesh, A. Biswas, C. M. Biwer, D. C. Francom, D. J. Luscher, A. Tripathi and S. C. Vogel. Posters for LDRD-DR mid-project review: Real-time Adaptive Acceleration of Dynamic Experimental Science. . (LA-UR-18-21341)

Banesh, D., C. M. Biwer, J. D. Lazarz, J. L. Barber, D. J. Walters, K. J. Ramos, A. Biswas, D. C. Francom, D. J. Luscher, P. J. Nichols, C. A. Bolme, R. L. Sandberg and J. P. Ahrens. Approaches to Indexing X-ray Diffraction Patterns from Low Symmetry Single Crystals on Dynamic Loading Platforms. . (LA-UR-19-21353)

Banesh, D., C. M. Biwer, J. D. Lazarz, J. L. Barber, D. J. Walters, K. J. Ramos, A. Biswas, D. C. Francom, D. J. Luscher, P. J. Nichols, C. A. Bolme, R. L. Sandberg and J. P. Ahrens. Analysis of the X-Ray Diffraction Experimental Parameter Space through Simulation Comparison using Geometric Hashing. Presented at *Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23047)

Biswas, A., C. M. Biwer, J. P. Ahrens, C. A. Bolme and R. L. Sandberg. Exploration of Ensemble Data Via Interactive User Inputs. Presented at *Stanford Synchrotron Radiation Lightsource (SSRL) and the Linac Coherent Light Source (LCLS) User Meeting 2017*, Menlo Park, California, United States, 2017-09-27 - 2017-09-29. (LA-UR-17-28808)

Biwer, C. M., S. C. Vogel, M. McKerns and J. P. Ahrens. Developing automation and data exploration capabilities for diffraction analysis. Presented at *LANSCE User Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30659)

Moran, K. R. and E. C. Lawrence. Improving experimental uncertainty via pre-built Gaussian process emulators (alternatively, shooting things with lasers and getting feedback really quickly). Presented at *DOE Computational Science Graduate Fellowship 2017 Annual Program Review*, Arlington, Virginia, United States, 2017-07-24 - 2017-07-27. (LA-UR-17-26057)

Orban, D. T., A. Biswas, D. H. Rogers, J. P. Ahrens and D. F. Keefe. Drag and Track: A Direct Manipulation Interface for Contextualizing Data Instances within a Continuous Parameter Space. Presented at *Student Symposium 2018*, Los Alamos, New Mexico, United States, 2018-07-30 - 2018-08-02. (LA-UR-18-26961)

Ramanathan, A., S. C. Vogel, D. W. Brown and M. Okuniewski. Treating nuclear fuels to make the world a safer place. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2017-08-09 - 2017-08-09. (LA-UR-17-27098)

Walters, D. J., D. J. Luscher, M. J. Cawkwell, F. L. Addessio, J. L. Barber, K. J. Ramos and C. A. Bolme. Modeling the anisotropic shock response of single-crystal RDX. Presented at *2017 SSRL/LCLS Users' Meeting at SLAC*, Menlo Park, California, United States, 2017-09-27 - 2017-09-29. (LA-UR-17-28664)

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.

Technical Outcomes

The research project developed revolutionary high-order hydrodynamic methods that have both excellent data locality and compute intensity, and that can accurately simulate complex multi-phase, multi-material flows. These novel methods are designed for performant calculations on advanced computer architectures such as graphics processing units (GPUs) that comprise exascale machines. The results from the project can benefit many programs of national importance ranging from simulating inertial confinement fusion (ICF) implosions to the design of high-explosive experiments.

Publications

Journal Articles

Abgrall, R., K. Lipnikov, N. R. Morgan and S. Tokareva. Multidimensional staggered grid residual distribution scheme for Lagrangian hydrodynamics. Submitted to *SIAM Journal on Scientific Computing*. (LA-UR-18-30342)

Abgrall, R., P. Bacigaluppi and S. Tokareva. "A Posteriori" Limited High Order and Robust Residual Distribution Schemes for Transient Simulations of Fluid Flows in Gas Dynamics. Submitted to *Journal of Computational Physics*. (LA-UR-19-21536)

Burton, D. E., N. R. Morgan, X. Liu, M. R. Berry, K. Lipnikov and E. Lieberman. A compatible Lagrangian discontinuous Galerkin hydrodynamic method for 2D and 3D gas dynamics on polytopal cells. Submitted to *Journal of Computational Physics*. (LA-UR-18-23834)

*Chiravalle, V. P. and N. R. Morgan. A 3D Lagrangian cell-centered hydrodynamic method with higher-order reconstructions for gas and solid dynamics. 2019. *Computers & Mathematics with Applications*. **78** (2): 298-317. (LA-UR-17-30750 DOI: 10.1016/j.camwa.2018.06.011)

*Lieberman, E. J., N. R. Morgan, D. J. Luscher and D. E. Burton. A higher-order Lagrangian discontinuous Galerkin hydrodynamic method for elastic–plastic flows. 2019. *Computers & Mathematics with Applications*. **78** (2): 318-334. (LA-UR-17-30257 DOI: 10.1016/j.camwa.2018.08.020)

*Lieberman, E. J., X. Liu, N. R. Morgan, D. J. Luscher and D. E. Burton. A higher-order Lagrangian discontinuous Galerkin hydrodynamic method for solid dynamics. 2019. *Computer Methods in Applied Mechanics and Engineering*. **353**: 467-490. (LA-UR-18-27653 DOI: 10.1016/j.cma.2019.05.006)

Lieberman, E., X. Liu, N. R. Morgan and D. E. Burton. A higher-order Lagrangian discontinuous Galerkin hydrodynamic method for high-explosive detonation physics. Submitted to *Journal of Computational Physics*. (LA-UR-19-26917)

Lipnikov, K. and N. Morgan. A high-order discontinuous Galerkin method for level set problems on polygonal meshes. 2019. *Journal of Computational Physics*. **397**: 108834. (LA-UR-18-29017 DOI: 10.1016/j.jcp.2019.07.033)

Lipnikov, K. and N. R. Morgan. A high-order conservative remap for DG schemes on curvilinear polygonal meshes. Submitted to *Journal of Computational Physics*. (LA-UR-18-31706)

Lipnikov, K. and N. R. Morgan. Conservative high-order discontinuous Galerkin remap scheme on curvilinear polytopal meshes. Submitted to *Journal of Computational Physics*. (LA-UR-20-20017)

Liu, X., J. Lou, H. Luo and H. Nishikawa. Reconstructed Discontinuous Galerkin Methods for Hyperbolic Diffusion Equations on Unstructured Grids. Submitted to *Communications in Computational Physics*. (LA-UR-19-20815)

Liu, X., L. Xuan, Y. Xia and H. Luo. A Reconstructed Discontinuous Galerkin Method for the Compressible Navier-Stokes Equations on 3D Hybrid Grids. Submitted to *Computers & Fluids*. (LA-UR-19-20828)

Liu, X., N. R. Morgan and D. E. Burton. A Lagrangian discontinuous Galerkin hydrodynamic method. Submitted to *AIAA Conference Proceedings*. (LA-UR-17-24651)

*Liu, X., N. R. Morgan and D. E. Burton. A Lagrangian discontinuous Galerkin hydrodynamic method. 2018. *Computers & Fluids*. **163**: 68-85. (LA-UR-17-24361 DOI: 10.1016/j.compfluid.2017.12.007)

Liu, X., N. R. Morgan and D. E. Burton. A high-order Lagrangian discontinuous Galerkin hydrodynamic method for quadratic cells : An accurate high-order face integral. Submitted to *journal of computational physics*. (LA-UR-18-28880)

*Liu, X., N. R. Morgan and D. E. Burton. Lagrangian discontinuous Galerkin hydrodynamic methods in axisymmetric coordinates. 2018. *Journal of Computational Physics*. **373**: 253-283. (LA-UR-18-21449 DOI: 10.1016/j.jcp.2018.06.073)

*Liu, X., N. R. Morgan and D. E. Burton. A high-order Lagrangian discontinuous Galerkin hydrodynamic method for quadratic cells using a subcell mesh stabilization scheme. 2019. *Journal of Computational Physics*. **386**: 110-157. (LA-UR-18-26689 DOI: 10.1016/j.jcp.2019.02.008)

Liu, X., N. R. Morgan and D. E. Burton. A WENO-based symmetry-preserving Lagrangian discontinuous Galerkin hydrodynamic method. Submitted to *Journal of Computational Physics*. (LA-UR-19-22578)

Liu, X., N. R. Morgan and D. E. Burton. A robust second-order accurate Lagrangian discontinuous Galerkin cell-centered hydrodynamic method on quadratic triangular cells. Submitted to *Computer Methods in Applied Mechanics and Engineering*. (LA-UR-19-25292)

Liu, X., Y. Xia and H. Luo. A reconstructed discontinuous Galerkin method for compressible turbulent flows on 3D curved grids. Submitted to *Computers & Fluids*. (LA-UR-19-20801)

Morgan, N. R., X. Liu and D. E. Burton. A Lagrangian discontinuous Galerkin hydrodynamic method for higher-order triangular elements. Submitted to *AIAA Conference Proceedings*. (LA-UR-17-24635)

*Morgan, N. R., X. Liu and D. E. Burton. Reducing spurious mesh motion in Lagrangian finite volume and discontinuous Galerkin hydrodynamic methods. 2018. *Journal of Computational Physics*. **372**: 35-61. (LA-UR-17-29885 DOI: 10.1016/j.jcp.2018.06.008)

*Petrella, M., S. Tokareva and E. F. Toro. Uncertainty quantification methodology for hyperbolic systems with application to blood flow in arteries. 2019. *Journal of Computational Physics*. **386**: 405-427. (LA-UR-18-27216 DOI: 10.1016/j.jcp.2019.02.013)

Tokareva, S., E. Toro, B. Saggiorato and A. Hidalgo. Low-dissipation centred schemes for hyperbolic equations in conservative and non-conservative form. Submitted to *Journal of Computational Physics*. (LA-UR-19-29379)

*Wu, T., M. Shashkov, N. Morgan, D. Kuzmin and H. Luo. An updated Lagrangian discontinuous Galerkin hydrodynamic method for gas dynamics. 2018. *Computers & Mathematics with Applications*. **78** (2): 258-273. (LA-UR-17-29217 DOI: 10.1016/j.camwa.2018.03.040)

Conference Papers

Liu, X., N. R. Morgan and D. E. Burton. A Lagrangian cell-centered discontinuous Galerkin hydrodynamic method for 2D Cartesian and RZ axisymmetric coordinates. Presented at *AIAA Science and Technology Forum and Exposition (SciTech 2018)*. (Kissimmee, Florida, United States, 2018-01-08 - 2018-01-12). (LA-UR-17-30900)

Liu, X., N. R. Morgan and D. E. Burton. A comparative study of two different methods for RZ axisymmetric coordinates in context of Lagrangian discontinuous Galerkin hydrodynamics. Presented at *AIAA Aviation and Aeronautics Forum and Exposition (AIAA AVIATION 2018)*. (Atlanta, Georgia, United States, 2018-06-25 - 2018-06-29). (LA-UR-18-24126)

Liu, X., N. R. Morgan and D. E. Burton. Exploration of consistent numerical integration for 2D cell-centered discontinuous Galerkin hydrodynamic method. Presented at *AIAA SciTech*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-24762)

Liu, X., N. R. Morgan and D. E. Burton. A robust and accurate third-order Lagrangian discontinuous Galerkin hydrodynamic method for the compressible Euler equations on curvilinear meshes. Presented at *AIAA Science and Technology Forum and Exposition (AIAA SciTech 2019)*. (San Diego, California, United States, 2019-01-06 - 2019-01-12). (LA-UR-18-25010)

Liu, X., N. R. Morgan and D. E. Burton. Exploration of the sub-cell stabilization scheme for the high-order Lagrangian discontinuous Galerkin hydrodynamic method. Presented at *AIAA Science and Technology Forum and Exposition (AIAA SciTech 2019)*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-31249)

Liu, X., N. R. Morgan and D. E. Burton. Exploration of Lagrangian discontinuous Galerkin method on curved triangular meshes using sub-cell mesh stabilization. Presented at

AIAA AVIATION Forum and Exposition. (Dallas, Texas, United States, 2019-06-17 - 2019-06-17). (LA-UR-19-24273)

Liu, X., N. R. Morgan and D. E. Burton. How to preserve symmetry of Hermite WENO scheme in Lagrangian hydrodynamics. Presented at *2020 AIAA SciTech Forum and Exposition*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-25338)

Liu, X., N. R. Morgan and D. E. Burton. Exploration of symmetry-preserving WENO limiters in Lagrangian hydrodynamics. Presented at *2020 AIAA SciTech Forum and Exposition*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-31975)

Liu, X., N. R. Morgan and D. E. Burton. Towards resolving the locking problems for triangular meshes in Lagrangian hydrodynamics. Presented at *The 11th International Conference on Computational Fluid Dynamics*. (Maui, Hawaii, United States, 2020-07-13 - 2020-07-17). (LA-UR-20-21483)

Morgan, N. R., S. Tokareva, X. Liu and A. Morgan. A machine learning approach for detecting shocks with high-order hydrodynamic methods. Presented at *AIAA SciTech Forum and Exposition*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-25154)

Morgan, N. R., X. Liu and D. E. Burton. A robust high-order Lagrangian discontinuous Galerkin hydrodynamic method for curvilinear meshes. Presented at *NECDC*. (Los Alamos, New Mexico, United States, 2018-10-15 - 2018-10-19). (LA-UR-18-24817)

Reports

Morgan, N. R. Physically consistent remap schemes for staggered grid hydrodynamic methods. Unpublished report. (LA-UR-19-23531)

Presentation Slides

Berry, M. R. GPU Performance (LDRD Review). Presented at *DG Methods LDRD Review*, Los Alamos, New Mexico, United States, 2019-01-22 - 2019-01-22. (LA-UR-19-20342)

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Advancing Predictive Capability for Brittle Failure Using Dynamic Graphs

Gowri Srinivasan
20170103DR

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.

Technical Outcomes

This project addressed the failure of brittle materials and fluid flow through fractures in brittle materials. We have developed machine learning (ML) algorithms that will predict failure times quicker and more accurately, and is relevant for weapons performance. We have also developed fast and accurate ML models for identifying gases such as Xenon that migrate upward to the atmosphere through fractures in real time, which is of utmost importance to our Nuclear Nonproliferation programs.

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

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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

Journal Articles

Bowen, C. M., N. A. Debardeleben, S. P. Blanchard and C. M. Anderson-Cook. Do Solar Proton Events Reduce the Number of Faults in Supercomputers?: A Comparative Analysis of Faults during and without Solar Proton Events. Submitted to *IEEE International Reliability Physics Symposium*. (LA-UR-19-31047)

Conference Papers

Blanchard, S. P., N. A. Debardeleben, P. Rech and D. Oliveira. Thermal Neutrons: A New Threat for Supercomputers and Safety Critical Applications. Presented at *SC'19*. (Denver, Colorado, United States, 2019-11-17 - 2019-11-17). (LA-UR-19-23232)

Reports

Wender, S. A., A. J. Couture and T. D. Fairbanks. Report on the Tin-II Thermal Neutron Detector. Unpublished report. (LA-UR-19-30822)

Presentation Slides

Bowen, C. M. Telling a Visual Story within Big Data: Case Studies on Interactive Visualizations for Supercomputer Data. Presented at *Rising Stars in Computational and Data Sciences*, Austin, Texas, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-22930)

Bowen, C. M. Telling a visual story within big data: case studies on interactive visualizations for supercomputer data. Presented at *21st Meeting of New Researchers in Statistics and Probability*, Fort Collins, Colorado, United States, 2019-07-24 - 2019-07-24. (LA-UR-19-26857)

Bowen, C. M., N. A. Debardeleben, S. P. Blanchard and C. M. Anderson-Cook. Do Solar Proton Events Reduce the Number of Faults in Supercomputers?: A Comparative Analysis of Faults during and without Solar Proton Events. Presented at *2019 Institute of Electrical and Electronics Engineers International Reliability Physics Symposium*, Monterey, California, United States, 2019-03-31 - 2019-03-31. (LA-UR-19-22250)

R. Mullin, E. R., S. F. Nowicki, N. A. Debardeleben, S. P. Blanchard, S. A. Wender and E. A. Baseman. Pre-deployment Characterization of Large Fast Neutron Detectors for High Performance Computing Fault Characterization. Presented at *2018 Symposium on Radiation Measurements and Applications (SORMA XVII)*, Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-14. (LA-UR-18-21582)

Ortega, S. P., N. A. Debardeleben and C. M. Bowen. Differential Privacy for Supercomputer Sensor Data. Presented at *USRC and HPC Symposia*, Los Alamos, New Mexico, United States, 2019-07-31 - 2019-08-01. (LA-UR-19-27434)

Posters

Bowen, C. M. Telling a Visual Story within Big Data: Case Studies on Interactive Visualizations for Supercomputer Data. Presented at *Spring Research Conference*, Blacksburg, Virginia, United States, 2019-05-22 - 2019-05-22. (LA-UR-19-24529)

Debardeleben, N. A. Data Analytics for Neutron Detection. Presented at *Ultrascale Systems Research Center Research Symposium*, Los Alamos, New Mexico, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-27103)

Ortega, S. P., N. A. Debardeleben and C. M. Bowen. Differential Privacy for Supercomputer Sensor Data. . (LA-UR-19-27097)

Schappert, O. M., S. P. Blanchard, N. A. Debardeleben, R. E. Lakis and A. Favalli. MCNP Simulations of Neutron Fluxes Through Trinity Supercomputer Nodes. . (LA-UR-19-27755)

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

Journal Articles

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)

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-19-22659)

C. Hebert, C. M., E. C. Lawrence, K. L. Myers, K. G. Bhat, J. P. Colgan and E. Judge. Non-negative matrix factorization for Modular Bayesian calibration of plasma compositions. Submitted to *Journal of the American Statistical Association*. (LA-UR-19-30403)

Presentation Slides

C. Hebert, C. M. Rocky beginnings: emulation for ChemCam data analysis. . (LA-UR-18-30744)

C. Hebert, C. M., K. L. Myers and E. C. Lawrence. Emulation for ChemCam data analysis. . (LA-UR-18-30784)

Klein, N. E. A statistics journey to Mars!. Presented at *UNM Graduate Statistics Club*, Albuquerque, New Mexico, United States, 2019-12-06 - 2019-12-06. (LA-UR-19-31807)

Lawrence, E. C. Computer Experiments at Los Alamos National Laboratory: Life on Mars and Really Big Computers. Presented at *The University of Michigan Department of Statistics Distinguished Alumni Speaker Series*, Ann Arbor, Michigan, United States, 2020-02-14 - 2020-02-14. (LA-UR-20-21574)

Lawrence, E. C., K. G. Bhat, N. E. Klein, C. Hebert, J. P. Colgan, E. Judge and K. L. Myers. Mars Attacked! Simulation-Based Disaggregation of LIBS Spectra. Presented at *Advanced Statistics meets Machine Learning-III*, Lemont, Illinois, United States, 2019-11-14 - 2019-11-14. (LA-UR-19-31457)

Myers, K. L., K. G. Bhat, E. C. Lawrence, E. Judge, J. P. Colgan and C. M. C. Hebert. Enabling Fast Disaggregation of Large Parameter Spaces. . (LA-UR-18-31077)

Posters

Bhat, K. G. Multi-Scale Uncertainty Quantification in the Physical Sciences and Engineering for Complex Models. Presented at *Joint Statistical Meetings*, Vancouver, Canada, 2018-07-29 - 2018-08-02. (LA-UR-18-26895)

Bhat, K. G., K. L. Myers, E. C. Lawrence, J. P. Colgan and E. Judge. Multi-Stage Emulation and Uncertainty Quantification for Disaggregation of LIBS Spectra. Presented at *Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21837)

Klein, N. E., E. C. Lawrence, K. L. Myers, J. P. Colgan and E. Judge. Is there ___ on Mars?: Disaggregation of LIBS spectra. Presented at *Conference on Data Analysis (CoDA)*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-27. (LA-UR-20-21301)

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

Journal Articles

Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Ex machina determination of structural correlation functions. Submitted to *Physical Review Letters*. (LA-UR-19-32446)

*Kidwell, N. M., B. Nebgen, L. V. Slipchenko and T. S. Zwier. The effects of site asymmetry on near-degenerate state-to-state vibronic mixing in flexible bichromophores. 2019. *The Journal of Chemical Physics*. **151** (8): 084313. (LA-UR-19-29710 DOI: 10.1063/1.5107423)

Nelson, T. R., B. T. Nebgen, A. J. White, Y. Zhang, H. Song, J. A. Bjorgaard, A. E. Sifain, B. Rodriguez-Hernandez, V. M. Freixas, S. Fernandez-Alberti, A. Roitberg, W. F. I. Malone and S. Tretiak. NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22362)

*Sifain, A. E., N. Lubbers, B. T. Nebgen, J. S. Smith, A. Y. Lokhov, O. Isayev, A. E. Roitberg, K. Barros and S. Tretiak. Discovering a Transferable Charge Assignment Model Using Machine Learning. 2018. *The Journal of Physical Chemistry Letters*. **9** (16): 4495-4501. (LA-UR-18-24683 DOI: 10.1021/acs.jpclett.8b01939)

*Smith, J. S., B. Nebgen, N. Lubbers, O. Isayev and A. E. Roitberg. Less is more: Sampling chemical space with active learning. 2018. *The Journal of Chemical Physics*. **148** (24): 241733. (LA-UR-18-22005 DOI: 10.1063/1.5023802)

*Smith, J. S., B. Nebgen, N. Lubbers, O. Isayev and A. E. Roitberg. Less is more: Sampling chemical space with active learning. 2018. *The Journal of Chemical Physics*. **148** (24): 241733. (LA-UR-18-30171 DOI: 10.1063/1.5023802)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, H. A. Nam, T. C. Germann, S. J. Fensin and K. M. Barros. Automated discovery of a robust interatomic potential for aluminum. Submitted to *Nature Communications*. (LA-UR-20-22194)

*Smith, J. S., B. T. Nebgen, R. Zubatyuk, N. Lubbers, C. Devereux, K. Barros, S. Tretiak, O. Isayev and A. E. Roitberg. Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. 2019. *Nature Communications*. **10** (1): 2903. (LA-UR-18-25687 DOI: 10.1038/s41467-019-10827-4)

Smith, J. S., R. Zubatyuk, B. T. Nebgen, N. E. Lubbers, K. M. Barros, A. E. Roitberg, O. Isayev and S. Tretiak. The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for organic molecules. Submitted to *Nature - Scientific Data*. (LA-UR-19-29769)

Tretiak, S., A. De Sio, E. Sommer, X. T. Nguyen, L. Gross, D. Popovi\xc4\x87, B. T. Nebgen, S. Fernandez-Alberti, S. Pittalis, A. Rozzi, E. Molinari, E. Mena-Osteritz, P. B\xc3\xa4uerle, T. Frauenheim and C. Lienau. Intermolecular conical intersections in molecular aggregates. Submitted to *Science*. (LA-UR-20-21416)

Zhou, G., B. T. Nebgen, N. E. Lubbers, W. F. I. Malone, A. M. Niklasson and S. Tretiak. GPU-Accelerated Semi-Empirical Born Oppenheimer Molecular Dynamics using PyTorch. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22394)

Zubatuk, T., B. T. Nebgen, N. E. Lubbers, J. S. Smith, R. Zubatuk, G. Zhou, C. F. Koh, K. M. Barros, O. Isayev and S. Tretiak. Machine Learned H\xc3\xbcckel Theory: Interfacing Physics and Deep Neural Networks. Submitted to *Chemical Science*. (LA-UR-19-29765)

Presentation Slides

Lubbers, N. E. Realizing Physical Principles in Atomistic Machine Learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-19 - 2019-02-21. (LA-UR-19-21277)

Lubbers, N. E., M. E. Gonzales, D. R. Byrd and B. T. Nebgen. Molecular Property modeling using Machine Learning. . (LA-UR-18-27401)

Nebgen, B. T., J. S. Smith, N. E. Lubbers, A. E. Sifain, K. M. Barros and S. Tretiak. Machines Learning Quantum Chemistry: Potentials, Properties, and P-Orbitals. Presented at *Telluride workshop: Multi-scale quantum mechanical analysis of condensed phase systems: methods and applications*, Telluride, Colorado, United States, 2018-07-23 - 2018-07-27. (LA-UR-18-26999)

Nebgen, B. T., J. S. Smith, N. Mathew, J. Chen, L. Burakovsky, S. J. Fensin and K. M. Barros. Automated generation of machine learning-based atomistic potentials for extreme conditions. Presented at *National Meeting of the American Physical Society*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22374)

Nebgen, B. T., J. S. Smith, N. Mathew, L. Burakovsky, S. J. Fensin, T. C. Germann, N. E. Lubbers, S. Tretiak and K. M. Barros. Machine Learning of Interatomic Potentials for Shock Compression Phenomena. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25529)

Nebgen, B. T., N. E. Lubbers, A. Lokhov, K. M. Barros and S. Tretiak. Machine Learning Optimal Effective Hamiltonians for Excited State Molecular Systems. Presented at *March APS*, Los Angeles, California, United States, 2018-03-05 - 2018-03-09. (LA-UR-18-21802)

Nebgen, B. T., N. E. Lubbers and S. Tretiak. Machines learning physics: deep tensor neural networks for dynamically optimized effective Hamiltonians. Presented at *ACS Boston*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-28121)

Nebgen, B. T., T. Zubatuk, S. I. Magedov, N. E. Lubbers, J. S. Smith, R. Zubatuk, G. Zhou, C. F. Koh, K. M. Barros, O. Isayev and S. Tretiak. Resurrecting Huckel Theory with Machine Learning. Presented at *Machine Learning and Informatics for Chemistry and Materials*, Telluride, Colorado, United States, 2019-09-30 - 2019-10-04. (LA-UR-19-29766)

Smith, J. S., B. T. Nebgen, N. E. Lubbers, O. Isayev and A. E. Roitberg. AI-ENABLED MD SIMULATIONS. . (LA-UR-19-31509)

Smith, J. S., K. M. Barros, S. Tretiak, S. J. Fensin, N. Mathew, T. C. Germann, L. Burakovsky, B. T. Nebgen and N. E. Lubbers. The importance of sampling for machine learning potentials. Presented at *American Chemical Society Conference*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-28758)

Smith, J. S., S. Tretiak, K. M. Barros, B. T. Nebgen, N. E. Lubbers, S. J. Fensin, T. C. Germann, O. Isayev, r. zubatyuk, A. Roitberg, C. Devereux, K. Ranashingha, H. Suwa, C. Batista and G. W. Chern. Accelerated Modeling of Atomistic Physics with Machine Learning. Presented at *American Chemical Society*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22830)

Tretiak, S. Machine Learning for Molecular Properties and Chemistry. Presented at *IMS Computational Data Science Approaches for Materials 2019*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23071)

Tretiak, S. Modeling of Electronic Properties in Organic and Hybrid Materials. . (LA-UR-19-28826)

Tretiak, S., B. T. Nebgen, J. S. Smith, N. E. Lubbers and A. Lokhov. Machine Learning for Quantum Mechanical Materials Properties. . (LA-UR-19-21738)

Posters

U. Chau, P. N., J. S. Smith, A. D. Migliori, S. Tretiak and C. A. Neale. Machine Learning in Molecular Dynamics Simulation. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26803)

Magedov, S. I., B. T. Nebgen, N. E. Lubbers, K. M. Barros and S. Tretiak. Prediction of bond orders using deep neural networks. Presented at *Meeting of the American Physical Society*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23861)

Nebgen, B. T., N. E. Lubbers, J. S. Smith, R. Zubatiuk, A. Lokhov, O. Isayev, K. M. Barros and S. Tretiak. Machine Learning For Quantitative H\xc3\xbcckel Theory. Presented at *Excited State Processes*, Santa Fe, New Mexico, United States, 2018-06-03 - 2018-06-07. (LA-UR-18-24826)

Smith, J. S., B. T. Nebgen, N. Mathew, J. Chen, N. E. Lubbers, L. Burakovsky, S. Tretiak, T. C. Germann, S. J. Fensin and K. M. Barros. Discovering physics from disorder: active learning a robust potential for aluminum. . (LA-UR-19-32169)

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

Journal Articles

Djidjev, H. N., E. A. R. Pelofske and G. Hahn. Decomposition algorithms for solving NP-hard problems on a quantum annealer. Submitted to *Journal of Signal Processing Systems*. (LA-UR-19-30809)

*Djidjev, H. N., G. Hahn, S. M. Mniszewski, C. F. Negre and A. M. Niklasson. Using Graph Partitioning for Scalable Distributed Quantum Molecular Dynamics. 2019. *Algorithms*. **12** (9): 187. (LA-UR-19-25278 DOI: 10.3390/a12090187)

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)

*Vyskocil, T. and H. Djidjev. Embedding Equality Constraints of Optimization Problems into a Quantum Annealer. 2019. *Algorithms*. **12** (4): 77. (LA-UR-19-20224 DOI: 10.3390/a12040077)

Conference Papers

Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihal\xc3\xa1k. Near-gathering of energy-constrained mobile agents. Presented at *26th International Colloquium on Structural Information and Communication Complexity SIROCCO 2019*. (L'Aquila, Italy, 2019-07-01 - 2019-07-04). (LA-UR-19-23906)

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)

Djidjev, H. N. and T. Vyskocil. Implementing constraints for quantum annealing optimization using finite state automata. Presented at *25th International Computing and Combinatorics Conference (COCOON)*. (Xian, China, 2019-07-29 - 2019-07-29). (LA-UR-19-22730)

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)

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)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Optimizing the spin reversal transform on the D-Wave 2000Q. Presented

at *ICRC 2019*. (San Mateo, California, United States, 2019-11-06 - 2019-11-08). (LA-UR-19-25307)

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Peering into the Anneal Process of a Quantum Annealer. Presented at *PDCAT 2019*. (Gold Coast, Australia, 2019-12-05 - 2019-12-07). (LA-UR-19-27870)

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)

Zbinden, S., A. Baertschi, H. N. Djidjev and S. J. Eidenbenz. Embedding Algorithms for Quantum Annealers with Chimera and Pegasus Connection Topologies. Presented at *ISC High Performance*. (Frankfurt, Germany, 2020-06-21 - 2020-06-25). (LA-UR-20-22259)

Reports

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

Presentation Slides

Baertschi, A., E. Bampas, J. Chalopin, S. Das, C. Karousatou and M. Mihal\xc3\xa1k. Near-gathering of energy-constrained mobile agents. Presented at *26th International Colloquium on Structural Information and Communication Complexity SIROCCO 2019*, L'Aquila, Italy, 2019-07-01 - 2019-07-04. (LA-UR-20-22307)

Francois, S., R. Andonov and H. N. Djidjev. Assembly of Chloroplast Genomes Using Global Optimization. Presented at *13th Annual Sequencing, Finishing, and Analysis in the Future (SFAF) Conference*, Santa Fe, New Mexico, United States, 2018-05-22 - 2018-05-22. (LA-UR-18-24468)

Pakin, S. D. Targeting Classical Code to a Quantum Annealer. Presented at *24th ACM International Conference on Architectural Support for Programming Languages and Operating Systems*, Providence, Rhode Island, United States, 2019-04-13 - 2019-04-17. (LA-UR-19-23060)

Posters

R. Pelofske, E. A., G. Hahn and H. N. Djidjev. Decomposition Algorithms for Scalable Quantum Annealing. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26700)

Massively-Parallel Acceleration of the Dynamics of Complex Systems: a Data-Driven Approach

Danny Perez
20190034ER

Project Description

Current atomistic modeling techniques are limited to extremely short timescales (on the order of microseconds or less), no matter the size of the computer that is used to carry out the simulations. This severely limits their ability to directly interpret experiments or to predict how materials will perform in real life. The key to addressing this problem is to find more efficient ways to exploit the computing power available via the Department of Energy's very large computers. We will develop and implement powerful massively-parallel algorithms deployed on thousands of processors in order to dramatically extend the range of systems that can be simulated over very long times. We will demonstrate the approach on a range of problems of interest to DOE, including the motion of dislocations in materials (materials failure in extreme conditions), the evolution of complex defects in nuclear materials (nuclear safety) and the evolution of bio-molecules (bio-security). In all of these cases, the lack of access to long-times has so far made computational materials design and drug design extremely challenging. Our goal is to use powerful algorithms and very-large-scale computing to directly tackle this challenge.

Publications

Journal Articles

Perez, D., A. Agarwal, A. F. Voter and S. Gnanakaran. Arbitrary accurate representation of atomistic dynamics via semi-Markov jump processes. Submitted to *TBD*. (LA-UR-19-29252)

Presentation Slides

Mathew, N., E. Martinez Saez and D. Perez. Accelerated Molecular Dynamics Simulations of Dislocation-Obstacle Interactions in Tungsten: Enabling Micro-Second Simulations. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22073)

Perez, D. Complex High-Dimensional Energy Landscapes. Presented at *Reunion workshop of the Complex High-Dimensional Energy Landscapes program.*, Lake Arrowhead, California, United States, 2019-06-10 - 2019-06-10. (LA-UR-19-25405)

Objective Flow Topology

Roxana Bujack
20190143ER

Project Description

High Explosives safety and surety and nuclear energy research rely heavily on computational simulations. DOE's supercomputers, expert scientists, and advanced hydrodynamics codes produce ever increasing datasets. This creates new challenges. First, while computational resources are increasing in modern high performance computing (HPC) architectures, the capacity for loading and storing data is not keeping pace- in effect, more data is produced than can be stored. The second problem is that scientists cannot view and comprehend ever larger amounts of flow data during visual analysis because human vision has finite resolution. Our proposed method will solve both problems by providing the means to better analyze big flow data by reducing it to its most essential structure. Firstly, it compresses the data, which helps overcome the Input/Output (I/O) bottleneck and allows the analysis of huge simulation data on a desktop machine with minimal loss of relevant information. Secondly, it produces a decluttered visualization of the fundamental behavior of the flow with minimal occlusion from less important regions.

Publications

Journal Articles

Bujack, R. B. and A. Middel. State of the Art in Flow Visualization in the Environmental Sciences. Submitted to *Environmental Earth Sciences*. (LA-UR-19-31637)

Conference Papers

Bujack, R. B., L. Yan, I. Hotz, C. Garth and B. Wang. Time-Dependent Flow Topology: Past, Present, and Future. Presented at *EuroVis*. (Lingkoeping, Sweden, 2020-06-03 - 2020-06-03). (LA-UR-19-30267)

Bujack, R. B., S. Dutta, D. Z. Zhang and T. Gunther. Objective Finite-Time Flow Topology from Flowmap Expansion and Contraction. Presented at *TopoInVis*. (Nyk\xc3\xb6ping, Sweden, 2019-06-17 - 2019-06-19). (LA-UR-19-23386)

Bujack, R. B., S. Dutta, I. B. Rojo, D. Z. Zhang and T. G \xc3\xbcnther. Objective Finite-Time Saddles and their Connection to FTLE. Presented at *EuroVis 2019*. (Porto, Portugal, 2019-06-03 - 2019-06-07). (LA-UR-19-21831)

Bujack, R. B., S. Sane, C. Garth and H. Childs. Survey of Seed Placement and Streamline Selection Techniques. Presented at *EuroVis*. (Linkoeping, Sweden, 2019-06-03 - 2019-06-03). (LA-UR-19-30263)

Dutta, S., R. X. Brady, M. E. Maltrud, P. J. J. Wolfram and R. B. Bujack. Leveraging Lagrangian Analysis for Discriminating Nutrient Origins. Presented at *Visualization in Environmental Sciences*. (Porto, Portugal, 2019-06-03 - 2019-06-03). (LA-UR-19-22455)

Yan, L., B. Wang and R. B. Bujack. Finite-time Saddles from Particle Origin and Destination. Presented at *Eurovis 2020*. (Norrk\xc3\xb6ping, Sweden, 2020-05-25 - 2020-05-25). (LA-UR-19-26219)

Books/Chapters

Bujack, R. B. Mathematical Foundations in Visualization. (LA-UR-19-29121)

Towards Memristor Supremacy with Novel Machine Learning Algorithms

Francesco Caravelli
20190195ER

Project Description

Memristors are the nanoscale equivalent of brain synapses: these are passive components able to learn, and their perspective application is in reproducing the capabilities of the brain. This project is a first step towards the integration of (hard) computational tasks in dense nanoscale analog circuits. The success of this project will show that the use of memristors without a complementary metal oxide semiconductor (CMOS), the base for current computational architectures, can still be used for storage and low-energy computation. The addition of CMOS hardware will then be used for hybrid brain-like and digital-like computers. This project is aligned with the goal of "Beyond Moore's Law" computation, one the Department of Energy missions. While some brain-like chips are currently available, their architecture is simple; the purpose of this project is to go beyond standard architectures.

Publications

Journal Articles

*Caravelli, F. Asymptotic Behavior of Memristive Circuits. 2019. *Entropy*. **21** (8): 789. (LA-UR-18-24748 DOI: 10.3390/e21080789)

Caravelli, F., C. Nisoli and G. Chern. Phase-change spin ice memory resistor. Submitted to *Physical Review Letters*. (LA-UR-19-27438)

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 J. P. Carbajal. Memristors for the Curious Outsiders. 2018. *Technologies*. **6** (4): 118. (LA-UR-18-27766 DOI: 10.3390/technologies6040118)

Sheldon, F. C., F. Caravelli and A. Kolchinsky. Feasibility, Optimality and Implementability of memory circuits for Reservoir Computing. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-20314)

Conference Papers

Coffrin, C. J., H. Nagarajan and R. W. Bent. Evaluating Ising Processing Units with Integer Programming. Presented at *Sixteenth International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Thessaloniki, Greece, 2019-06-04 - 2019-06-07). (LA-UR-19-22000)

Pang, Y., C. J. Coffrin, A. Lokhov and M. D. Vuffray. The Potential of Quantum Annealing for Rapid Solution Structure Identification. Presented at *17th International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. (Vienna, Austria, 2020-05-26 - 2020-05-29). (LA-UR-19-31884)

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)

Presentation Slides

Caravelli, F. Memristive Networks. Presented at *Talk @ICTP Trieste*, Trieste, Italy, 2019-09-23 - 2019-09-23. (LA-UR-19-29539)

Coffrin, C. J. Beyond Moore’s Law: Exploring the Future of Computation. . (LA-UR-19-21268)

Coffrin, C. J. Novel Computing Platforms: Potential and Challenges for Discrete Optimization. . (LA-UR-19-21267)

Coffrin, C. J. Challenges with Chains: Testing the Limits of a D-Wave Quantum Annealer for Discrete Optimization. . (LA-UR-19-21739)

Coffrin, C. J. Harnessing Analog Noise: A Hybrid Algorithm for Binary Quadratic Optimization with Uncertainty. . (LA-UR-19-24684)

Coffrin, C. J. The Potential of Quantum Annealing for Rapid Solution Structure Identification. . (LA-UR-20-21046)

Lokhov, A. Uncovering the behavior of quantum annealers with statistical learning. Presented at *APS march meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-22165)

Lokhov, A. Uncovering the behavior of quantum annealers with statistical learning. Presented at *At the crossroads of physics and machine learning*, Santa Barbara, California, United States, 2019-02-11 - 2019-02-11. (LA-UR-19-22163)

Posters

Lokhov, A. Optimal deployment of resources for maximizing impact in spreading processes. Presented at *APS march meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-22164)

Stable, Conservative, High-Order Numerical Methods for Direct Numerical Simulations (DNS) in Complex Geometries

Peter Brady
20190227ER

Project Description

Numerical simulations play a key role in stockpile stewardship. The large scale industrial simulations that are required for understanding the complex regimes arising from stockpile stewardship considerations employ a variety simplified physical models. The development and assessment of these models can be greatly enhanced by reliable databases produced by more focused, high-fidelity simulations. This project will extend the capabilities of high-fidelity, exa-scale simulations to the complex configurations that are typically encountered in engineering applications.

Publications

Journal Articles

Brady, P. T. and D. Livescu. Foundations for High-Order, Conservative Cut-Cell Methods: Stable Discretizations on Degenerate Meshes. Submitted to *Journal of Computational Physics*. (LA-UR-20-22279)

Conference Papers

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-Cell Methods. Presented at *AIAA Scitech*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-29984)

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-Cell Methods. Presented at *AIAA SciTech Forum*. (San Diego, California, United States, 2019-01-07 - 2019-01-11). (LA-UR-18-31402)

Sharan, N., P. T. Brady and D. Livescu. Stable and conservative boundary treatment for difference methods, with application to cut-cell discretizations. Presented at *2020 AIAA SciTech Forum*. (Orlando, Florida, United States, 2020-01-06 - 2020-01-10). (LA-UR-19-32707)

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. Numerical Study of the Properties of a Ghost-Cell Method. Presented at *American Institute of Aeronautics and Astronautics*. (Orlando, Florida, United States, 2020-01-07 - 2020-01-11). (LA-UR-19-28614)

Reports

Brady, P. T. and D. Livescu. High-Order, Stable, and Conservative Boundary Schemes for Central and Compact Finite Differences. Unpublished report. (LA-UR-19-20056)

Presentation Slides

Brady, P. T. and D. Livescu. A Foundation for High-Order Cut-Cell Methods: Stable Derivatives on Degenerate Meshes. Presented at *APS DFD*, Atlanta, Georgia, United States, 2018-11-18 - 2018-11-20. (LA-UR-18-30896)

Brady, P. T. and D. Livescu. Stable, High-Order and Conservative Cut-cell Methods. Presented at *AIAA Scitech*, San Diego, California, United States, 2019-01-07 - 2019-01-07. (LA-UR-19-20057)

Brady, P. T. and D. Livescu. High-Order Cut-Cell Methods in Multiple Dimensions. Presented at *72nd APS DFD meeting*, Seattle, Washington, United States, 2019-11-23 - 2019-11-23. (LA-UR-19-31797)

Sharan, N., P. T. Brady and D. Livescu. High-order energy-stable boundary treatment for finite-difference cut-cell method. Presented at *72nd Annual Meeting of the APS Division of Fluid Dynamics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31665)

Sharan, N., P. T. Brady and D. Livescu. Stable and conservative boundary treatment for difference methods, with application to cut-cell discretizations. Presented at *2020 AIAA SciTech Forum*, Orlando, Florida, United States, 2020-01-06 - 2020-01-06. (LA-UR-20-20086)

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. High-Order Ghost-Cell Method for Non-Conforming Boundaries. Presented at *American Physical Society Division of Fluid Dynamics*, Seattle, Washington, United States, 2019-11-23 - 2019-11-26. (LA-UR-19-31645)

Posters

Shrestha, P., P. T. Brady, V. Gyrya and D. Livescu. High-Order Ghost-Point Method for Non-Conforming Boundaries. Presented at *Los Alamos Post-doc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28565)

Statistical Learning in Cyberphysical Systems

Nathan Lemons
20190351ER

Project Description

The overarching goal of this project is to develop novel data-driven algorithms for statisical learning of an effective high-fidelity representation of cyberphysical systems. This will allow applications such as real-time detection and classification of anomalies, state estimation for damage-recovery operations, and optimal expansion of the system. We expect our work to be highly relevant to those tasked with operating and protecting large networked cyberphysical systems, such as electric grids. This research is directly relevant to the program office "Cybersecurity for Energy Delivery Systems" within the Office of Electricity in the Department of Energy. It is expected that members of the Intelligence Community will also be interested in this work. We also expect to contribute to the state of the art in machine learning and statistical learning through publications and presentations at top conferences.

Publications

Journal Articles

Gy\xc5\x91ri, E., N. W. Lemons, N. Salia and O. Zamora. The Structure of Hypergraphs without long Berge cycles. Submitted to *Electronic Journal of Combinatorics*. (LA-UR-18-31512)

Keszegh, B., N. W. Lemons, R. R. Martin, D. P\xc3\xa1lv \xc3\xb6lgyi and B. Patk\xc3\xb3s. Induced and non-induced poset saturation problems. Submitted to *SIAM Journal on Discrete Mathematics*. (LA-UR-20-22232)

Likhosherstov, V., Y. Maximov and M. Chertkov. Tractable Minor-free Generalization of Planar Zero-field Ising Models. Submitted to *IEEE Transactions on Information Theory*. (LA-UR-19-30102)

Conference Papers

Deka, D., U. Hashmi, L. Pereira, A. Busic and S. N. Backhaus. Co-optimizing Energy Storage for Prosumers using Convex Relaxations. Presented at *ISAP Conference 2019*. (New Delhi, India, 2019-12-10 - 2019-12-14). (LA-UR-19-29297)

Deka, D. and S. Misra. Learning for DC-OPF: Classifying active sets using neural nets. Presented at *Powertech 2019*. (milan, Italy, 2019-06-23 - 2019-06-27). (LA-UR-19-24726)

Hannon, C. M., D. Deka, D. Jin, M. D. Vuffray and A. Lokhov. Real-time Anomaly Detection and Classification in Streaming PMU Data. Presented at *XXI Power Systems Computation Conference*. (Porto, Portugal, 2020-06-29 - 2020-07-03). (LA-UR-19-31329)

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)

Reports

Belyy, A., A. Sholokhov, M. R. Amini and Y. Maximov. MEMOIR: Multi-class Extreme Classification with Inexact Margin. Unpublished report. (LA-UR-19-21219)

Burashnikova, A., Y. Maximov and M. R. Amini. Sequential Learning over Implicit Feedback for Robust Large-Scale Recommender Systems. Unpublished report. (LA-UR-19-21349)

Krechetov, M., Y. Maximov, J. Marecek and M. Takac. Entropy-Penalized Semidefinite Programming. Unpublished report. (LA-UR-18-24430)

Likhosherstov, V., Y. Maximov and M. Chertkov. Inference and Sampling of K33-free Ising Models. Unpublished report. (LA-UR-19-26932)

Likhosherstov, V., Y. Maximov and M. Chertkov. A New Family of Tractable Ising Models. Unpublished report. (LA-UR-19-24712)

Presentation Slides

Hannon, C. M., D. Deka, M. D. Vuffray and A. Lokhov. Real-time Modeling and Anomaly Detection in Cyber-physical Systems. . (LA-UR-20-22487)

Posters

Hannon, C., D. Deka and A. Lokhov. Realtime Modeling and Anomaly Detection in Cyber-Physical Systems. Presented at *NeurIPS*, Los Alamos, New Mexico, United States, 2019-12-08 - 2019-12-14. (LA-UR-19-32246)

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.

Technical Outcomes

This project has developed, prototyped, and open-sourced (https://quinoacomputing.org) a new modern massively parallel software architecture for physics simulations using the Charm++ runtime system. Using adaptive methods for hydrodynamics, which result in inefficiencies in large-scale simulations that are representative of all multi-physics simulations, we have demonstrated excellent scaling to large supercomputers, relying on automatic load balancing that does not require physics or computer science expertise. The follow-on work is planned by adding new coupled physics.

Publications

Journal Articles

Bakosi, J., R. F. Bird, F. Gonzalez, C. Junghans, W. Li, H. Luo, A. K. Pandare and J. I. Waltz. Asynchronous distributed-memory task-parallel algorithm for compressible flows on unstructured 3D Eulerian grids. Submitted to *Computers & Fluids*. (LA-UR-20-21450)

*Pandare, A. K., H. Luo and J. Bakosi. An enhanced AUSM+-up scheme for high-speed compressible two-phase flows on hybrid grids. 2019. *Shock Waves*. **29** (5): 629-649. (LA-UR-18-24062 DOI: 10.1007/s00193-018-0861-x)

Reports

Bakosi, J., O. Certik, J. Barnett and G. Collins. Vectorize! Bridging the Performance-Productivity Gap of Vectorization. Unpublished report. (LA-UR-17-29524)

Bakosi, J., R. F. Bird, C. Junghans, A. K. Pandare, R. S. Pavel, J. I. Waltz, W. Li, H. Luo, E. Bohm, L. Kale, E. Mikida, E. Ramos, J. Barnett, G. Collins and A. Pakki. Asynchronous Navier-Stokes Solver on 3D Unstructured Grids for the Exascale Era. Unpublished report. (LA-UR-19-29712)

Pandare, A. K., J. I. Waltz and J. Bakosi. A Reconstructed Discontinuous Galerkin method for Multi-Material Flows with Sharp-Interfaces. Unpublished report. (LA-UR-19-20312)

Presentation Slides

Bakosi, J. Unstructured-mesh CFD, Stochastic methods for turbulence, Production codes. . (LA-UR-17-26808)

Bakosi, J., A. K. Pandare, R. F. Bird, J. I. Waltz, W. Li, H. Luo, E. Bohm, L. V. Kal\xc3\xa9, E. Mikida and E. Ramos. Adaptive Computational Fluid Dynamics with Charm++. Presented at *Supercomputing 2019*, Denver, Colorado, United States, 2019-11-17 - 2019-11-22. (LA-UR-19-31534)

Bakosi, J., R. F. Bird, C. Junghans, A. K. Pandare and H. Luo. Concept-based runtime polymorphism with Charm++ chare arrays using value semantics. Presented at *16th Annual Workshop on Charm++ and its Applications*, Urbana-Champaign, Illinois, United States, 2018-04-11 - 2018-04-12. (LA-UR-18-22990)

Bakosi, J., R. F. Bird, C. Junghans, R. S. Pavel, J. I. Waltz, F. Gonzalez and B. Rogers. Quinoa: Adaptive Computational Fluid Dynamics. Presented at *15th Annual Workshop on Charm++ and its Applications*, Urbana-Champaign, Illinois, United States, 2017-04-17 - 2017-04-19. (LA-UR-17-22931)

Bakosi, J., R. F. Bird, C. Junghans and J. I. Waltz. Quinoa: Adaptive Hydrodynamics on Charm++. Presented at *2018 Applied Computer Science and Programming Models/Co-Design Meeting at Sandia National Labs*, Albuquerque, New Mexico, United States, 2018-02-12 - 2018-02-16. (LA-UR-18-20947)

Li, W., A. K. Pandare, J. Bakosi and H. Luo. Adaptive Discontinuous Galerkin Method for Compressible Flow Using Charm++. Presented at *17th Annnual Workshop on Charm++ and its Applications*, Urbana-Champaign, Illinois, United States, 2019-05-01 - 2019-05-02. (LA-UR-19-24060)

Pandare, A. K., J. Bakosi and H. Luo. Progress towards development of discontinuous Galerkin finite-element methods for compressible flows using Charm++. Presented at *16th Annual Workshop on Charm++ and its Applications*, Urbana-Champaig, Illinois, United States, 2018-04-11 - 2018-04-12. (LA-UR-18-22989)

Waltz, J. I., A. K. Pandare and J. Bakosi. A direct finite element ALE method for non-equilibrium multi-material flows. Presented at *AIAA Sci Tech Meeting*, Orlando, Florida, United States, 2020-01-06 - 2020-01-10. (LA-UR-19-25355)

Waltz, J. I., J. Bakosi and A. K. Pandare. A finite element ALE method for multi-material flows. Presented at *Finite Elements in Fluids*, Chicago, Illinois, United States, 2019-04-01 - 2019-04-03. (LA-UR-19-22884)

Posters

Bakosi, J., O. Certik, J. Barnett and G. Collins. Vectorize! Bridging the Performance-Productivity Gap of Vectorization. . (LA-UR-17-29526)

Pandare, A. K., J. I. Waltz and J. Bakosi. Multi-Material Shock Hydrodynamics using a Reconstructed Discontinuous Galerkin Method. . (LA-UR-19-28581)

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.

Technical Outcomes

The main technical outcome was the proof-of-concept demonstration that a model of cortical development based on sparse coding could be used for the unsupervised learning of depth-selective spatiotemporal/binocular features from stereo video and that such features could in turn be used for object detection tasks. Additional technical outcomes included the proof-of-concept demonstration that the same cortical development models could be used for the unsupervised learning of features on a diverse set of data.

Publications

Journal Articles

*Yoon, B., T. Bhattacharya and R. Gupta. Machine learning estimators for lattice QCD observables. 2019. *Physical Review D*. **100** (1): 014504. (LA-UR-18-26411 DOI: 10.1103/PhysRevD.100.014504)

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)

Conference Papers

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)

Carroll, J. A., N. T. Carlson and G. Kenyon. Phase Transitions in Image Denoising via Sparsely Coding Convolutional Neural Networks. Presented at *workshop on Advances in Modeling and Learning Interactions from Complex Data, Neural Information Processing Systems*. (Long Beach, California, United States, 2017-12-04 - 2017-12-04). (LA-UR-19-32591)

Kenyon, G., M. Mitchell and S. Y. Lundquist. Sparse Coding of Stereo Video for Object Detection. Presented at *Neural Information Processing Systems*. (Long Beach, California, United States, 2017-12-04 - 2017-12-04). (LA-UR-19-32502)

Kenyon, G., N. T. T. Nguyen-Fotiadis, J. S. Moore, E. S. Michalak, P. T. Hraber and G. E. Getzelman. Detecting Real vs Synthetic Faces: Robustness of Deep Neural Networks vs. Sparse Coding against Universal Adversarial Perturbations. Presented at *Workshop on Deep Learning for Detecting AudioVisual Fakes, ICML 2019*. (Long Beach, California, United States, 2019-06-15 - 2019-06-15). (LA-UR-19-24168)

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)

Teti, M. A., E. E. Meyer and G. Kenyon. Can lateral inhibition for sparse coding help explain V1 neuronal responses to natural stimuli?. Presented at *Southwest Symposium on Image Analysis and Interpretation (SSIAI)*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29). (LA-UR-20-22286)

Wang, D. A., C. M. S. Strauss, J. M. Springer, A. M. Thresher, H. P. J. Pritchard and G. Kenyon. Sparse MP4. Presented at *Southwest Symposium on Image Analysis and Interpretation (SSIAI)*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2020-03-29). (LA-UR-20-22060)

Wang, D. A., G. Kenyon, H. P. J. Pritchard, J. M. Springer, A. M. Thresher and C. Strauss. Compression of Video Portraits using Spatiotemporal Sparse Coding. Presented at *Southwest Symposium on Image Analysis and Interpretation*. (Santa Fe, New Mexico, United States, 2020-03-29 - 2019-11-17). (LA-UR-19-32339)

Watkins, Y. Z., A. M. Thresher, P. F. Schultz, A. Wild, A. T. Sornborger and G. Kenyon. Unsupervised Dictionary Learning via a Spiking Locally Competitive Algorithm. Presented at *ICONS '19 Proceedings of the International Conference on Neuromorphic Systems*. (Knoxville, Tennessee, United States, 2019-07-23 - 2019-07-23). (LA-UR-18-31520)

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)

Presentation Slides

Getzelman, G. E., G. Kenyon, E. S. Michalak, J. S. Moore, M. J. Dixon, P. T. Hraber and N. T. T. Nguyen-Fotiadis. Adversarially-Robust Sparse Coding for GAN Detection. Presented at *DARPA MediFor PI meeting*, Menlo Park, California, United States, 2019-07-09 - 2019-07-09. (LA-UR-19-26394)

Kenyon, G. Strategic Implications of Artificial Intelligence/ Deep Learning Deep Threats and Deep Fakes. Presented at *Atlantic Council*, Washington, District Of Columbia, United States, 2019-09-20 - 2019-09-20. (LA-UR-19-29520)

Posters

Wang, D. A. PetaVision: Interpolating Video and Up-Sampling Simulations. . (LA-UR-19-27303)

Yoon, B., G. Kenyon and P. F. Schultz. PetaVision Neural Simulation Toolbox on Intel KNLs. Presented at *SC17*, Denver, Colorado, United States, 2017-11-12 - 2017-11-17. (LA-UR-17-26794)

Yoon, B., G. Kenyon and P. F. Schultz. Executing Large-Scale Neuromorphic Models on the Trinity Supercomputer. Presented at *IEEE International Conference on Rebooting Computing (ICRC)*, McLean, Virginia, United States, 2017-11-08 - 2017-11-08. (LA-UR-17-30188)

Yoon, B., P. F. Schultz and G. Kenyon. Implementing a Sparse Prediction Machine on the Trinity Supercomputer. Presented at *NIPS2017*, Long Beach, California, United States, 2017-12-09 - 2017-12-09. (LA-UR-17-31142)

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.

Technical Outcomes

This project developed new image analysis algorithms that enable extracting rare and subtle signatures of Space Resident Objects (RSO). The main results are the new Point Spread Function (PSF) estimation algorithm based on convolutional sparse coding and improved moving source detection and localization. These algorithms enable an order of magnitude improvement in the astrometry of the end point localization. This project also created a software repository that provides baseline implementations of the new algorithms.

Publications

Journal Articles

*Sun, Y., B. Wohlberg and U. S. Kamilov. An Online Plug-and-Play Algorithm for Regularized Image Reconstruction. 2019. *IEEE Transactions on Computational Imaging*. **5** (3): 395-408. (LA-UR-18-28977 DOI: 10.1109/TCI.2019.2893568)

Conference Papers

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., 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)

Wozniak, P. R., L. Prasad and B. E. Wohlberg. Moving point source detection and localization in wide-field images. Presented at *Advanced Maui Optical and Space Surveillance Technologies Conference (AMOS 2018)*. (Wailea, Hawaii, United States, 2018-09-11 - 2018-09-14). (LA-UR-18-28308)

Presentation Slides

Carrera, D., A. Foi, G. Boracchi and B. E. Wohlberg. On the Weighting for Convolutional Sparse Coding. Presented at *Signal Processing with Adaptive Sparse Structured Representations (SPARS)*, Toulouse, France, 2019-07-01 - 2019-07-01. (LA-UR-19-25474)

Wohlberg, B. E. Structured Sparsity for Convolutional Representations. Presented at *Workshop on Recent Developments on Mathematical/Statistical approaches in DAta Science (MSDAS)*, Dallas, Texas, United States, 2019-06-01 - 2019-06-02. (LA-UR-19-25475)

Posters

Wozniak, P. R., L. Prasad and B. E. Wohlberg. Moving point source detection and localization in wide-field images. Presented at *Advanced Maui Optical and Space Surveillance Technologies Conference (AMOS 2018)*, Wailea, Hawaii, United States, 2018-09-11 - 2018-09-14. (LA-UR-18-28357)

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 the Department of Energy such as environmental management (EM), the National Nuclear Security Administration(NNSA), Office of Nuclear Energy (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.

Technical Outcomes

At the completion of this project we have a computational tool for developing new parameterizations for quantum chemistry calculations. This new capability has been used for developing modeling tools for light elements and for uranium and plutonium simulations in aqueous solution. The new modeling tool has allowed us to perform the longest quantum-chemistry based molecular dynamics simulation of UO2 in aqueous solution, to date.

Publications

Journal Articles

Carlson, R. K., M. J. Cawkwell, P. Yang and E. R. Batista. Actinides in Solution: DFTB for U, O, and H Chemistry. Submitted to *Chemical Science*. (LA-UR-19-30522)

Aguirre Castiblanco, N. F., A. L. Morgenstern, M. J. Cawkwell, E. R. Batista and P. Yang. Development of Density Functional Tight-Binding Parameters Using Relative Energy Fitting and Particle Swarm Optimization. 2020. *Journal of Chemical Theory and Computation*. acs.jctc.9b00880. (LA-UR-19-26772 DOI: 10.1021/acs.jctc.9b00880)

Liu, C., E. R. Batista, N. F. Aguirre Castiblanco, P. Yang, M. J. Cawkwell and E. Jakubikova. Benchmarking and optimization of SCC-DFTB parameters for iron complexes. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-19-28865)

Presentation Slides

Cawkwell, M. J. Fast Quantum Molecular Dynamics Simulations of Heavy Elements in Solution (w17_solutionqmd). . (LA-UR-19-21930)

Cawkwell, M. J., N. F. Aguirre Castiblanco, P. Yang and E. R. Batista. Fast Quantum Molecular Dynamics Simulations of Heavy Elements in Solution (w17_solutionqmd). . (LA-UR-18-21224)

Posters

Carlson, R. K., M. J. Cawkwell, E. R. Batista and P. Yang. DFTB for Actinide Chemistry in Solution. Presented at *Basic Energy Sciences-Heavy Element Chemistry Onsite Review*, Los Alamos, New Mexico, United States, 2019-06-11 - 2019-06-11. (LA-UR-19-25160)

Liu, C. Optimization of Fe-C parameters in DFTB. . (LA-UR-18-26167)

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.

Technical Outcomes

Our methods have made substantial contributions and placed Los Alamos at the forefront of mixed integer non linear programming (MINLP). Our results include key advances in the fundamentals of optimization theory, application of techniques to DOE mission areas in critical infrastructure, and one open source software (Alpine.jl). The approaches are two orders of magnitudes faster than existing approaches and have solved benchmark MINLP problems for which there were no known solutions prior to this work.

Publications

Journal Articles

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)

*Nagarajan, H., M. Lu, S. Wang, R. Bent and K. Sundar. An adaptive, multivariate partitioning algorithm for global optimization of nonconvex programs. 2019. *Journal of Global Optimization*. **74** (4): 639-675. (LA-UR-17-25666 DOI: 10.1007/s10898-018-00734-1)

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., R. Bent and P. Van Hentenryck. Optimization of Structural Flood Mitigation Strategies. 2019. *Water Resources Research*. **55** (2): 1490-1509. (LA-UR-18-21506 DOI: 10.1029/2018WR024362)

Wang, S., R. W. Bent, C. J. Coffrin, S. Eksioglu 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)

Conference Papers

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. Eksioglu 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)

Sundar, K., S. G. Manyam, D. Casbeer and P. Sujit. Coordinated Air-Ground Vehicle Routing with Timing Constraints. Presented at *Indian Control Conference*. (Hyderabad, India, 2019-12-18 - 2019-12-20). (LA-UR-19-28660)

Presentation Slides

Bent, R. W., S. Krishna Kanth Hari, K. Sundar, H. Nagarajan and S. N. Backhaus. Hierarchical Predictive Control Algorithms for Optimal Design and Operation of Microgrids. Presented at *Power Systems Computation Conference*, Dublin, Ireland, 2018-06-11 - 2018-06-15. (LA-UR-18-24985)

Hijazi, H. L. Gravity: A Modeling Language for Mathematical Optimization and Machine Learning. Presented at *INFORMS Optimization*, Denver, Colorado, United States, 2018-03-23 - 2018-03-26. (LA-UR-18-22284)

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 the Department of Energy.

Technical Outcomes

The main result of this project is an algorithm enabling modeling of the adiabatic molecular dynamics in sufficiently large molecular systems with substantially higher accuracy than standard computational methods without a significant increase in the computational cost. The algorithm provides a novel capability for predictive first-principles based large-scale molecular dynamics simulations beyond the ground state that can be applied to numerous problems involving photo-induced phenomena.

Publications

Journal Articles

*Baskov, R., A. J. White and D. Mozyrsky. Improved Ehrenfest Approach to Model Correlated Electron–Nuclear Dynamics. 2019. *The Journal of Physical Chemistry Letters*. **10** (3): 433-440. (LA-UR-18-26927 DOI: 10.1021/acs.jpclett.8b03061)

*Bjorgaard, J. A., D. Sheppard, S. Tretiak and A. M. N. Niklasson. Extended Lagrangian Excited State Molecular Dynamics. 2018. *Journal of Chemical Theory and Computation*. **14** (2): 799-806. (LA-UR-17-27227 DOI: 10.1021/acs.jctc.7b00857)

*Chubukov, A. V. and D. Mozyrsky. Evolution of the dynamics of neutral superconductors between BCS and BEC regimes: The variational approach. 2018. *Low Temperature Physics*. **44** (6): 528-533. (LA-UR-18-23263 DOI: 10.1063/1.5037555)

*Freixas, V. M., D. Ondarse-Alvarez, S. Tretiak, D. V. Makhov, D. V. Shalashilin and S. Fernandez-Alberti. Photoinduced non-adiabatic energy transfer pathways in dendrimer building blocks. 2019. *The Journal of Chemical Physics*. **150** (12): 124301. (LA-UR-18-31806 DOI: 10.1063/1.5086680)

*Mozyrsky, D. and A. V. Chubukov. Dynamic properties of superconductors: Anderson-Bogoliubov mode and Berry phase in the BCS and BEC regimes. 2019. *Physical Review B*. **99** (17): 174510. (LA-UR-19-21884 DOI: 10.1103/PhysRevB.99.174510)

Nelson, T. R., A. J. White, J. A. Bjorgaard, A. E. Sifain, Y. Zhang, B. T. Nebgen, S. Fernandez-Alberti, D. V. Mozyrsky, S. Tretiak and A. E. Roitberg. Non-adiabatic Excited State Molecular Dynamics: theory and applications for modeling photophysics in extended molecular materials. Submitted to *Chemical Reviews*. (LA-UR-19-25569)

*Nelson, T. R., D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. F. Galindo, V. D. Kleiman, S. Fernandez-Alberti, A. E. Roitberg and S. Tretiak. Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. 2018. *Nature Communications*. **9** (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, D. W. Gao, O. V. Prezhdo, S. Fernandez-Alberti, A. E. Roitberg and S. Tretiak. Photoexcited Nonadiabatic Dynamics of Solvated Push–Pull \xcf \x80-Conjugated Oligomers with the NEXMD Software. 2018. *Journal of Chemical Theory and Computation*. **14** (8): 3955-3966. (LA-UR-18-20388 DOI: 10.1021/acs.jctc.8b00103)

*Sifain, A. E., W. Linjun, S. Tretiak and O. V. Prezhdo. Numerical tests of coherence-corrected surface hopping methods using a donor-bridge-acceptor model system. 2019. *The Journal of Chemical Physics*. **150** (19): 194104. (LA-UR-19-20761 DOI: 10.1063/1.5092999)

Towards Operationalized Data Fusion for Activity-Based Intelligence (U)

Geoffrey Fairchild
20190603ER

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 and meetings with Department of Defense partners have 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 work will prepare the Lab with the capability to meet national needs regarding this problem.

Technical Outcomes

This project resulted in a number of firsts for LANL and the DOE complex: 1) the first access to several classified data streams and services at LANL, 2) the first access to one classified data stream in particular in the entire DOE complex, 3) the first C2S classified cloud-based data analytics infrastructure (C2S) at LANL, and 4) external guidance and follow-on funding from multiple U.S. Combatant Commands.

Publications

Presentation Slides

Del Valle, S. Y. Heterogeneous Computing & Data Fusion for Global Dynamics. Presented at *DoD-DOE Data Analytics Technical Exchange*, Arlington, Virginia, United States, 2019-05-29 - 2019-05-29. (LA-UR-19-24177)

Posters

Del Valle, S. Y., J. R. Conrad, A. R. Daughton, G. Fairchild, J. Gafur, E. N. A. Generous, K. C. Kempfert, C. A. Manore, K. Martinez, D. A. Osthus and N. K. Parikh. Heterogeneous Computing & Data Fusion for Global Dynamics. Presented at *DoD-DOE Data Analytics Technical Exchange*, Arlington, Virginia, United States, 2019-05-29 - 2019-05-29. (LA-UR-19-24260)

Variational Quantum Eigensolver for Single-Point Water Electronic Energy Calculation

Pavel Dub
20190607ER

Project Description

In the next 5 years, quantum computers are expected to cross a threshold beyond which classical simulation of the devices will become impossible. This next generation of quantum hardware needs to be applied to addressing problems of grand-challenge science. The bridging approach proposed in this proposal is one way to reach that goal. Variational Quantum Eigensolver (VQE) that can improve upon best-in-class classical results should enable researchers to address a number of scientific challenges.

Technical Outcomes

VQE is based on preparation of trial states based on a quantum ansatz and measuring an average value of a qubit Hamiltonian. We used a Los Alamos-machine learning algorithm (Cincio, L. et al. New. J. Phys. 2018, 20, 113022) and discovered that the simplest ansatz affects only 3 qubits out of 14 (H2O molecule, sto-3g basis set) thus significantly reducing complexity of the problem.

Publications

Presentation Slides

Dub, P. The role of the metal-bound N–H functionality in Noyori-type molecular catalysts. Presented at *meeting with PNNL scientists*, Richmond, Washington, United States, 2019-08-07 - 2019-08-07. (LA-UR-19-27936)

Physics-Based Machine Learning for Electric Power Outage Prediction

Carleton Coffrin

20190630ER

Project Description

Machine learning is currently being used as a black box for performing various tasks such as predicting power outages, classifying images or identifying an intruder, to name a few. Scientists are not able to easily incorporate physical constraints into existing prediction algorithms, leading to situations where predictions violate simple laws of physics giving rise to poor prediction results. The goal of this project is to incorporate physical constraints into the learning algorithms so that they are satisfied by construction. This will lead to a new generation of robust and explainable predictors based on scalable constrained-optimization algorithms.

Technical Outcomes

Novel machine learning algorithms were developed for image classification. A proof of concept validation was conducted on a seminal dataset of hand written digits (MNIST). The preliminary results on digit classification are promising with comparable accuracy of state of the alternatives.

Statistical Numerics for Predictive Science

Michael Grosskopf
20190635ER

Project Description

Computer simulation of physical systems plays a critical role in modern science and engineering. Building trust in the use of simulator results requires a deep understanding of the different aspects of uncertainty that result from the use of imperfect models and solvers with unknown parameters that are used to match noisy data. This project will build on new results in probabilistic numerical methods to coherently incorporate solver uncertainty with other forms of statistical and epistemic uncertainty to push the boundaries of modern predictive science.

Technical Outcomes

We explored the properties of the state-of-the-art in probabilistic numerical methods and attempted to extend the methodology to simulation of shock hydrodynamics. While the success at development of a probabilisitic shock solver was limited, the development of R code and understanding for implementing modern probabilistic numerical methods is an important step forward in uncertainty quantification capabilities at the Laboratory. Additionally, lessons learned in extending to shock hydro offer new exciting future opportunities.

Searching for ConText: Microtasking to Solve Computationally Unsolvable Problems

Kari Sentz

20190637ER

Project Description

Concomitant with the increased adoption of classified computing, Department of Energy (DOE) as a complex is generating potentially classified information at a rate that our human derivative classifier resources cannot possibly match. The unintentional release of classified information is a significant source of security incidents across the complex. Such releases pose a serious threat to national and international security interests and our critical DOE assets. Automated computational tools are a requirement to keep pace with the growing needs of the community. DOE and National Nuclear Security Administration (NNSA) are not alone in this vulnerability. The protection of sensitive information is common to the missions of all government organizations and those that serve them.

Technical Outcomes

The research developed computational statistics/machine learning and human-in-the-loop methods for semantically structuring large unstructured data sets hierarchically. Specifically, we advanced new more meaningful ways of capturing hidden structure in unstructured text data; cross-leveraged complementary methods through advanced approaches to modelling and fusing information; identified opportunities to use human interaction to continually improve semantically structured representations; and developed a prototype for extracting information from users with a search engine.

Publications

Conference Papers

Nguyen, Q., R. B. Porter and B. Zimmer. Trade-offs Between Inference and Learning in Image Segmentation. Presented at *Applications of Machine Learning, SPIE Optical Engineering and Applications*. (San Diego, California, United States, 2019-08-13 - 2019-08-14). (LA-UR-19-27865)

Reports

Sentz, K., J. E. J. Powell, A. N. Skurikhin and R. B. Porter. Searching for ConText: Microtasking to Solve Computationally Unsolvable Problems. Unpublished report. (LA-UR-19-30118)

Posters

Skurikhin, A. N. and T. L. Burr. Learning Ensembles of Graphical Models for Context-Aware Pattern Recognition. Presented at *Data and Information Fusion Conference*, Santa Fe, New Mexico, United States, 2019-08-20 - 2019-08-22. (LA-UR-19-28145)

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).

Publications

Journal Articles

Berrone, S., J. D. Hyman and S. Pieraccini. Multilevel Monte Carlo predictions of first passage times in three-dimensional discrete fracture networks: A graph-based approach. Submitted to *Water Resources Research*. (LA-UR-19-29755)

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., H. Rajaram, S. Srinivasan, N. Makedonska, S. Karra, H. S. Viswanathan and G. Srinivasan. Matrix Diffusion in Fractured Media: New Insights Into Power Law Scaling of Breakthrough Curves. 2019. *Geophysical Research Letters*. (LA-UR-19-23625 DOI: 10.1029/2019GL085454)

Hyman, J. D., J. Jimenez-Martinez, C. W. Gable, P. H. Stauffer and R. J. Pawar. Characterizing the Impact of Fractured Caprock Heterogeneity on Supercritical CO2 Injection. 2020. *Transport in Porous Media*. **131** (3): 935-955. (LA-UR-19-25316 DOI: 10.1007/s11242-019-01372-1)

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)

Hyman, J. D., M. Dentz, A. A. Hagberg and P. Kang. Emergence of Stable Laws for First Passage Times in Random Three-Dimensional Fracture Networks. Submitted to *Physical Review Letters*. (LA-UR-19-23405)

*Hyman, J. D., M. Dentz, A. Hagberg and P. K. Kang. Linking Structural and Transport Properties in Three-Dimensional Fracture Networks. 2019. *Journal of Geophysical Research: Solid Earth*. **124** (2): 1185-1204. (LA-UR-18-27717 DOI: 10.1029/2018JB016553)

Kang, P. K., J. D. Hyman, W. S. Han and M. Dentz. Anomalous Transport in Three-Dimensional Discrete Fracture Networks: Interplay between Aperture Heterogeneity and Particle Injection Modes. Submitted to *Physical Review Fluids*. (LA-UR-20-20512)

Osthus, D. A., J. D. Hyman, S. Karra, N. Panda and G. Srinivasan. A Probabilistic Clustering Approach for Identifying Primary Subnetworks of Discrete Fracture Networks with Quantified Uncertainty. Submitted to *SIAM/ASA Journal on Uncertainty Quantification*. (LA-UR-19-27288)

Romano, V., S. Bigi, F. Carnevale, J. D. Hyman, S. Karra, A. J. Valocchi, M. Tartarello and M. Battaglia. Hydraulic characterization of a fault zone from fracture distribution. Submitted to *Journal of Structural Geology*. (LA-UR-19-32302)

*Sherman, T., J. D. Hyman, D. Bolster, N. Makedonska and G. Srinivasan. Characterizing the impact of particle behavior at fracture intersections in three-dimensional discrete fracture networks. 2019. *Physical Review E*. **99** (1): 013110. (LA-UR-18-29382 DOI: 10.1103/PhysRevE.99.013110)

Sherman, T., J. D. Hyman, M. Dentz and D. Bolster. Characterizing the Influence of Fracture Density on

Network Scale Transport. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-19-27671)

Srinivasan, S., E. Cawi, J. D. Hyman, D. A. Osthus, A. A. Hagberg, H. S. Viswanathan and G. Srinivasan. Physics-Informed Machine Learning for Backbone Identification in Discrete Fracture Networks. Submitted to *Computational Geosciences*. (LA-UR-19-28357)

Sweeney, M. R., C. W. Gable, S. Karra, P. H. Stauffer, R. J. Pawar and J. D. Hyman. Upscaled discrete fracture matrix model (UDFM): an octree-refined continuum representation of fractured porous media. Submitted to *Computational Geosciences*. (LA-UR-19-25805)

Sweeney, M. R. and J. D. Hyman. Stress effects on flow and transport in three-dimensional fracture networks. Submitted to *Journal of Geophysical Research: Solid Earth*. (LA-UR-19-30234)

Presentation Slides

Hyman, J. D. Applications of Graph Theory and Machine Learning to Discrete Fracture Networks. . (LA-UR-18-31148)

Hyman, J. D. The Influence of Multiple Scales in Fractured Media on Flow and Transport Properties. . (LA-UR-18-30105)

Hyman, J. D. FRAM. Presented at *dfnWorkShop*, SANTA FE, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29484)

Hyman, J. D. pydfnworks. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29482)

Hyman, J. D. background slides for dfnWorkShop. Presented at *dfnworkshop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29494)

Hyman, J. D., H. Rajaram, S. Srinivasan, N. Makedonska, S. Karra, H. S. Viswanathan and G. Srinivasan. The role of advection and matrix diffusion in power-law scaling behavior of first passage times in three-dimensional discrete fracture networks. Presented at *AGU fall Meeting*, San Fransisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-31973)

Hyman, J. D., J. Jimenez-Martinez and R. J. Pawar. Characterizing the Impact of Fracture Geometry and Network Structure on Multiphase Flow through Fractured Media. Presented at *AGU Fall Meeting*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31334)

Sweeney, M. R. Modeling discrete fracture networks in porous media using a continuum approach. Presented at *Arizona - Los Alamos Days*, Tucson, Arizona, United States, 2019-04-20 - 2019-04-21. (LA-UR-19-23513)

Sweeney, M. R. Leveraging the dfnWorks software suite for continuum modeling of fractured porous media. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29299)

Sweeney, M. R., J. D. Hyman, C. W. Gable, S. Karra, N. Makedonska and R. J. Pawar. Octree-refined continuum representation of discrete fracture networks. Presented at *SIAM Geoscience 2019*, Houston, Texas, United States, 2019-03-11 - 2019-03-11. (LA-UR-19-22018)

Posters

Kang, P., J. D. Hyman and M. Dentz. Anomalous Transport in 3D Discrete Fracture Networks (DFN): Interplay between Aperture Heterogeneity and Particle Injection Modes. Presented at *AGU Fall Meeting*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31476)

Sherman, T. J., D. Bolster, N. Makedonska, G. Srinivasan and J. D. Hyman. Characterizing the impact of Lagrangian particle behavior at fracture intersections on transport through three-dimensional fracture networks. Presented at *American Geophysical Union Fall 2018*, Washington DC, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31288)

Sweeney, M. R. and J. D. Hyman. How do different stress regimes affect transport in three-dimensional discrete fracture networks?. Presented at *LANL Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28466)

Sweeney, M. R. and J. D. Hyman. How do different stress networks affect transport in three-dimensional discrete fracture networks?. Presented at *dfnWorkShop*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-23. (LA-UR-19-29295)

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.

Technical Outcomes

Extensions to a Poisson matrix factorisation (PMF) model were developed to improve graph link prediction. The extensions includes scenarios that are commonly encountered in cyber and national security applications yet not accounted for in existing models. The use of generative hyper-heuristic search algorithms to automate the selection and generation of customized link prediction algorithms according to the specific problem and data set were also developed.

Publications

Journal Articles

Turcotte, M., F. Sanna Passino and N. A. Heard. GRAPH LINK PREDICTION IN COMPUTER NETWORKS USING POISSON MATRIX FACTORISATION. Submitted to *Annals of Applied Statistics*. (LA-UR-20-20567)

Conference Papers

Pope, A. S., D. R. Tauritz and M. Turcotte. Automated Design of Tailored Link Prediction Heuristics for Applications in Enterprise Network Security. Presented at *The Genetic and Evolutionary Computation Conference*. (Prague, Czech Republic, 2019-07-13 - 2019-07-17). (LA-UR-19-23176)

Reports

Pope, A. S. The Automated Design of Network Graph Algorithms with Applications in Cybersecurity. Unpublished report. (LA-UR-20-20273)

Presentation Slides

Y. Hallgren, K. L. and M. Turcotte. Robust Bayesian change detection for cyber-security applications. . (LA-UR-20-20324)

Sanna Passino, F., M. Turcotte and N. Heard. Some ideas on Bayesian modelling of networks for cyber-security applications. Presented at *Focused Research Workshop*, Bristol, United Kingdom, 2019-03-25 - 2019-03-28. (LA-UR-19-23198)

Turcotte, M. Latent Feature Models for Network Link Prediction with Labelled Nodes. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-27 - 2019-07-27. (LA-UR-19-27254)

Posters

Sanna Passino, F. and M. Turcotte. Latent feature models for network link prediction with labelled nodes. . (LA-UR-18-26824)

Machine Learning of Quantum Computing Algorithms

Patrick Coles
20180628ECR

Project Description

Building a quantum computer has been compared to the Manhattan Project, in that achieving the goal will have widespread effects, even at the geo-political level. Quantum computers promise to revolutionize various fields like pharmaceutical design and big-data analysis. A quantum computer would impact both financial and national security, since it could be used to break our current methods for encrypted communication. Furthermore, our national nuclear security could benefit from quantum computers, since they may speed up our ability to optimize weapons design and to simulate explosion dynamics. However, none of these impacts will be realized without well-designed algorithms. In other words, exploiting recent advances in quantum computing hardware (e.g., made by US companies like Google, IBM, and Intel) will require efficient software. Our work will address this software issue by automating the process of designing quantum computing algorithms. Our software will determine the fastest algorithm for a specific hardware and a specific application. For example, suppose one wants to use a quantum computer to simulate a biological molecule. Our software will find the fastest algorithm for this – taking into account the imperfections of the hardware. This will be a crucial tool for using real quantum computers in the future.

Publications

Journal Articles

Bravo-Prieto, C., R. LaRose, M. V. S. Cerezo de la Roca, Y. Subasi, L. Cincio and P. J. Coles. Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems. Submitted to *arXiv*. (LA-UR-19-29101)

Coles, P. J., J. Kubler, A. T. Arrasmith and L. Cincio. An Adaptive Optimizer for Measurement-Frugal Variational Algorithms. Submitted to *arXiv; Quantum*. (LA-UR-19-29383)

*Coles, P. J., M. Cerezo and L. Cincio. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states. 2019. *Physical Review A*. **100** (2): 022103. (LA-UR-19-22724 DOI: 10.1103/PhysRevA.100.022103)

Khatri, S., R. LaRose, A. Poremba, L. Cincio, A. T. Sornborger and P. J. Coles. Quantum-assisted quantum compiling. 2019. *Quantum*. **3**: 140. (LA-UR-18-25861 DOI: 10.22331/q-2019-05-13-140)

*LaRose, R., A. Tikku, E. O'Neel-Judy, L. Cincio and P. J. Coles. Variational quantum state diagonalization. 2019. *npj Quantum Information*. **5** (1): 57. (LA-UR-18-29266 DOI: 10.1038/s41534-019-0167-6)

S. Cerezo de la Roca, M. V., A. Poremba, L. Cincio and P. J. Coles. Variational quantum fidelity estimation. Submitted to *Physical Review Letters*. (LA-UR-19-25585)

S. Cerezo de la Roca, M. V., A. Sone, T. J. Volkoff, L. Cincio and P. J. Coles. Cost-Function-Dependent Barren Plateaus in Shallow Quantum Neural Networks. Submitted to *Nature Communications*. (LA-UR-19-32681)

Sharma, K., S. Khatri, M. V. S. Cerezo de la Roca and P. J. Coles. Noise Resilience of Variational Quantum Compiling. Submitted to *New Journal of Physics*. (LA-UR-19-28095)

*Subasi, Y., L. Cincio and P. J. Coles. Entanglement spectroscopy with a depth-two quantum circuit. 2019. *Journal of Physics A: Mathematical and Theoretical*. **52** (4): 44001. (LA-UR-18-25483 DOI: 10.1088/1751-8121/aaf54d)

Di Tulio, M., R. Rossignoli and M. V. S. Cerezo de la Roca. Fermionic entanglement in the Lipkin model. Submitted to *Physical Review A*. (LA-UR-19-27998)

Zhang, Y., P. J. Coles, A. Winick, J. Lin and N. Lutkenhaus. Security proof of practical quantum key distribution with detection-efficiency mismatch. Submitted to *Physical Review A*. (LA-UR-20-22369)

Posters

S. Cerezo de la Roca, M. V., A. Poremba, L. Cincio and P. J. Coles. Variational Quantum Fidelity Estimation (VQFE). . (LA-UR-19-28193)

S. Cerezo de la Roca, M. V., L. Cincio and P. J. Coles. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states Or, how to compare two quantum states on a quantum computer. . (LA-UR-19-24875)

Numerical Methods for Radiation Hydrodynamics Simulations on Current and Future Advanced Parallel Architectures

Jonas Lippuner
20190519ECR

Project Description

To ensure the safety and reliability of the United States nuclear stockpile, large-scale, sophisticated, multi-physics computer simulations of nuclear explosions are necessary since the US does not conduct nuclear tests anymore. To perform these simulations, the Department of Energy operates the largest supercomputers in the world. The computing hardware in these supercomputers has changed dramatically in the last decade and most of the computing power (up to 95%) is now in special, advanced architecture chips, such as graphics processing units (GPUs). The simulation codes used today were designed long before these chips were invented and the methods and algorithms used in our codes are not necessarily the best suited ones for the current and future hardware. This project seeks to investigate which methods perform most efficiently on this advanced hardware and to develop new such methods. The results of this work will be crucial to decide the future direction of the various programmatic simulation code development efforts of the National Nuclear Security Administration. The new methods developed as part of this project will also help ensure that our large-scale physics simulations run efficiently on current and future supercomputers.

Improving Predictions of Complex Systems with Predictive Discrepancy Models and Data Fusion

David Osthus
20190546ECR

Project Description

Disease spread represents a vulnerability and risk to our national security. Pandemics don't respect borders and pose a significant burden on our populace and infrastructure. Intervention strategies are only successful if deployed in a timely, efficient, and targeted manner. Preferably, interventions are proactive rather than reactive. Before we can proactively counter disease spread, however, we have to be able to forecast its spread. Thus, disease forecasting capabilities constitute a significant link in the national security chain. This project will develop state, regional, and national flu forecasting models that will be deployed in real-time to maximize impact with public health decision makers. These models will push the limits of disease forecasting by bringing together state-of-the-art mathematical modeling with numerous data sources. The mathematical modeling advances are relevant to many applications with incomplete theory, experimental data, and the need to make predictions with quantified uncertainties. As such, this work has broad applicability to Department of Energy and ational Nuclear Security Administration applications, such as nuclear weapons, nonproliferation, and energy, as well as direct applications in National Institutes of Health and Centers for Disease Control and Prevention.

Publications

Journal Articles

Gibson, G. C., D. A. Osthus, K. R. Moran and N. G. Reich. Improving Probabilistic Infectious Disease Forecasting Through Coherence. Submitted to *PLOS Computational Biology*. (LA-UR-19-32598)

Osthus, D. A. and K. R. Moran. Multiscale influenza forecasting. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-19-28977)

Presentation Slides

Osthus, D. A. Dante: An Applied Statistician's Approach to Flu Forecasting. Presented at *FluSight Seasonal Influenza Forecasting Workshop*, Atlanta, Georgia, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28213)

Osthus, D. A. Dante: An Applied Statistician's Approach to Flu Forecasting. . (LA-UR-19-28798)

Osthus, D. A. and K. R. Moran. Multiscale Flu Forecasting. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-28 - 2019-07-28. (LA-UR-19-27237)

Posters

Osthus, D. A. 2018/19 FluSight Challenge Dante and DBM +. Presented at *FluSight Seasonal Influenza Forecasting Workshop*, Atlanta, Georgia, United States, 2019-08-20 - 2019-08-20. (LA-UR-19-28198)

Optimizing Scientific Codes in the Presence of Extreme Heterogeneity Using Machine Learning

Eun Jung Park
20190566ECR

Project Description

Existing hint-based approaches to optimizing the translation of human code to machine code for complex scientific codes have been effective at generating efficient code for traditional architectures, but emerging heterogeneous architectures have proven too complex for existing techniques. This project will leverage emerging machine learning techniques to perform code translation for complex, heterogeneous machine architectures. The resulting techniques will be one critical step in supporting scientific computing on the non-traditional computer architectures expected to replace existing supercomputing platforms in the post-Exascale era.

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.

Technical Outcomes

We developed a novel inverse modeling technique that enables the accurate reconstruction of signals from small sets of measurements by learning a mathematical model that exploits properties of the reconstruction space. The reconstruction is represented in terms of sums of convolutions with so called dictionary filters. The convolutional model optimizes over the entire signal, yielding near-optimal and sparse representations. The result is a considerable advance in the reconstruction of a broad range of experimental data.

Publications

Journal Articles

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)

*Liu, J., C. Garcia-Cardona, B. Wohlbereg and W. Yin. First- and Second-Order Methods for Online Convolutional Dictionary Learning. 2018. *SIAM Journal on Imaging Sciences*. **11** (2): 1589-1628. (LA-UR-17-27611 DOI: 10.1137/17M1145689)

Conference Papers

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*. (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)

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)

Presentation Slides

Garcia Cardona, C. Generalized Convolutional Representation for Field Data on Graphs. Presented at *SIAM Conference on Computational Science and Engineering*, Atlanta, Georgia, United States, 2017-02-27 - 2017-02-27. (LA-UR-17-22319)

Garcia Cardona, C. Convolutional Dictionary Learning for Inverse Problems. Presented at *SIAM Conference on Computational Science and Engineering*, Spokane, Washington, United States, 2019-02-25 - 2019-03-01. (LA-UR-19-21427)

Skau, E. W. and C. Garcia Cardona. Convolutional Dictionary Learning for Tomography. Presented at *2018 IEEE Image, Video, and Multidimensional Signal Processing (IVMSP) Workshop*, Zagori, Greece, 2018-06-10 - 2018-06-12. (LA-UR-18-24894)

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.

Technical Outcomes

This project developed novel algorithms for large-scale nonlinear optimization. Mathematical insights where leveraged to improve the scalability of optimization algorithms which were developed into solvers that can be applied to a wide-range of optimization tasks faced by the Department of Energy. These solvers were made available to the broader community as open-source software. The outcomes of this project have made significant progress on several open grand-challenge problems relating to optimization of critical infrastructure networks.

Publications

Journal Articles

Hijazi, H., C. Coffrin and P. V. Hentenryck. Convex quadratic relaxations for mixed-integer nonlinear programs in power systems. 2017. *Mathematical Programming Computation*. **9** (3): 321-367. (LA-UR-18-21065 DOI: 10.1007/s12532-016-0112-z)

Conference Papers

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)

Reports

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

Tasseff, B. A., C. J. Coffrin, A. Waechter and C. Laird. Exploring Benefits of Linear Solver Parallelism on Modern Nonlinear Optimization Applications. Unpublished report. (LA-UR-19-28981)

Presentation Slides

Coffrin, C. J. PowerModels.jl: A Framework for Exploring Power Flow Formulations (presentation). Presented at *20th Power Systems Computation Conference*, Dublin, Ireland, 2018-06-11 - 2018-06-15. (LA-UR-18-25317)

Coffrin, C. J. Convex Relaxations of the Power Flow Equations: A Brief Introduction. . (LA-UR-19-24682)

Coffrin, C. J. Optimization Based Bound Tightening for Power Network Optimization. Presented at *IISE Anual Conference and Expo*, Orlando, Florida, United States, 2019-05-18 - 2019-05-21. (LA-UR-19-24683)

Coffrin, C. J., M. D. Vuffray and A. Lokhov. Comparison of Three D-Waves. . (LA-UR-18-23860)

Coffrin, C. J. and L. A. Roald. A Brief Introduction to AC Power Flow Relaxations. . (LA-UR-18-24847)

Kroger, O., C. J. Coffrin, H. L. Hijazi and H. Nagarajan. Juniper: An Open-Source Nonlinear Branch-and-Bound Solver in Julia (presentation). 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-18-25318)

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.

Publications

Journal Articles

*Caravelli, F. Locality of interactions for planar memristive circuits. 2017. *Physical Review E*. **96** (5): 052206. (LA-UR-17-23533 DOI: 10.1103/PhysRevE.96.052206)

Caravelli, F. Asymptotic behavior of memristive circuits and combinatorial optimization. Submitted to *Proceeding of the National Academy of Science*. (LA-UR-17-30617)

*Caravelli, F. Asymptotic Behavior of Memristive Circuits. 2019. *Entropy*. **21** (8): 789. (LA-UR-18-24748 DOI: 10.3390/e21080789)

Caravelli, F. On a ``continuum" formulation of the Ising model partition function. Submitted to *Journal of Statistical Mechanics: Theory and Experiment*. (LA-UR-19-28192)

Caravelli, F. Spin-Dot interactions in Artificial Spin Ice: population inversion as an entropic effect. Submitted to *Physical Review Letters*. (LA-UR-19-31351)

Caravelli, F., C. Nisoli and G. Chern. Phase-change spin ice memory resistor. Submitted to *Physical Review Letters*. (LA-UR-19-27438)

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. 2018. *Technologies*. **6** (4): 118. (LA-UR-18-27766 DOI: 10.3390/technologies6040118)

*Caravelli, F. and P. Barucca. A mean-field model of memristive circuit interaction. 2018. *EPL (Europhysics Letters)*. **122** (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)

*Cui, T., F. Caravelli and C. Ududec. Correlations and clustering in wholesale electricity markets. 2018. *Physica A: Statistical Mechanics and its Applications*. **492**: 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)

Sheldon, F. C., F. Caravelli and A. Kolchinsky. Feasibility, Optimality and Implementability of memory circuits for Reservoir Computing. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-20-20314)

Presentation Slides

Caravelli, F. Non-equilibrium properties of memristive networks. Presented at *Applied Statistical Physics*, Santa Fe, New Mexico, United States, 2017-05-01 - 2017-05-05. (LA-UR-17-23642)

Caravelli, F. Information Theory and (F)RG. Presented at *FRG Conference*, Trento, Italy, 2019-09-16 - 2019-09-16. (LA-UR-19-29327)

Caravelli, F. Memristive Networks. Presented at *Talk @ICTP Trieste*, Trieste, Italy, 2019-09-23 - 2019-09-23. (LA-UR-19-29539)

Optimal Control of Quantum Machines

Davide Girolami
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.

Technical Outcomes

The first important result of the project is the exact calculation of the minimum energy and time required for experimentally creating quantum correlations, such as entanglement. This finding advances our understanding of quantum processes, improving our ability to run quantum computers more efficiently. A second significant result is a quantum algorithm for discovering causal relations in complex data sets. The protocol paves the way for harnessing quantum causal links as a resource for quantum technologies.

Publications

Journal Articles

*Girolami, D. How Difficult is it to Prepare a Quantum State?. 2019. *Physical Review Letters*. **122** (1): 010505. (LA-UR-18-27400 DOI: 10.1103/PhysRevLett.122.010505)

Girolami, D. Quantifying Causation. Submitted to *Physical Review Letters*. (LA-UR-19-26319)

*Yadin, B., P. Bogaert, C. E. Susa and D. Girolami. Coherence and quantum correlations measure sensitivity to dephasing channels. 2019. *Physical Review A*. **99** (1): 012329. (LA-UR-18-29513 DOI: 10.1103/PhysRevA.99.012329)

Presentation Slides

Girolami, D. Detecting metrologically useful asymmetry and entanglement by a few local measurements.. Presented at *SQUINT Workshop*, Santa Fe, New Mexico, United States, 2018-02-22 - 2018-02-22. (LA-UR-18-21362)

Girolami, D. Characterizing genuine multipartite correlations and their pattern complexity. Presented at *APS March Meeting 2018*, Los Angeles, California, United States, 2018-03-05 - 2018-03-05. (LA-UR-18-21555)

Girolami, D. Characterizing genuine multipartite correlations and their pattern complexity. Presented at *ICCS 2018*, Cambridge, Massachusetts, United States, 2018-07-22 - 2018-07-22. (LA-UR-18-26801)

Girolami, D. Characterizing genuine multipartite correlations and their pattern complexity. Presented at *Information Engines at the Frontiers of Nanoscale Thermodynamics*, Telluride, Colorado, United States, 2018-07-19 - 2018-07-26. (LA-UR-18-26800)

Girolami, D. Quantum Resources for Information Processing. . (LA-UR-19-20054)

Girolami, D. Quantum Resources for Information Processing. . (LA-UR-19-20055)

Girolami, D. Quantum Resources for Information Processing. . (LA-UR-19-21941)

Girolami, D. A Quantum Law of Requisite Variety. Presented at *APS March Meeting 2019*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-21940)

Girolami, D. How difficult is it to [re[are a quantum state?. . (LA-UR-19-23651)

Girolami, D. Quantum Resources for Noisy Information Processing. . (LA-UR-19-24297)

Girolami, D. Quantum Resources for Noisy Information Processing. . (LA-UR-19-27815)

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

Journal Articles

Mansbach, R. A., C. A. Lopez Bautista, N. W. Hengartner, G. Malloci, J. Mehla, I. V. Leus, P. Ruggerone, H. I. Zgurskaya, V. Rybenkov and S. Gnanakaran. Application of a Fragment-Based Algorithm for Drug Design to Antibiotics for Resistant Bacteria. Submitted to *Nature Communications*. (LA-UR-19-24832)

Mansbach, R. A., I. V. Leus, J. Mehla, C. A. Lopez Bautista, J. K. Walker, V. V. Rybenkov, N. W. Hengartner, H. I. Zgurskaya and S. Gnanakaran. Machine Learning Algorithm Identifies an Antibiotic Vocabulary for Permeating Gram-Negative Bacteria. Submitted to *Journal of Chemical Information and Modeling*. (LA-UR-20-22055)

*Mansbach, R. A., T. Travers, J. M. Fair and S. Gnanakaran. Snails In Silico: A Review of Computational Studies on the Conopeptides. 2019. *Marine Drugs*. **17** (3): 145. (LA-UR-19-21315 DOI: 10.3390/md17030145)

Mansbach, R. A., T. Travers, S. Chakraborty and S. Gnanakaran. A Graph-Directed Approach for Creation of a Homology Modeling Library: Application to Conotoxin Structure Prediction. Submitted to *Structure*. (LA-UR-19-26210)

Mehla, J., G. Malloci, R. A. Mansbach, C. A. Lopez Bautista, P. D. Manrique Charry, R. Tsivkovski, S. B. Grindstaff, R. H. Cascella, N. W. Hengartner, L. K. Herndon, A. Atzori, A. V. Vargiu, F. Cardamone, O. Lomovskaya, P. Ruggerone, S. Gnanakaran, V. V. Rybenkov and H. I. Zgurskaya. Physico-chemical and molecular descriptors of efflux substrates, inhibitors and avoiders in Pseudomonas aeruginosa. Submitted to *ACS Infectious Diseases*. (LA-UR-20-21086)

Schmilovich, K., R. A. Mansbach and A. L. Ferguson. The Search for Shine: Active learning identifies optimal pi-conjugated peptide chemistries for optoelectronics. Submitted to *Chemical Science*. (LA-UR-19-27326)

Reports

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)

Presentation Slides

Mansbach, R. A., C. A. Lopez Bautista, N. W. Hengartner and S. Gnanakaran. A Fragment Library for Drug Activity in Gram Negative Bacteria. . (LA-UR-19-20062)

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.

Technical Outcomes

There are two main technical outcomes: (1) the development of tensor network techniques for studying quantum many-body problems. In particular, I developed scalable algorithms for analyzing topological order as well as other emergent phenomena in quantum many-body physics; (2) the development of machine learning tools for quantum algorithm discovery. These tools help finding short-depth (possibly approximate) algorithms for near-term noisy quantum computers. Such algorithms are crucial for reducing computational error on current quantum devices.

Publications

Journal Articles

Berman, G. P., V. N. Gorshkov, V. V. Tereshchuk, V. I. Tsifrinovich and M. Merkli. Two-Component Axionic Dark Matter Halos. Submitted to *Physical Review D*. (LA-UR-20-20772)

Bravo-Prieto, C., R. LaRose, M. V. S. Cerezo de la Roca, Y. Subasi, L. Cincio and P. J. Coles. Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems. Submitted to *arXiv*. (LA-UR-19-29101)

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

*Cincio, L., Y. Subasi, A. T. Sornborger and P. J. Coles. Learning the quantum algorithm for state overlap. 2018. *New Journal of Physics*. **20** (11): 113022. (LA-UR-18-21984 DOI: 10.1088/1367-2630/aae94a)

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)

*Coles, P. J., M. Cerezo and L. Cincio. Strong bound between trace distance and Hilbert-Schmidt distance for low-rank states. 2019. *Physical Review A*. **100** (2): 022103. (LA-UR-19-22724 DOI: 10.1103/PhysRevA.100.022103)

Francuz, A., J. Dziarmaga, G. Vidal and L. Cincio. Determining topological order from infinite projected entangled pair states. Submitted to *Physical Review Letters*. (LA-UR-19-29100)

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*. **96** (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. 2019. *Quantum*. **3**: 140. (LA-UR-18-25861 DOI: 10.22331/q-2019-05-13-140)

*LaRose, R., A. Tikku, E. O'Neel-Judy, L. Cincio and P. J. Coles. Variational quantum state diagonalization. 2019. *npj Quantum Information*. **5** (1): 57. (LA-UR-18-29266 DOI: 10.1038/s41534-019-0167-6)

*Rams, M. 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 X*. **8** (4): 041033. (LA-UR-18-20465 DOI: 10.1103/PhysRevX.8.041033)

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)

Roberts, D., L. Cincio, A. B. Saxena, A. Petukhov and S. Knysh. Noise amplification at spin-glass bottlenecks of quantum annealing:a solvable 1+1D model. Submitted to *Physical Review A*. (LA-UR-19-28446)

S. Cerezo de la Roca, M. V., A. Poremba, L. Cincio and P. J. Coles. Variational quantum fidelity estimation. Submitted to *Physical Review Letters*. (LA-UR-19-25585)

*Subasi, Y., L. Cincio and P. J. Coles. Entanglement spectroscopy with a depth-two quantum circuit. 2019. *Journal of Physics A: Mathematical and Theoretical*. **52** (4): 44001. (LA-UR-18-25483 DOI: 10.1088/1751-8121/aaf54d)

Reports

Cincio, L., I. M. Vitev, D. A. Neill and B. Yoon. proposal: Toward Quantum Computation of Hadronization in QCD. Unpublished report. (LA-UR-19-24958)

Cincio, L. and D. Spier Moreira Alves. Renormalization of Entanglement in Quantum Field Theories. Unpublished report. (LA-UR-19-23645)

Cincio, L. and P. J. Coles. proposal: Advancing Integrated Development Environments for Quantum Computing through Fundamental Research (AIDE-QC). Unpublished report. (LA-UR-19-24953)

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)

Presentation Slides

Cincio, L. Tensor networks. Presented at *Zakopane school of Theoretical Physics*, Zakopane, Poland, 2017-06-13 - 2017-06-21. (LA-UR-17-24609)

Cincio, L. Automating quantum algorithm discovery. Presented at *Informal meeting at UCSD*, San Diego, California, United States, 2018-01-10 - 2018-01-10. (LA-UR-18-20145)

Cincio, L. Simulating real-time evolution on classical and quantum computers. Presented at *Santa Fe meeting*, Santa Fe, New Mexico, United States, 2018-07-10 - 2018-07-10. (LA-UR-18-26692)

Posters

Cincio, L., Y. Subasi, A. T. Sornborger and P. J. Coles. Automating Quantum Algorithms Design. Presented at *squint*, Santa Fe, New Mexico, United States, 2018-02-22 - 2018-02-24. (LA-UR-18-21361)

Nortier, F. M., R. Bhandia, E. R. Birnbaum, J. C. Cooley, K. D. John, C. A. Martinez, E. M. O'Brien, E. R. Olivas, B. Stein and C. Vermeulen. Proton Beam Production of Curie Scale Ac-225 at 100 MeV and Below. Presented at *11th International Symposium on Targeted Alpha Therapy (TAT11)*, Ottawa, Canada, 2019-04-01 - 2019-04-01. (LA-UR-19-21984)

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.

Technical Outcomes

The goal of this fellowship was to study trace elements in geological materials using techniques available on the ChemCam and SuperCam instruments. Both ChemCam and SuperCam use Laser-Induced Breakdown Spectroscopy (LIBS) and SuperCam also uses luminescence spectroscopy to analyze trace elements in geological samples. This work produced quantitative modeling for chromium using LIBS, an expanded LIBS database for additional trace elements, and developed the luminescence technique in preparation for the upcoming Mars mission in 2020.

Publications

Presentation Slides

Ollila, A. M. Luminescence spectroscopy: A new analytical tool for Mars exploration. . (LA-UR-17-30938)

Ollila, A. M., R. C. Wiens, S. M. Clegg, N. L. Lanza, O. Beyssac, M. Gautier, S. Sharma, A. Misra, S. Maurice and O. Gasnault. Luminescence Spectroscopy: Rare Earth Elements (and Friends) as Potential Biosignatures on Mars. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31080)

Materials for the Future

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

Neil Harrison
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.

Publications

Journal Articles

Balakirev, F. F., S. M. Ennaceur, R. J. Migliori and A. Migliori. Resonant ultrasound spectroscopy: The essential toolbox. 2019. *Review of Scientific Instruments*. **90** (12): 121401. (LA-UR-19-28447 DOI: 10.1063/1.5123165)

Harrison, N. Electronically driven collapse of the bulk modulus in delta-plutonium. Submitted to *Proceedings of the National Academy of Sciences of the United States of America*. (LA-UR-19-32035)

Harrison, N., J. B. Betts, F. F. Balakirev, S. Richmond, M. Jaime and P. H. Tobash. Twin source of electronic disorder in plutonium. Submitted to *TBD*. (LA-UR-19-20229)

Harrison, N. and M. Jaime. Hidden valence transition in uranium ruthenium two silicon two. Submitted to *Nature Communications*. (LA-UR-19-21055)

Joyce, J. J., K. S. Graham, J. Zhu, G. H. Lander, T. Durakiewicz, J. M. Wills, P. H. Tobash, E. D. Bauer, J. N. Mitchell and H. Choi. Competing Electronic Configurations for PuTe and New Insight on Plutonium Metal. Submitted to *Physical Review Letters*. (LA-UR-19-20178)

Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Physical Review X*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

Tutchton, R. M., W. Chiu, R. C. Albers, G. Kotliar and J. Zhu. Supplementary Information: Electronic Correlation Induced Expansion of Compensated Electron and Hole Fermi Pockets in d-Plutonium. Submitted to *Nature Communications*. (LA-UR-19-29905)

Tutchton, R. M., W. Chiu, R. C. Albers, G. Kotliar and J. Zhu. Electronic Correlation Induced Expansion of Compensated Electron and Hole Fermi Pockets in delta-Plutonium. Submitted to *Nature Communications*. (LA-UR-19-29904)

Conference Papers

Harrison, N., J. B. Betts, P. H. Tobash and M. Jaime. Magnetostriction of Ga-stabilized delta-plutonium. Presented at *Plutonium Futures*. (San Diego, California, United States, 2018-09-09 - 2018-09-14). (LA-UR-18-26836)

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the electronic and magnetic structure of Pu6Fe. Presented at *Pu Futures 2018*. (San Diego, California, United States, 2018-09-09 - 2018-09-09). (LA-UR-18-23453)

Maiorov, B. A., J. B. Betts, F. F. Balakirev and A. Migliori. Temperature dependent and Real Time Studies of Elastic Moduli of \xce\xb4-239Pu and alloys. Presented at *Plutonium Futures*. (san diego, California, United States, 2018-09-09 - 2018-09-14). (LA-UR-18-25818)

Tobash, P. H., E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, S. Richmond, D. Wheeler and T. Albrecht-Schmitt. Progress on the Thermophysical Properties of Some Plutonium Alloys and Compounds. Presented at *Pu Futures 2018*. (San Diego, California, United States, 2018-09-09 - 2018-09-09). (LA-UR-18-23371)

Books/Chapters

Tobash, P. H. and S. Bobev. Chemical Bonding and Structural Relationships in Extended Solids. (LA-UR-18-28530)

Reports

Nelson, C. A. Uncovering the role of 5f-electron magnetism in plutonium using capacitive dilatometry. Unpublished report. (LA-UR-19-20411)

Presentation Slides

Harrison, N. Magnetostriction of delta-plutonium. Presented at *Plutonium futures*, san diego, California, United States, 2018-09-09 - 2018-09-09. (LA-UR-18-28499)

Harrison, N. Magnetostriction of delta plutonium 2. Presented at *Plutonium Futures*, San Diengo, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28630)

Harrison, N., P. H. Tobash, M. Jaime, S. Richmond, J. B. Betts and M. R. Wartenbe. Phase stabilization by electronic entropy in plutonium. Presented at *American Physical Society March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21885)

Hernandez, S. C. Insights into point-defects of \xce\xb4-Pu and \xce\xb4-Pu-Ga alloys using density functional theory. Presented at *Uppsala University*, Uppsala, Sweden, 2018-06-08 - 2018-06-08. (LA-UR-18-24654)

Hernandez, S. C. Overview of using density functional theory for material science applications on Pu and its compounds. Presented at *Computational Data Science Approaches for Materials*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23136)

Hernandez, S. C. Density functional theory study of aging of Pu. . (LA-UR-20-21880)

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the Electronic and Magnetic Structure of Pu6Fe. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21830)

Kushwaha, S. K., M. K. Chan, N. Harrison, P. Ferrari Silveira Rosa, S. M. Thomas, E. D. Bauer, F. Ronning, J. Park and J. D. Thompson. Magnetic field induced Fermi liquid in a candidate topological Kondo insulator. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22244)

Maiorov, B. A., J. B. Betts, F. F. Balakirev, F. J. Freibert and A. Migliori. Temperature Dependent and Real Time Studies of Elastic Moduli of \xce\xb4-239Pu and Alloys. Presented at *Plutonium Futures*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-29991)

Migliori, A. and S. M. Ennaceur. Toward an understanding of aging in plutonium from direct measurements of stored energy. . (LA-UR-18-31769)

Tobash, P. H., E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, T. Albrecht-Schmitt and D. Wheeler. Thermophysical Property Studies on Pu Alloys and Compounds. Presented at *MRS 2018*, Phoneix, Arkansas, United States, 2018-04-02 - 2018-04-02. (LA-UR-18-22563)

Tobash, P. H., S. Richmond, E. D. Bauer, J. N. Mitchell, D. S. Schwartz, F. J. Freibert, D. Wheeler and T. Albrecht-Schmitt. Progress on the Thermophysical Properties of Some Plutonium Alloys and Compounds. Presented at *Pu Futures 2018*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28267)

Tutchton, R. M. Correlation and Electron-phonon coupling in the Electronic structure of Plutonium. Presented at *Science in 3*, Los Alamos, New Mexico, United States, 2018-06-13 - 2018-06-13. (LA-UR-18-26227)

Tutchton, R. M., J. Julien, Q. Si and J. Zhu. First Principles Study of the Fermi Surface Topology of CeCu2Si2. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22188)

Tutchton, R. M., J. Zhu and W. Chiu. Data Diversity as a Tool In the Search for d-Pu’s Missing Magnetism. Presented at *Computational Data Science Approaches for Materials*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-26601)

Tutchton, R. M. and J. Zhu. Fermi Surface Topology and Correlation Effects in the Electronic Structure of Plutonium. Presented at *APS March meeting*, Boston, Massachusetts, United States, 2019-03-03 - 2019-03-08. (LA-UR-19-21868)

Wartenbe, M. R., P. H. Tobash, N. Harrison, J. B. Betts, J. Singleton and L. E. W. Stritzinger. Plutonium in high magnetic fields. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22254)

Posters

Hernandez, S. C. and J. M. Wills. First Principles Investigation of the Electronic and Magnetic Structure of Pu6Fe. Presented at *Pu Futures 2018*, San Diego, California, United States, 2018-09-10 - 2018-09-10. (LA-UR-18-28384)

Nelson, C. A., M. R. Wartenbe, S. M. Thomas, G. M. Schmiedeshoff, N. Harrison and P. H. Tobash. Assembling and Calibrating a Capacitive Dilatometer for Magnetostriction and Thermal Expansion Measurements. . (LA-UR-18-26970)

Richmond, S. (U) Plutonium sample processing, grain growth and extraction by hydriding. . (LA-UR-19-21170)

Tutchton, R. M. and J. Zhu. Fermi Surface Topology and Correlation Effects in the Electronic Structures of Plutonium. Presented at *LRDR review*, Los Alamos, New Mexico, United States, 2019-02-26 - 2019-02-26. (LA-UR-19-21439)

Tutchton, R. M. and J. Zhu. Temperature Dependent Phonon Dispersions of Non-magnetic delta-Plutonium. Presented at *Theory Frontiers in Actinide Sciences: Chemistry and*

Materials, Santa Fe, New Mexico, United States, 2020-02-02 - 2020-02-05. (LA-UR-20-20745)

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

Sergei Tretiak
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.

Publications

Journal Articles

*Appavoo, K., W. Nie, J. -. Blancon, J. Even, A. D. Mohite and M. Y. Sfeir. Ultrafast optical snapshots of hybrid perovskites reveal the origin of multiband electronic transitions. 2017. *Physical Review B*. **96** (19): 195308. (LA-UR-17-29873 DOI: 10.1103/PhysRevB.96.195308)

*Blancon, J. -., A. V. Stier, H. Tsai, W. Nie, C. C. Stoumpos, B. Traore, L. Pedesseau, M. Kepenekian, F. Katsutani, G. T. Noe, J. Kono, S. Tretiak, S. A. Crooker, C. Katan, M. G. Kanatzidis, J. J. Crochet, J. Even and A. D. Mohite. Scaling law for excitons in 2D perovskite quantum wells. 2018. *Nature Communications*. **9** (1): 2254. (LA-UR-18-30029 DOI: 10.1038/s41467-018-04659-x)

Blancon, J. R., A. V. Stier, H. Tsai, W. Nie, C. Stoumpos, B. Traore, L. Pedesseau, M. Kepenekian, S. Tretiak, S. A. Crooker, C. Katan, M. G. Kanatzidis, J. J. Crochet, A. Mohite and J. Even. Strongly bound excitons in Ruddlesden-Popper 2D perovskites. Submitted to *arXiv*. (LA-UR-17-29656)

Canicoba, N., N. Zagni, F. Liu, K. Fernando, H. Belleza, B. Traor \xc3\xa9, R. Rogel, H. Tsai, L. L. Brizoual, W. Nie, J. J. Crochet, S. Tretiak, C. Katan, J. Even, M. Kanatzidis, B. W. Alphenaar, J. C. Blancon, M. A. Alam and A. D. Mohite. Halide Perovskite High-k Field Effect Transistors with Dynamically Reconfigurable Ambipolarity. 2019. *ACS materials letters*. **1** (6): 633-640. (LA-UR-19-28793 DOI: 10.1021/acsmaterialslett.9b00357)

Collins, L., E. Muckley, H. Tsai, D. Ghosh, A. J. Neukirch, S. Tretiak, S. Kalinin, W. Nie and I. Ivanov. Understanding Multiscale Charge Dynamics in Mixed Ionic Electronic Conductors: Linking Hysteresis with Local Functionality. Submitted to *Nature Materials*. (LA-UR-19-28377)

Fernando, K., C. N. Devesa, J. C. Blancon, H. Tsai, J. Even, P. M. Ajayan, M. G. Kanatzidis, M. A. Alam, W. Nie, B. W. Alphenaar and A. D. Mohite. Origin of intrinsic unipolar memristors action on a single-grain of halide perovskite. Submitted to *Nature Communications*. (LA-UR-19-20524)

*Kepenekian, M., B. Traore, J. Blancon, L. Pedesseau, H. Tsai, W. Nie, C. C. Stoumpos, M. G. Kanatzidis, J. Even, A. D. Mohite, S. Tretiak and C. Katan. Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. 2018. *Nano Letters*. **18** (9): 5603-5609. (LA-UR-18-20158 DOI: 10.1021/acs.nanolett.8b02078)

Kinigstein, E. D., H. Tsai, W. Nie, J. C. Blancon, K. G. Yager, K. Appavoo, J. Even, M. G. Kanatzidis, A. D. Mohite and M. Y. Sfeir. Edge States Drive Exciton Dissociation in Hot Cast Ruddlesden-Popper Lead Halide Perovskite Thin Films. Submitted to *ACS Nano*. (LA-UR-20-21239)

Leveillee, J. A., A. J. Neukirch, S. Tretiak, C. Katan, L. Zhou, J. Even, A. Schleife and A. Mohite. Influence of \xcf\x80-conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. Submitted to *Physical Review Materials*. (LA-UR-18-22811)

Leveillee, J. A., C. Katan, J. Even, A. Mohite, S. Tretiak, A. Schleife and A. J. Neukirch. First principles survey of organic spacer candidates for tuned light emission from layered hybrid perovskite materials. Submitted to *ACS Energy Letters*. (LA-UR-19-20225)

Lewis, S. G., F. Liu, W. Nie, L. Zhou, N. A. Moody, A. Mohite, S. Tretiak and A. J. Neukirch. Cesium coated halide perovskites as new photocathode material. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-20077)

*Li, X., J. Hoffman, W. Ke, M. Chen, H. Tsai, W. Nie, A. D. Mohite, M. Kepenekian, C. Katan, J. Even, M. R. Wasielewski, C. C. Stoumpos and M. G. Kanatzidis. Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, (NH3CmH2mNH3)(CH3NH3)(n-1)PbnI3n+1 (m=4-9; n=1-4). 2018. *Journal of* *the American Chemical Society*. **140** (38): 12226-12238. (LA-UR-19-20437 DOI: 10.1021/jacs.8b07712)

Liu, F., M. A. Hoffbauer, S. G. Lewis, A. J. Neukirch, V. Pavlenko, H. Tsai, W. Nie, P. M. Ajayan, M. Kanatzidis, J. J. Crochet, N. A. Moody, J. R. Blancon and A. Mohite. Highly-efficient and regenerative electron sources using halide perovskite semiconductor thin films. Submitted to *Science*. (LA-UR-19-32662)

Liu, F., M. D. Yoho, H. Tsai, K. Fernando, J. T. Tisdale, S. Shrestha, J. K. S. Baldwin, A. Mohite, S. Tretiak, D. T. Vo and W. Nie. The Working Principle of Hybrid Perovskite Single Crystal Detector for Gamma-Ray Photon Counting. Submitted to *Nature Communications*. (LA-UR-19-25920)

Liu, F., S. G. Lewis, A. J. Neukirch, V. Pavlenko, M. A. Hoffbauer, H. Tsai, W. Nie, J. Even, S. Tretiak, M. G. Kanatzidis, J. J. Crochet, N. A. Moody, J. C. Blancon and A. D. Mohite. Highly-efficient and regenerative electron sources using halide perovskite semiconductor thin films. Submitted to *Science*. (LA-UR-19-32491)

Neukirch, A. J., D. Ghosh, D. Acharya, L. Zhou, W. Nie, O. V. Prezhdo and S. Tretiak. Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-28376)

Neukirch, A. J., D. Ghosh, L. Zhou, O. Prezhdo and S. Tretiak. Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Submitted to *ACS Energy Letters*. (LA-UR-19-26479)

*Neukirch, A. J., I. I. Abate, L. Zhou, W. Nie, H. Tsai, L. Pedesseau, J. Eyen, J. J. Crochet, A. D. Mohite, C. Katan and S. Tretiak. Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. 2018. *The Journal of Physical Chemistry Letters*. **9** (24): 7130-7136. (LA-UR-18-30565 DOI: 10.1021/acs.jpclett.8b03343)

Neukirch, A. J., J. A. Leveillee, J. Even, D. Ghosh, W. Nie, A. Mohite, S. Tretiak and A. Schleife. Tuning electronic structure in layered hybrid perovskites with organic spacer substitution. Submitted to *Nano Letters*. (LA-UR-19-28375)

Park, M., A. J. Neukirch, S. E. Reyes-Lillo, M. Lai, S. Ellis, D. Dietze, J. Neaton, P. Yang, S. Tretiak and R. Mathies. Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. Submitted to *Nature Communications*. (LA-UR-18-25906)

*Park, M., A. J. Neukirch, S. E. Reyes-Lillo, M. Lai, S. R. Ellis, D. Dietze, J. B. Neaton, P. Yang, S. Tretiak and R. A. Mathies. Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. 2018. *Nature Communications*. **9** (1): 2525. (LA-UR-17-31256 DOI: 10.1038/s41467-018-04946-7)

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Boom or Bust? Predicting Explosive Safety under Impacts

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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.

Publications

Journal Articles

Addessio, F. L., M. J. Cawkwell, K. J. Ramos and D. J. Luscher. Investigation of Plate Impact Experiments on Single-Crystal RDX Above the Phase Transformation Pressure. Submitted to *Journal of Applied Physics*. (LA-UR-20-22056)

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Walters, D. J., K. J. Ramos, F. L. Addessio, C. E. Armenta, J. L. Barber, C. A. Bolme, M. J. Cawkwell, L. Dresselhaus-Cooper, A. E. Gleason Holbrook, A. C. Golder, E. L. Hartline, B. J. Jensen, H. J. Lee, D. J. Luscher, C. S. Meredith, I. Nam, T. H. Pierce, C. Pulham, P. Rigg, R. L. Sandberg, M. Seaberg, N. Sinclair and G. K. Windler. Mesoscale Mechanics of Energetic Materials: A Coordinated Experiment-theory Effort Using New In Situ Probes. Presented at *16th International Detonation Symposium*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-20). (LA-UR-18-25734)

Reports

Mohan, N., M. J. Cawkwell, F. L. Addessio, K. J. Ramos and D. J. Luscher. Characterizing Grain-Size Effects in the Shock Heating of Idealized PBXs. Unpublished report. (LA-UR-19-28308)

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Addessio, F. L., N. Mohan, D. J. Luscher, M. J. Cawkwell and K. J. Ramos. Theory and Model Development for Single-Crystals of RDX: Phase Transformations through Damage. Presented at *LANL workshop on predicting HE safety under impacts*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-21. (LA-UR-19-21305)

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Cawkwell, M. J., N. Mohan, D. J. Luscher, R. T. Perriot and K. J. Ramos. Atomic-scale Simulations of Explosives: Applications to EOS, thermal transport, surface energies, and crystal plasticity. Presented at *LANL workshop on predicting HE safety under impacts*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-21. (LA-UR-19-21233)

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Driven Quantum Matter: A Route Towards Novel Phases

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20190026DR

Project Description

The discovery of new materials has played a significant part in nearly every technological leap forward. To date, these advances have relied on conventional materials, which are now reaching their intrinsic limits. Quantum materials can enable us to overcome this, as they offer a host of unique properties that could be the basis of the next technological revolution, impacting areas including quantum computing and energy-efficient sensing. However, it has been difficult to tailor them for such applications, likely because conventional equilibrium tuning methods (e.g., temperature and pressure) make it difficult to realize a desired state of matter. Intense, transient electromagnetic (EM) fields have recently emerged as an exciting alternative for driving quantum materials into new states. However, these states have thus far been discovered by chance, making it vital to develop new approaches for predicting and controlling EM-driven phases. The objective of this project is to move beyond serendipitous discovery to demonstrate a world-leading capability for predicting and realizing novel EM-driven quantum phases, accomplished by pursuing an integrated theoretical and experimental approach focusing on three representative classes of quantum materials. This will impact a wide range of mission-relevant objectives, including novel materials for energy-efficient sensing, data storage, and computation.

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Presentation Slides

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Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials

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20190043DR

Project Description

Testing of refurbished (aka Lifetime Extension), reused, or newly designed weapon components is central to the mission of the Enhanced Capabilities for Subcritical Experiments (ECSE) project. While the ECSE accelerator will produce an excellent x-ray sources that will be used for weapons radiography, a great deal of leverage (both in terms of cost and radiographic quality) comes from what happens in the radiographic imaging system. This project proposes to produce a new scintillator material, the most important component in the imaging system, that provides options to improve the performance of ECSE. Perhaps it goes without stating, but greater radiographic system performance for ECSE will vastly increase the value of the experiments performed there. Looking further afield, a deeper understanding of the important interplay between the atomic and condensed matter physics that determines scintillator performance will help us to improve these materials for other missions relevant to the National Nuclear Security Administration as well as Department of Energy writ large.

Publications

Journal Articles

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Books/Chapters

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Presentation Slides

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Uberuaga, B. P. Brighter, Faster, Tougher: Adaptive Co-design of Resilient Radiation Detector Materials. Presented at *MSTS Nevada Working Group*, Las Vegas, Nevada, United States, 2019-07-15 - 2019-07-17. (LA-UR-19-26531)

Uberuaga, B. P. Physics-Based Machine Learning Models for High Throughput Screening of Novel Scintillator Chemistries: Materials that Glow. Presented at *Materials Science & Technology 2019*, Portland, Oregon, United States, 2019-09-29 - 2019-09-29. (LA-UR-19-29653)

Uberuaga, B. P. Fundamental studies of radiation effects in materials. . (LA-UR-19-27963)

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Posters

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Talapatra, A. A. and R. Arroyave. Experiment Design Frameworks for Materials Discovery. Presented at *Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23119)

Williams, L., E. Kioupakis and G. Pilania. Machine Learning with Local Environment Descriptors to Predict New Scintillator Materials. Presented at *Michigan Institute for Computational Discovery in Engineering*, Ann Arbor, Michigan, United States, 2019-04-10 - 2019-04-10. (LA-UR-19-23018)

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

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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/macroscale networks.

Technical Outcomes

The program has contributed significantly to the Science Strength of the Laboratory. We produced a multiscale photonics theory for understanding/identifying photon-plasmon interaction regimes for new functionality. We developed advanced quantum emitters (doped-CNTs and heterostructured-QDs), especially telecom-wavelength single-photon sources. We developed multiscale integration and assembly (scanning-probe-nanolithography and hierarchically-ordered polymer templating). We demonstrated field-induced intensity/decay rate enhancement, directionality and polarization control, and photon near-indistinguishability. We developed a multiscale structural theory for soft-hard-hybrid assemblies/composites and soft-matter non-equilibrium dynamics.

Publications

Journal Articles

Abudayyeh, H., B. Lubotzky, R. Rapaport, A. V. Blake, J. Wang, S. Majumder, J. A. Hollingsworth, R. Bose and A. V. Malko. Highly Directional Quantum Emission by Deterministic Placing of Quantum Dots in Bullseye Nanoantennas. Submitted to *ACS Photonics*. (LA-UR-19-29840)

Abudayyeh, H., B. Lubotzky, S. Majumder, J. A. Hollingsworth and R. Rapaport. Purification of single photons by temporal heralding of quantum dot sources. Submitted to *arXiv*. (LA-UR-18-28801)

*Abudayyeh, H., B. Lubotzky, S. Majumder, J. A. Hollingsworth and R. Rapaport. Purification of Single Photons by Temporal Heralding of Quantum Dot Sources. 2019. *ACS Photonics*. **6** (2): 446-452. (LA-UR-19-29784 DOI: 10.1021/acsphotonics.8b01396)

*Bagge-Hansen, M., S. Bastea, J. A. Hammons, M. H. Nielsen, L. M. Lauderbach, R. L. Hodgin, P. Pagoria, C. May, S. Aloni, A. Jones, W. L. Shaw, E. V. Bukovsky, N. Sinclair, R. L. Gustavsen, E. B. Watkins, B. J. Jensen, D. M. Dattelbaum, M. A. Firestone, R. C. Huber, B. S. Ringstrand, J. R. I. Lee, T. van Buuren, L. E. Fried and T. M. Willey. Detonation synthesis of carbon nano-onions via liquid carbon condensation. 2019. *Nature Communications*. **10** (1): 3819. (LA-UR-20-21965 DOI: 10.1038/s41467-019-11666-z)

*Dawood, F., J. Wang, P. A. Schulze, C. J. Sheehan, M. R. Buck, A. M. Dennis, S. Majumder, S. Krishnamurthy, M. Ticknor, I. Staude, I. Brener, P. M. Goodwin, N. A. Amro and J. A. Hollingsworth. The Role of Liquid Ink Transport in the Direct Placement of Quantum Dot Emitters onto Sub-Micrometer Antennas by Dip-Pen Nanolithography. 2018.

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*Dennis, A. M., M. R. Buck, F. Wang, N. F. Hartmann, S. Majumder, J. L. Casson, J. D. Watt, S. K. Doorn, H. Htoon, M. Sykora and J. A. Hollingsworth. Role of Interface Chemistry in Opening New Radiative Pathways in InP/CdSe Giant Quantum Dots with Blinking-Suppressed Two-Color Emission. 2019. *Advanced Functional Materials*. **29** (37): 1809111. (LA-UR-18-28614 DOI: 10.1002/adfm.201809111)

Doorn, S. K., S. Ozden, A. Saha, Y. Kim, K. Thurman, J. L. Blackburn and H. Htoon. Route to sp3 Functionalization of Polyfluorene Polymer-Wrapped Single-Wall Carbon Nanotubes. Submitted to *Journal of the American Chemical Society*. (LA-UR-19-26407)

*Dreier, T. A., B. S. Ringstrand, S. Seifert and M. A. Firestone. Synthesis and application of a metal ion coordinating ionic liquid monomer: Towards size and dispersity control of nanoparticles formed within a structured polyelectrolyte. 2018. *European Polymer Journal*. **107**: 275-286. (LA-UR-18-27591 DOI: 10.1016/j.eurpolymj.2018.08.017)

*Gifford, B. J., A. E. Sifain, H. Htoon, S. K. Doorn, S. Kilina and S. Tretiak. Correction Scheme for Comparison of Computed and Experimental Optical Transition Energies in Functionalized Single-Walled Carbon Nanotubes. 2018. *The Journal of Physical Chemistry Letters*. **9** (10): 2460-2468. (LA-UR-18-21776 DOI: 10.1021/acs.jpclett.8b00653)

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*Gifford, B. J., X. He, M. Kim, H. Kwon, A. Saha, A. E. Sifain, Y. Wang, H. Htoon, S. Kilina, S. K. Doorn and S. Tretiak. Optical Effects of Divalent Functionalization of Carbon Nanotubes. 2019. *Chemistry of Materials*. **31** (17): 6950-6961. (LA-UR-18-31887 DOI: 10.1021/acs.chemmater.9b01438)

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Htoon, H., Z. Hu, Y. Kim, S. Krishnamurthy, I. D. Avdeev, M. O. Nestoklon, A. Singh, A. V. Malko, S. Goupalov and J. A. Hollingsworth. Intrinsic Exciton Photophysics of PbS Quantum Dots Revealed by Low-Temperature Single Nanocrystal Spectroscopy. 2019. *Nano Letters*. (LA-UR-19-29763 DOI: 10.1021/acs.nanolett.9b02937)

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Krishnamurthy, S., Z. Hu, A. Singh, Y. Kim, A. V. Blake, E. Dolgopolova, J. R. McBride, A. Piryatinski, A. V. Malko, H. Htoon, M. Sykora and J. A. Hollingsworth. PbS/CdS Quantum Dot Room-Temperature Single-Photon Emitters Reach the Telecom O and S Bands. Submitted to *Nature Materials*. (LA-UR-19-29782)

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*Ma, X., A. R. James, N. F. Hartmann, J. K. Baldwin, J. Dominguez, M. B. Sinclair, T. S. Luk, O. Wolf, S. Liu, S. K. Doorn, H. Htoon and I. Brener. Solitary Oxygen Dopant Emission from Carbon Nanotubes Modified by Dielectric Metasurfaces. 2017. *ACS Nano*. **11** (6): 6431-6439. (LA-UR-18-21087 DOI: 10.1021/acsnano.7b02951)

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Saeboe, A. M., R. Toufanian, J. C. Kays, A. Piryatinski, A. Nikiforov, A. H. Mahler, M. Chern and A. M. Dennis. Indium Phosphide Quantum Shells for Multiplexed Near Infrared Imaging. Submitted to *Nano Letters*. (LA-UR-18-20931)

Sinitsyn, N. Computing with a single qubit faster than the computation quantum speed limit. Submitted to *Physics Letters. Section A: General, Atomic and Solid State Physics*. (LA-UR-18-30503)

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J. Welch, P. M., T. Dreier, H. D. Magurudeniya, M. Firth, J. Ilavsky, S. Seifert, A. Rahman, A. Singh, B. S. Ringstrand, C. J. Hanson, J. A. Hollingsworth and M. A. Firestone. Determination of sub-surface, 3D volumetric structural hierarchy induced by polymerizing from a quantum-dot ionic liquid monomer conjugate. Submitted to *Materials Horizons*. (LA-UR-19-29846)

*Welch, P. M., K. O. Rasmussen and C. F. Welch. Describing nonequilibrium soft matter with mean field game theory. 2019. *The Journal of Chemical Physics*. **150** (17): 174905. (LA-UR-18-30104 DOI: 10.1063/1.5081829)

Conference Papers

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)

Books/Chapters

Doorn, S. K., H. Htoon and S. Tretiak. Photophysics and Quantum Emission Behaviors of Covalently-Introduced Defects in Single-Wall Carbon Nanotubes. (LA-UR-17-31069)

Gifford, B. J. Functionalized Carbon Nanotube Excited States and Optical Properties. (LA-UR-19-23110)

Reports

Zhang, J. Final Co-op Report. Unpublished report. (LA-UR-19-31956)

Presentation Slides

Dreier, T. Control of Nanoparticles in Composite Polymer Matricies. . (LA-UR-18-26557)

Dreier, T. Control of Nanoparticles in Composite Polymer Matricies. Presented at *ACS National Meeting*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-23. (LA-UR-18-27774)

Dreier, T. Applications of Organic Chemistry in Nanoscience. . (LA-UR-19-20649)

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Dreier, T. Materials Control via Molecular Manipulation. . (LA-UR-19-26507)

Firestone, M. A. Engineered nanophase materials: Detonation-derived nanoparticles and synthetic scaffolds for nanocomposite fabrication. Presented at *Departmental seminar Mechanical Engineering*, Las Cruces, New Mexico, United States, 2019-02-15 - 2019-02-15. (LA-UR-19-21130)

Firestone, M. A., A. Joshi, J. A. Hollingsworth and K. Kwock. Preparation of heterofunctional (binary) nanoparticle polymer composites for solid-state photonics. Presented at *10th ECNP International Conference on Nanostructured Polymers and Nanocomposites*, San Sebastian, Spain, 2018-10-03 - 2018-10-03. (LA-UR-18-29085)

Firestone, M. A., J. A. Hollingsworth, A. Joshi and P. M. J. Welch. Synthetic approaches for preparation of binary, heterogeneous nanoparticle composites for solid state photonics. Presented at *ACS Spring National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22868)

Hollingsworth, J. A. Effects of Shape, Crystal Structure and Defect Engineering on Photophysical Properties of Single Inorganic Semiconductor Nanocrystals. Presented at *International Conference on Photochemistry*, Strasbourg, France, 2017-07-16 - 2017-07-21. (LA-UR-17-25529)

Hollingsworth, J. A. Non-blinking Nanomaterials: Experimental Success Invites Theoretical Inquiry. Presented at *Nanomaterials: Computation, Theory, and Experiment*, Telluride, Colorado, United States, 2017-07-11 - 2017-07-15. (LA-UR-17-25527)

Hollingsworth, J. A. Hybrid Photonic-Plasmonic Materials. . (LA-UR-18-21608)

Hollingsworth, J. A. Building single-photon sources and collective emitters using synthetically engineered quantum dots. Presented at *NanoKorea*, Seoul, Korea, South, 2019-07-02 - 2019-07-05. (LA-UR-19-26102)

Hollingsworth, J. A. Heterostructured Nanomaterials: Understanding & Controlling Light-Emission Properties From the Inside Out. . (LA-UR-19-26101)

Hollingsworth, J. A. Directly correlating synthesis parameters with nanostructure and optical properties. Presented at *American Chemical Society (VIRTUAL SYMPOSIUM)*, Philadelphia, New Mexico, United States, 2020-03-22 - 2020-03-23. (LA-UR-20-22499)

Hollingsworth, J. A., H. Htoon, M. Sykora, S. Rosenthal, J. McBride, N. J. Orfield, S. Majumder, A. Singh and N. Mishra. Controlling the Generation and Fate of Photons in Semiconductor Nanocrystals. Presented at *EMN Summer Meeting 2017*, Havana, Cuba, 2017-05-03 - 2017-05-08. (LA-UR-17-23402)

Hu, Z., A. Singh, J. A. Hollingsworth and H. Htoon. Relations between morphology and emission properties in single colloidal nanoplatelets. Presented at *253rd American Chemical Society NATIONAL MEETING*, San Francisco, California, United States, 2017-04-01 - 2017-04-07. (LA-UR-17-23184)

Hu, Z., A. Singh, J. A. Hollingsworth and H. Htoon. Probing the morphological effects on photoluminescence properties in single colloidal nanoplatelets. Presented at *2017 CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2017-09-25 - 2017-09-27. (LA-UR-17-28400)

Magurudeniya, H. D., A. Joshi, B. S. Ringstrand, D. J. Williams, J. A. Hollingsworth and M. A. Firestone. Engineered synthetic scaffolds for precision geometric placement of nanoconstituents: Formation of durable polymer binary nanoparticle composites. Presented at *FFSCI on Nanoscience*, Dubrovnik, Croatia, 2017-05-04 - 2017-05-04. (LA-UR-17-23584)

Singh, A., S. Krishnamurthy, Z. Hu, A. Joshi, Y. Kim, M. Sykora, A. Malko, H. Htoon and J. A. Hollingsworth. Ultra-photostable lead chalcogenide giant quantum dots (gQDs) for telecom wavelength. Presented at *MRS Spring Meeting*, Phoenix, New Mexico, United States, 2018-04-02 - 2018-04-06. (LA-UR-18-22888)

Wang, J., F. Dawood, P. A. Schulze, C. J. Sheehan, S. Majumder, S. Krishnamurthy, I. Staude, I. Brener, N. Amro, P. M. Goodwin and J. A. Hollingsworth. Integration of quantum emitters and 3D nanoantennas by dip-pen nanolithography. Presented at *2018 CINT User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-24. (LA-UR-18-28841)

Wang, J., F. Dawood, P. Schulze, C. J. Sheehan, I. Staude, I. Brener, N. Amro and J. A. Hollingsworth. Integration of colloidal giant quantum dots and 3D nanoantennas by dip-pen nanolithography. Presented at *256th ACS National Meeting*, Boston, Massachusetts, United States, 2018-08-19 - 2018-08-19. (LA-UR-18-26451)

J. Welch, P. M. Playing Games on Mean Fields - Structure Theory-. Presented at *LDRD-DR Program Review: Hybrid Photonic-Plasmonic Materials*, Los Alamos, New Mexico, United States, 2018-03-01 - 2018-03-01. (LA-UR-18-21583)

Posters

Blake, A. V., J. Wang, R. Bose, Y. Kim, H. A. Abudayyeh, R. Rapaport, A. V. Malko, H. Htoon and J. A. Hollingsworth. Nanoscale Integration Attains New Heights with Dip-Pen Nanolithography. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29474)

Dreier, T., B. Ringstrand and M. A. Firestone. Control of Nanoparticles in Composite Polymer Matricies. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28912)

Dreier, T., B. S. Ringstrand and M. A. Firestone. Precise Placement of Nanoparticles in Polymer Composites via Pre-Coordination. . (LA-UR-18-21601)

Dreier, T., B. S. Ringstrand and M. A. Firestone. Precise Placement of Nanoparticles in Polymer Composites via Pre-Coordination. Presented at *Inorganic Chemistry Gordon Research Conference*, Biddeford, Maine, United States, 2018-06-17 - 2018-06-22. (LA-UR-18-25258)

Dreier, T., S. I. F. Diouf, D. J. Williams, T. Elkin and M. A. Firestone. Nanostructured Feed-stocks for Fused Deposition Modeling. . (LA-UR-19-24293)

Gary, D. C., S. Krishnamurthy, Z. Hu, A. Singh, Y. Kim, A. V. Blake, A. V. Malko, H. Htoon and J. A. Hollingsworth. Quantum Dots Reach the Telecom O and S Bands as Room-Temperature Single-Photon Emitters. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-24. (LA-UR-19-29438)

Hanson, C. J., N. F. Hartmann, X. Ma, A. Singh, S. Krishnamurthy, Z. Hu, R. Iyer, S. M. Jeffery, J. K. Grey, A. Piryatinski, A. V. Malko, H. Htoon and J. A. Hollingsworth. Fully Automated Batch Reactor System (FABRS) for Giant Quantum Dot Materials Development, Optimization, and Scale-up. . (LA-UR-18-21591)

Joshi, A., H. D. Magurudeniya, C. J. Hanson, J. A. Hollingsworth and M. A. Firestone. Directed Organization of Giant Quantum Dots (gQDs) during Polymerization of Ionic Liquid (IL) Crystalline Mesophases. Presented at *LDRD-DR meeting*, Los Alamos, New Mexico, United States, 2018-03-01 - 2018-03-02. (LA-UR-18-21559)

Kim, Y., X. He, A. Saha, I. Sarpkaya, S. K. Doorn and H. Htoon. Temperature Dependent Single Dopant Spectroscopy in CNT. Presented at *CINT User Meeting*, Santa Fe, New Mexico, United States, 2017-09-25 - 2017-09-27. (LA-UR-17-28396)

Kim, Y., X. He, A. Saha, M. Kim, Y. Wang, S. K. Doorn and H. Htoon. Excitonic fine structure of solitary defects in CNT revealed by magneto-PL spectroscopy. Presented at *DR (Hybrid Photonic-Plasmonic Materials) review and the Workshop*, Los Alamos, New Mexico, United States, 2018-03-01 - 2018-03-02. (LA-UR-18-21558)

I. Madrid, R. J. Evaluating Thermal Response of "Giant" Quantum Dots. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2017-08-02 - 2017-08-02. (LA-UR-17-26684)

Majumder, S., A. Singh, N. J. Orfield, J. A. Hollingsworth and H. Htoon. Deconstructing the Giant Quantum Dot Architecture: Fabricating Superior Quantum Emitters by Design. Presented at *Hybrid Photonic-Plasmonic Materials Workshop (LDRD, DR review)*, Los Alamos, New Mexico, United States, 2018-03-01 - 2018-03-02. (LA-UR-18-21593)

Piryatinski, A., O. Roslyak, H. Li and E. Bittner. Cooperative Dynamics of Quantum Emitters in Plasmonic Cavity. Presented at *LANL Materials for the Future Capability Review (MCR)*, Los Alamos, New Mexico, United States, 2018-04-08 - 2018-04-11. (LA-UR-18-21983)

Sheely, A. B. Studying the Effect of Edge Functionalization in Graphene Quantum Dots. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-32081)

Singh, A., S. Majumder, N. J. Orfield, K. Bustillo, J. Ciston, H. Htoon and J. A. Hollingsworth. Interface and Defect Engineering of Heterostructured Semiconductor Quantum Dots. Presented at *MRS Spring 2018*, Phoenix, Arizona, United States, 2018-04-02 - 2018-04-06. (LA-UR-18-22800)

Singh, A., Z. Hu, A. Joshi, Y. Kim, H. Htoon and J. A. Hollingsworth. Fabrication and Design Concepts toward Hybrid Plasmonics -Transformed Single Quantum Emitters for Telecom Wavelengths. Presented at *LDRD DR Review*, Los Alamos, New Mexico, United States, 2018-03-01 - 2018-03-02. (LA-UR-18-21615)

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Weight, B. M., B. J. Gifford and S. Tretiak. Interacting Pairs of Surface Defects on Carbon Nanotubes. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27817)

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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.

Technical Outcomes

This project was an experimental, theoretical, and computational modeling effort aimed at building a mechanistic understanding of how grain boundary (GB) structure affects dynamic damage evolution in a model BCC metal, namely tantalum(Ta). Dynamic damage evolution was quantified using plate-impact driven spallation testing. A single crystal plasticity model for BCC materials and a macroscale damage model with micro-inertial effects were developed to represent the material behavior and boundary conditions more accurately in meso-scale simulations.

Publications

Journal Articles

Bronkhorst, C. A., H. Cho, P. W. Marcy, S. A. Vander Wiel, V. Livescu and G. T. I. Gray. Local Damage Stress Conditions in Tantalum subjected to Light Shock Loading via Soft Scale-Coupling. Submitted to *International Journal of Plasticity*. (LA-UR-18-31564)

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Conference Papers

Fensin, S. J., G. T. I. Gray, N. Bourne and R. S. Hixson. Microstructure Based Failure Criterion For Ductile Materials. Presented at *Dymat*. (Arcachon, France, 2018-09-09 - 2018-09-14). (LA-UR-18-21825)

I. Gray, G. T., C. M. Knapp, D. R. Jones, V. Livescu, S. J. Fensin, B. M. Morrow, C. P. Trujillo, D. T. Martinez and J. A. Valdez. Structure / Property Characterization of Spallation in Wrought and Additively Manufactured Tantalum. Presented at *2017 Shock Compression of Condensed Matter Conference Proceedings*. (St. Louis, Missouri, United States, 2017-07-10 - 2017-07-10). (LA-UR-17-28190)

I. Gray, G. T., V. Livescu, C. M. Knapp, D. R. Jones, S. J. Fensin, S. Chen, C. M. Cady, C. P. Trujillo and D. T. Martinez. Structure / Property (Constitutive and Dynamic Strength / Damage) Behavior of Additively Manufactured Tantalum. Presented at *DYMAT 2018 Conference*. (Arcachon, France, 2018-09-09 - 2018-09-14). (LA-UR-18-21100)

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Books/Chapters

Bronkhorst, C. A., H. Cho, P. W. Marcy, S. A. Vander Wiel, V. Livescu and G. T. I. Gray. Local Stress and Damage Response of Polycrystal Materials to Light Shock Loading Conditions via Soft Scale-Coupling. (LA-UR-18-30872)

Reports

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Presentation Slides

Black, A. N. AWS D20.1: A First Attempt at AM Qualification in Industry. Presented at *IMOG Meeting on Additive Manufacturing*, Augusta, Georgia, United States, 2019-05-21 - 2019-05-22. (LA-UR-19-24519)

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Bronkhorst, C. A., G. T. I. Gray, V. Livescu, H. M. Mourad, D. Versino, H. Cho and D. R. Jones. Physical and Computational Aspects of Engineering Damage Mechanics. Presented at *TMS Annual Meeting*, Phoenix, Arizona, United States, 2018-03-12 - 2018-03-16. (LA-UR-18-21882)

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Bronkhorst, C. A., H. Cho, S. J. Fensin, G. T. I. Gray, D. R. Jones, V. Livescu, P. W. Marcy, E. N. Hahn, H. M. Mourad, B. S. Runnels, S. A. Vander Wiel and S. S. Zentgraf. Inter-

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Chen, J., E. N. Hahn, D. R. Jones and S. J. Fensin. Towards Predicting A Microstructure's Susceptibility To Spall: NEMD Simulations Of\xc2\xa0Additively\xc2\xa0Manufactured \xc2\xa0Tantalum. Presented at *Plasticity*, Panama City, Panama, 2019-01-02 - 2019-01-09. (LA-UR-18-31791)

Cho, H., C. A. Bronkhorst and H. M. Mourad. Deformations of tantalum: crystal plasticity models. . (LA-UR-18-22678)

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I. Gray, G. T., C. A. Bronkhorst, H. M. Mourad, H. Cho, V. Livescu, S. J. Fensin, D. R. Jones, E. N. Hahn, C. M. Knapp, S. A. Vander Wiel, P. W. Marcy and N. Li. Structure / Property (Constitutive and Dynamic Strength / Damage) Characterization of Wrought and Additively Manufactured Tantalum. Presented at *2018 NNSA/CEA-DAM Postdoctoral Exchange Workshop -- Paris-France*, Paris, France, 2018-05-15 - 2018-05-18. (LA-UR-18-24031)

I. Gray, G. T., C. M. Knapp, D. R. Jones, V. Livescu, R. A. Beal, S. J. Fensin, B. M. Morrow, C. P. Trujillo, D. T. Martinez and J. A. Valdez. Structure / Property (Constitutive and Dynamic Strength / Damage) Characterization of Wrought and Additively Manufactured Tantalum. Presented at *Condensed Matter Shock Conference - GSCCM 2017*, St. Louis, Missouri, United States, 2017-07-09 - 2017-07-14. (LA-UR-17-25292)

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I. Gray, G. T., S. J. Fensin, C. M. Knapp, D. R. Jones, V. Livescu, B. M. Morrow, B. G. Ndefru and J. A. Valdez. Structure / Property Behavior of Additively Manufactured (AM) Materials: Opportunities and Challenges. Presented at *Society for Engineering Mechanics Conference - invited Keynote talk*, Greenville, South Carolina, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-24812)

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I. Gray, G. T., V. Livescu, C. Knapp, D. R. Jones, S. J. Fensin, S. Chen, E. N. Hahn, C. M. Cady, C. P. Trujillo and D. T. Martinez. Role of Grain Boundaries on Damage Evolution in Wrought and Additively Manufactured (AM) Tantalum. Presented at *MS&T-18 Fall Materials Meeting*, Columbus, Ohio, United States, 2018-10-15 - 2018-10-18. (LA-UR-18-29638)

I. Gray, G. T., V. Livescu, R. A. Beal, J. A. Valdez, J. S. Carpenter, C. M. Knapp, B. Morrow and D. R. Jones. Dynamic Response of Additively Manufactured Bulk Metals and Alloys: 316L SS, 304L SS, Ti-6Al-4V, Ta. Presented at *Joint DoD/NNSA Additive Manufacturing Workshop -- at LLNL*, Livermore, California, United States, 2017-02-07 - 2017-02-09. (LA-UR-17-20646)

I. Gray, G. T., V. Livescu, T. J. Nizolek, J. A. Valdez, C. Liu and R. A. Beal. Compact-Forced-Simple-Shear(CFSS) Sample for Studying the Shear Response and Microstructure Evolution in Additively Manufactured Ta, Wrought Ta, and High-Hard Armor Steel. Presented at *Nordmetall Colloquium*, Chemnitz, Germany, 2019-12-01 - 2019-12-06. (LA-UR-19-31777)

Hahn, E. N., S. J. Fensin, T. C. Germann, M. A. Meyers, R. J. Ravelo and J. E. Hammerberg. Dynamic Tensile Failure of Nanocrystalline Tantalum. Presented at *TMS 2017*, San Diego, California, United States, 2017-02-26 - 2017-02-26. (LA-UR-17-21315)

Hahn, E. N., S. J. Fensin and T. C. Germann. The influence of grain boundary orientation on the strength and failure of tantalum bicrystals. Presented at *20th Biennial APS Shock Compression of Condensed Matter Conference*, St. Louis, Missouri, United States, 2017-07-09 - 2017-07-09. (LA-UR-17-25613)

Hahn, E. N., S. J. Fensin and T. C. Germann. Towards Predicting a Microstructure's Susceptibility to Spall: Non-Equilibrium Molecular Dynamics Simulations of Tantalum. Presented at *International Conference on Plasticity, Damage, and*

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Hahn, E. N. and T. C. Germann. Large-Scale Molecular Dynamics Studies of Materials Dynamics. . (LA-UR-18-29707)

Jones, D. R., R. M. Martinez and V. Livescu. Analysis of Low Oxygen AM Tantalum. . (LA-UR-19-24536)

Jones, D. R., S. J. Fensin and G. T. I. Gray. Shock Response and Damage in Tantalum: Wrought vs. Additive Manufactured. Presented at *TMS 2018*, Phoenix, Arizona, United States, 2018-03-11 - 2018-03-11. (LA-UR-18-22025)

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Li, N., J. Weaver, D. R. Jones, S. J. Fensin, N. Mara, C. A. Bronkhorst and G. T. I. Gray. Quantifying the role of grain boundaries in Ta. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-29101)

Livescu, V. Processing-Driven Microstructures in Additively Manufactured Tantalum. Presented at *International Conference on Plasticity, Damage, and Fracture*, San Juan, Puerto Rico, United States, 2018-01-03 - 2018-01-09. (LA-UR-17-31394)

Livescu, V., C. Liu, R. M. Martinez, B. G. Ndefru, S. S. Zentgraf and G. T. I. Gray. Deformation and Damage in Polycrystalline Tantalum. Presented at *TMS 2019 Annual Meeting and Exhibition*, San Antonio, Texas, United States, 2019-03-10 - 2019-03-15. (LA-UR-19-22044)

Livescu, V., D. R. Jones, C. A. Bronkhorst and G. T. I. Gray. EBSD Characterization for the Development of Ductile Damage Models. Presented at *Electron Backscatter Diffraction Topical Conference 2018*, Ann Arbor, Michigan, United States, 2018-05-23 - 2018-05-25. (LA-UR-18-24237)

Marcy, P. W. Bayesian Gaussian Process Models on Spaces of Sufficient Dimension Reduction. Presented at *Statistical Perspectives of Uncertainty Quantification*, Atlanta, Georgia, United States, 2017-05-29 - 2017-05-30. (LA-UR-17-24278)

Marcy, P. W., S. A. Vander Wiel, C. A. Bronkhorst and V. Livescu. Statistical Analysis of Stress Patterns Within Simulated Tantalum. Presented at *International Conference on Plasticity, Damage, and Fracture 2018*, San Juan, Puerto Rico, United States, 2018-01-03 - 2018-01-03. (LA-UR-18-20010)

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Trujillo, C. P., G. T. I. Gray, E. K. Cerreta, V. Livescu, D. T. Martinez, M. W. Burkett and S. Chen. Influence of Temperature Effects on the Dynamic Tensile Extrusion of Molybdenum \xc2\xa0. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25710)

Weaver, J., D. R. Jones, N. Li, S. J. Fensin, G. T. I. Gray and N. Mara. Quantifying the role of grain boundaries in Ta: micropillars and nanoindentation. Presented at *TMS 2018*, Phoenix, Arizona, United States, 2018-03-11 - 2018-03-15. (LA-UR-18-22353)

Vander Wiel, S. A., P. W. Marcy, C. A. Bronkhorst, V. Livescu and C. B. Storlie. Fitting Stress Fields in Polycrystalline Materials -- Statistical Art and Science. Presented at *2018 Joint Research Conference on Statistics in Quality, Industry, and Technology*, Santa Fe, New Mexico, United States, 2018-06-12 - 2018-06-14. (LA-UR-18-25121)

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Zentgraf, S. S. Developing a Mesoscale Toolset to Isolate Grain Boundary Effects in Material Failure. . (LA-UR-17-27262)

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Jones, D. R., S. J. Fensin, D. T. Martinez, C. P. Trujillo and G. T. I. Gray. Stress and Strain-Rate Effects on Incipient Spall in Tantalum. Presented at *DYMAT 2018*, Arcachon, France, 2018-09-10 - 2018-09-10. (LA-UR-18-27755)

Martinez, R. M., V. Livescu, G. T. I. Gray and L. M. Hull. Study of Damage Evolution in Tantalum using EBSD. Presented at *EBSD 2018 Topical Conference*, Ann Arbor, Michigan, United States, 2018-05-23 - 2018-05-25. (LA-UR-18-23950)

Miramontes-Carrera, E., C. P. Gonzales, D. R. Jones, D. T. Martinez and C. P. Trujillo. Shock Experiments on Additively Manufactured and Wrought Tantalum. . (LA-UR-18-26950)

Vander Wiel, S. A., C. A. Bronkhorst, R. C. Foster, V. Livescu and P. W. Marcy. Three Statistical Challenges in Materials Mechanics: Microstructure to Performance. Presented at *Joint Statistical Meetings*, Baltimore, Maryland, United States, 2017-07-29 - 2017-08-03. (LA-UR-17-26440)

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 though 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.

Technical Outcomes

We have significantly enhanced our experimental capabilities to measure and our theoretical capabilities to predict shock induced chemistry in high explosives. The experiments have begun to validate the theoretical predictions of early time chemistry with a one to one correspondence for the first time.

Publications

Journal Articles

*Bowlan, P., M. Powell, R. Perriot, E. Martinez, E. M. Kober, M. J. Cawkwell and S. McGrane. Probing ultrafast shock-induced chemistry in liquids using broad-band mid-infrared absorption spectroscopy. 2019. *The Journal of Chemical Physics*. **150** (20): 204503. (LA-UR-19-20976 DOI: 10.1063/1.5092242)

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)

*Cawkwell, M. J. and R. Perriot. Transferable density functional tight binding for carbon, hydrogen, nitrogen, and oxygen: Application to shock compression. 2019. *The Journal of Chemical Physics*. **150** (2): 24107. (LA-UR-18-29043 DOI: 10.1063/1.5063385)

*Krishnapriyan, A., P. Yang, A. M. N. Nildasson and M. J. Cawkwell. Numerical Optimization of Density Functional Tight Binding Models: Application to Molecules Containing Carbon, Hydrogen, Nitrogen, and Oxygen. 2017. *Journal of Chemical Theory and Computation*. **13** (12): 6191-6200. (LA-UR-17-25536 DOI: 10.1021/acs.jctc.7b00762)

*Martinez, E., R. Perriot, E. M. Kober, P. Bowlan, M. Powell, S. McGrane and M. J. Cawkwell. Parallel replica dynamics simulations of reactions in shock compressed liquid benzene. 2019. *The Journal of Chemical Physics*. **150** (24): 244108. (LA-UR-19-20743 DOI: 10.1063/1.5092209)

Mcgrane, S. D., M. J. Cawkwell, R. T. Perriot, E. Martinez Saez, E. M. Kober, P. Yang, J. Su, A. M. Niklasson, S. M. Mniszewski, P. R. Bowlan, M. S. Powell, K. E. Brown, C. A. Bolme, D. S. Moore, K. J. Ramos and A. E. Gleason Holbrook. Shocked Chemical Dynamics in High Explosives Project. Submitted to *Weapons Engineering Science Journal*. (LA-UR-19-29921)

Mniszewski, S. M., R. T. Perriot, E. H. Rubensson, C. F. A. Negre, M. J. Cawkwell and A. M. Niklasson. Linear scaling pseudo Fermi-operator expansion for fractional occupation. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-18-28187)

*Moore, D. S. Shock physics at the nanoscale [Invited]. 2018. *Journal of the Optical Society of America B*. **35** (10). (LA-UR-18-24007 DOI: 10.1364/JOSAB.35.0000B1)

Perriot, R. T., M. J. Cawkwell, E. Martinez Saez, E. M. Kober and S. D. Mcgrane. Reaction rates in nitromethane under high pressure from density functional tight binding molecular dynamics simulations. Submitted to *Journal of Physical Chemistry A*. (LA-UR-19-32543)

*Powell, M. S., P. R. Bowlan, S. F. Son, C. A. Bolme, K. E. Brown, D. S. Moore and S. D. McGrane. A benchtop shock physics laboratory: Ultrafast laser driven shock spectroscopy and interferometry methods. 2019. *Review of Scientific Instruments*. **90** (6): 063001. (LA-UR-18-31447 DOI: 10.1063/1.5092244)

*Zuanetti, B., S. D. McGrane, C. A. Bolme and V. Prakash. Measurement of elastic precursor decay in pre-heated aluminum films under ultra-fast laser generated shocks.

2018. *Journal of Applied Physics*. **123** (19): 195104. (LA-UR-18-21409 DOI: 10.1063/1.5027390)

Conference Papers

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)

Mcgrane, S. D., P. R. Bowlan, M. S. Powell, K. E. Brown, C. A. Bolme and M. J. Cawkwell. Broadband mid-infrared measurements for shock induced chemistry. Presented at *Shock Compression of Condensed Matter*. (St. Louis, Missouri, United States, 2017-07-09 - 2017-07-09). (LA-UR-17-28315)

Moore, D. S., C. A. Bolme, K. E. Brown, M. T. Greenfield and S. D. Mcgrane. A comparison of infrared, Raman, and coherent Raman spectroscopies in studies of shock-induced chemistry. Presented at *Proceedings of the APS Topical Conference on Shock Compression Condensed Matter 2019*. (Portland, Oregon, United States, 2019-06-17 - 2019-06-17). (LA-UR-19-25921)

Perriot, R. T., C. F. A. Negre, S. D. Mcgrane and M. J. Cawkwell. Density functional tight binding calculations for the simulation of shocked nitromethane with LATTE-LAMMPS. Presented at *APS SCCM 2017*. (St Louis, Missouri, United States, 2017-07-09 - 2017-07-09). (LA-UR-17-27832)

Perriot, R. T., M. J. Cawkwell, E. M. Kober and S. D. Mcgrane. Density Functional Tight Binding Calculations for the Simulation of High Explosive Detonation. Presented at *16th International Detonation Symposium*. (Cambridge, Maryland, United States, 2018-07-15 - 2018-07-15). (LA-UR-18-25689)

Powell, M. S., P. R. Bowlan, S. F. Son and S. D. Mcgrane. Ultrafast Mid-Infrared Spectroscopy on Shocked Thin Film Explosive Crystals. Presented at *16th International Detonation Symposium*. (Chesapeake, Maryland, United States, 2018-07-15 - 2018-07-20). (LA-UR-18-25792)

Books/Chapters

Cawkwell, M. J., E. M. Kober and E. Martinez Saez. Accelerated Molecular Dynamics Simulations of Shock-induced Chemistry: Application to Liquid Benzene. (LA-UR-17-27034)

Reports

Moore, D. S. Why do some explosives detonate?. Unpublished report. (LA-UR-18-31112)

Powell, M. S. ULTRAFAST BROADBAND MIDINFRARED ABSORPTION SPECTROSCOPY ON SHOCKED ENERGETIC MATERIALS. Unpublished report. (LA-UR-19-21226)

Presentation Slides

El Atwani, O., E. Martinez Saez, E. V. Esquivel, E. Aydogan, Y. Wang, B. P. Uberuaga, S. A. Maloy, M. Efe and C. Taylor. Does sink efficiency unequivocally characterize how grain boundaries impact radiation damage?. Presented at *TMS 2018*, Phoenix, Arizona, United States, 2018-03-11 - 2018-03-11. (LA-UR-18-21864)

Bolme, C. A., K. E. Brown, M. J. Cawkwell, A. E. Gleason Holbrook, A. C. Golder, E. M. Kober, S. D. Mcgrane, A. M. Niklasson, K. J. Ramos and P. Yang. X-ray absorption spectroscopy of chemical dynamics in shocked energetic materials. Presented at *LANL Workshop on Shocked Chemical Dynamics in High Explosives*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20848)

Bowlan, P. R., S. A. Trugman, X. Wang, N. J. Hur, S. Cheong, A. J. Taylor, D. A. Yarotski and R. P. Prasankumar. Probing ultrafast spin dynamics in antiferromagnetsusing THz pulses. Presented at *SPIE: Optics and Photonics*, San Diego, California, United States, 2017-08-09 - 2017-08-09. (LA-UR-17-27638)

Brown, K. E. Laser-driven Flyer Plate Implementation. Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20648)

Brown, K. E. Picosecond to Nanosecond Spectroscopy of Shocked Reactive Materials. Presented at *Energetic Materials Gordon Research Conference*, Newry, Maine, United States, 2018-06-03 - 2018-06-03. (LA-UR-18-24713)

Brown, K. E. Picosecond to Nanosecond Spectroscopy of Shocked Reactive Materials. Presented at *Seminars at Cornell and Coe Colleges*, Mount Vernon, Iowa, United States, 2019-02-21 - 2019-02-21. (LA-UR-19-21400)

Brown, K. E. Probing the Chemistry of Shocked Energetic Materials at Picosecond to Nanosecond Timescales. Presented at *Invited seminar at University of Missouri*, Columbia, Missouri, United States, 2019-09-27 - 2019-09-27. (LA-UR-19-29634)

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, 2018-07-16 - 2018-07-16. (LA-UR-18-26399)

Brown, K. E., M. S. Powell and S. D. Mcgrane. Pairing Ultrafast Spectroscopy to Nanosecond Shock Generation. Presented at *21st Biennial APS Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25319)

Brown, K. E., M. S. Powell and S. D. Mcgrane. Pairing Ultrafast Spectroscopy to Nanosecond Shock Generation. Presented at *University Workshop on Damage, Shock, and*

Characterization, Los Alamos, New Mexico, United States, 2019-07-30 - 2019-07-30. (LA-UR-19-27168)

Cawkwell, M. J. Shocked Chemical Dynamics in High Explosives: Theory aims and overview. Presented at *LANL workshop on Shocked Chemical Dynamics in High Explosives*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20745)

Cawkwell, M. J. Linear Scaling Tight Binding Molecular Dynamics for Organic Materials. Presented at *Symposium to Celebrate the Life and Work of David Pettifor, CBE, FRS*, Oxford, United Kingdom, 2018-07-10 - 2018-07-11. (LA-UR-18-26127)

Cawkwell, M. J. Large-scale Accelerated Quantum Molecular Dynamics (w17_latteqmd). . (LA-UR-19-21928)

Cawkwell, M. J. Understanding the transferability of non-orthogonal tight binding models for molecules and metals. Presented at *Fall Materials Research Society (MRS) Meeting*, Boston, Massachusetts, United States, 2019-12-02 - 2019-12-02. (LA-UR-19-31891)

Cawkwell, M. J., A. Krishnapriyan, E. Martinez Saez, R. T. Perriot, S. M. Mniszewski, A. M. Niklasson and E. M. Kober. Large Scale Accelerated Quantum Molecular Dynamics (W17_latteqmd). . (LA-UR-18-21124)

Cawkwell, M. J., N. F. Aguirre Castiblanco, E. R. Batista, R. K. Carlson, A. Krishnapriyan, V. W. Manner, A. M. Niklasson, R. T. Perriot and P. Yang. Optimized DFTB models for molecular dynamics simulations of energetic materials. Presented at *IMS Computational Data Science Approaches for Materials 2019*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23153)

Kober, E. M. Reduced Order Models for Reactions of Energetic Materials. Presented at *CNLS Seminar*, Los Alamos, New Mexico, United States, 2017-11-06 - 2017-11-06. (LA-UR-17-30149)

Kober, E. M. Reduced Order Models for Reactions of Energetic Materials. Presented at *Mesoscale Modeling of Explosives Initiation*, Santa Fe, New Mexico, United States, 2017-09-26 - 2017-09-26. (LA-UR-17-28724)

Kober, E. M. Reduced Order Models for Reactions of Energetic Materials. Presented at *LDRD DR Mid-term review*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20801)

Kober, E. M. Formulating Reduced Order Chemistry Models from Reactive Molecular Dynamics. Presented at *Gordon Research Conference on Energetic Materials*, Newry, Maine, United States, 2018-06-03 - 2018-06-03. (LA-UR-18-24768)

Mcgrane, S. D. Shocked chemical dynamics in high explosives (HE). Presented at *LDRD Review*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20676)

Mcgrane, S. D. Shock induced chemistry in explosives. . (LA-UR-19-31186)

Mcgrane, S. D., D. S. Moore, P. R. Bowlan and M. S. Powell. Ultrafast spectroscopy of shocked explosives. Presented at *ONR MURI review*, Arlington, Virginia, United States, 2017-06-12 - 2017-06-12. (LA-UR-17-24498)

Mcgrane, S. D., D. S. Moore, P. R. Bowlan and M. S. Powell. Ultrafast spectroscopy of shocked explosives. . (LA-UR-17-31235)

Mcgrane, S. D., D. S. Moore, P. R. Bowlan and M. S. Powell. Ultrafast spectroscopy of shocked explosives. Presented at *ONR MURI project review*, online WebEx, District Of Columbia, United States, 2018-07-09 - 2018-07-09. (LA-UR-18-26011)

Mcgrane, S. D., D. S. Moore, P. R. Bowlan and M. S. Powell. Ultrafast spectroscopy of shocked explosives. Presented at *Office of Naval Research Multi University Research Project Review*, Arlington, Virginia, United States, 2019-01-14 - 2019-01-14. (LA-UR-19-20177)

Mcgrane, S. D., P. R. Bowlan, K. E. Brown, C. A. Bolme and M. J. Cawkwell. Broadband mid-infrared measurements for shock induced chemistry. Presented at *Shock Compression of Condensed Matter*, St. Louis, Missouri, United States, 2017-07-10 - 2017-07-10. (LA-UR-17-25368)

Mcgrane, S. D. and D. S. Moore. Ultrafast spectroscopy of shocked explosives- update 170220. . (LA-UR-17-21382)

Moore, D. S. Elucidation of shock-initiation chemistry through spectroscopy. Presented at *Energetic Materials Gordon Research Conference*, Newry, Maine, United States, 2018-06-03 - 2018-06-03. (LA-UR-18-23994)

Moore, D. S. Dynamic compression induced chemistry. Presented at *Dynamic Compression Summer School*, Chicago, Illinois, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-26654)

Moore, D. S. Shock physics at the nanoscale. Presented at *High Power Laser Ablation 2018*, Santa Fe, New Mexico, United States, 2018-03-26 - 2018-03-26. (LA-UR-18-22032)

Moore, D. S., C. A. Bolme, K. E. Brown, M. T. Greenfield and S. D. Mcgrane. A comparison of infrared, Raman and coherent Raman spectroscopies in studies of shock-induced chemistry. Presented at *APS Topical Conference on Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25000)

Niklasson, A. M. Shadow Hamiltonian dynamics for non-linear self-consistent field models, a coordinated design approach to scientific computing. . (LA-UR-18-30995)

Niklasson, A. M. Density Matrix Perturbation Theory. . (LA-UR-19-20666)

Perriot, R. T. Investigation of shock-induced chemistry in reactive materials using LATTE-LAMMPS\xc2\xa0. Presented at *Shocked Chemical Dynamics in High Explosives Workshop*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20831)

Perriot, R. T. MOLECULAR DYNAMICS SIMULATIONS OF SHOCK INDUCED CHEMISTRY IN ORGANIC MATERIALS. Presented at *APS March Meeting*, Los Angeles, California, United States, 2018-03-04 - 2018-03-04. (LA-UR-18-21759)

Perriot, R. T. What we can learn from quantum molecular dynamics simulations of detonation chemistry: extracting reaction rates, and the search for intermediates. . (LA-UR-19-24410)

Perriot, R. T., C. F. A. Negre, E. M. Kober, S. D. Mcgrane and M. J. Cawkwell. Density Functional Tight Binding Simulations of Reaction Chemistry in Nitromethane with LATTE-LAMMPS. Presented at *MRS Fall meeting*, Boston, Massachusetts, United States, 2017-11-26 - 2017-11-26. (LA-UR-17-30629)

Perriot, R. T., E. M. Kober, E. Martinez Saez, P. R. Bowlan, M. S. Powell, S. D. Mcgrane and M. J. Cawkwell. Molecular Dynamics Simulations of the Detonation Chemistry of Energetic Materials. Presented at *Europyro*, Tours, France, 2019-06-03 - 2019-06-03. (LA-UR-19-24411)

Perriot, R. T., E. M. Kober, S. M. Mniszewski, E. Martinez Saez, A. M. Niklasson, P. Yang, S. D. Mcgrane and M. J. Cawkwell. Reaction Analysis of Shocked Nitromethane using Extended Lagrangian Born-Oppenheimer Molecular Dynamics. Presented at *APS SCCM*, St Louis, Missouri, United States, 2017-07-09 - 2017-07-09. (LA-UR-17-25306)

Perriot, R. T., M. J. Cawkwell, E. M. Kober and S. D. Mcgrane. TEMPERATURE- AND PRESSURE-DEPENDENT REACTION RATES IN NITROMETHANE AND PETN FROM DENSITY FUNCTIONAL TIGHT BINDING MOLECULAR DYNAMICS SIMULATIONS. Presented at *16th International Detonation Symposium*, Cambridge, Maryland, United States, 2018-07-15 - 2018-07-15. (LA-UR-18-25688)

Perriot, R. T., M. J. Cawkwell, E. Martinez Saez and S. D. Mcgrane. Reaction Rates in Shocked Nitromethane from Density Functional Tight Binding Simulations. Presented at *APS MArch Meeting*, Denver, Colorado, United States, 2020-03-01 - 2020-03-01. (LA-UR-20-21937)

Powell, M. S. Ultrafast Broadband Mid-Infrared Absorption Spectroscopy on Shock Energetic Materials. . (LA-UR-19-21300)

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Powell, M. S., P. R. Bowlan, S. F. Son, C. A. Bolme, K. E. Brown, D. S. Moore, M. J. Cawkwell, A. Strachan and S. D. Mcgrane. Ultrafast Shock Induced Mid-Infrared Vibrational Changes in Thin Film Explosives. Presented at *APS Topical Group on Shock Compression of Condensed Matter (GSCCM)*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25243)

Powell, M. S. and S. D. Mcgrane. Update for TriService Review for MURI topic PCP@Xtreme. . (LA-UR-19-28165)

Martinez Saez, E., B. P. Uberuaga, O. El Atwani and B. D. Wirth. Atomistic modeling of helium segregation to grain boundaries in tungsten and its effect on de-cohesion. Presented at *MMM-2018*, Osaka, Japan, 2018-10-29 - 2018-11-02. (LA-UR-18-30313)

Martinez Saez, E., C. F. A. Negre, E. M. Kober, M. J. Cawkwell, D. Perez, A. F. Voter and A. M. Niklasson. Accelerated Quantum Molecular Dynamics. Presented at *Euromat 2017*, Thessaloniki, Greece, 2017-09-17 - 2017-09-17. (LA-UR-17-28294)

Martinez Saez, E., C. F. A. Negre, M. J. Cawkwell, D. Perez, A. F. Voter and A. M. Niklasson. Accelerated Quantum Molecular Dynamics. Presented at *TMS2018*, Phoenix, Arizona, United States, 2018-03-11 - 2018-03-11. (LA-UR-18-21782)

Posters

Armenta, C. E., C. A. Bolme, M. J. Cawkwell, A. C. Golder, T. H. Pierce, K. J. Ramos and G. K. Windler. LANL High Explosive Crystal Laboratory. Presented at *LDRD DR Review*, Los Alamos, New Mexico, United States, 2018-02-06 - 2018-02-06. (LA-UR-18-20803)

Bowlan, P. R., M. S. Powell, R. T. Perriot, E. Martinez Saez, E. M. Kober, M. J. Cawkwell and S. D. Mcgrane. Probing ultrafast shock-induced chemistry using broad-band mid-infrared absorption spectroscopy. Presented at *Shock Compression of Condensed Matter*, portland, Oregon, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25544)

Bowlan, P. R., S. D. Mcgrane, M. S. Powell, K. E. Brown, C. A. Bolme and M. J. Cawkwell. Broad-band mid-infrared measurements for time resolving shock-induced chemical reactions. Presented at *Ultrafast Optics*, Jackson Hole, Wyoming, United States, 2017-10-09 - 2017-10-13. (LA-UR-17-29151)

Cawkwell, M. J., A. Krishnapriyan, R. T. Perriot, A. M. Niklasson and P. Yang. Optimized DFTB Parameterizations for Organic Materials. Presented at *Workshop of Shocked Chemical Dynamics in High Explosives*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20512)

Perriot, R. T., E. M. Kober, S. M. Mniszewski, E. Martinez Saez, A. M. Niklasson, P. Yang, S. D. Mcgrane and M. J. Cawkwell. Reaction Analysis of Shocked Nitromethane using Extended Lagrangian Born-Oppenheimer Molecular Dynamics. Presented at *LANL Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2017-08-29 - 2017-08-29. (LA-UR-17-27750)

Powell, M. S., P. R. Bowlan, R. T. Perriot, E. M. Kober, M. J. Cawkwell and S. D. Mcgrane. Probing Ultrafast, Shock-induced Chemistry Using Extremely Broad Band, Ultrashort Mid-infrared Pulses. Presented at *Center for Laser Electro Optics (CLEO*, San Jose, California, United States, 2019-05-05 - 2019-05-10. (LA-UR-19-23866)

Powell, M. S., P. R. Bowlan, S. D. Mcgrane, K. E. Brown, C. A. Bolme and M. J. Cawkwell. Overview of Mid-Infrared Generation for Probing Shocked Chemistry. Presented at *20170070DR Project Appraisal*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20677)

Powell, M. S., P. R. Bowlan, S. D. Mcgrane, K. E. Brown, C. A. Bolme and M. J. Cawkwell. Time Resolved Broad-Band Mid-Infrared Shock Induced Chemistry Measurements on Nitromethane. Presented at *20170070DR Project Appraisal*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-05. (LA-UR-18-20829)

Powell, M. S., P. R. Bowlan, S. F. Son and S. D. Mcgrane. Ultrafast Mid-Infrared Spectroscopy on Shocked Thin Film Explosives. Presented at *Gordon Research Conference*, Newry, Maine, United States, 2018-06-02 - 2018-06-08. (LA-UR-18-24726)

Martinez Saez, E., R. T. Perriot, E. M. Kober, P. R. Bowlan, M. S. Powell, S. D. Mcgrane and M. J. Cawkwell. Accelerated Quantum Molecular Dynamics Simulations of Shock-induced Chemistry in Liquid Benzene. Presented at *Carbon in Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-10-28 - 2019-10-30. (LA-UR-19-30485)

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 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

Journal Articles

Asaba, T., Y. Su, M. Janoschek, J. D. Thompson, S. M. Thomas, E. D. Bauer, S. Lin and F. Ronning. Large Tunable Anomalous Hall Effect in kagome Antiferromagnet U3Ru4Al12. Submitted to *Nature Communications*. (LA-UR-19-25889)

*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. Ultrahigh-resolution neutron spectroscopy of low-energy spin dynamics in UGe2. 2019. *Physical Review B*. **99** (1): 014429. (LA-UR-18-20542 DOI: 10.1103/PhysRevB.99.014429)

Jeong, J., S. Lin, Y. Lee, C. Lee, J. W. Choi, Y. H. Jeong, H. J. Chang and J. Kim. Hard skyrmions in a rare earth permanent magnet. Submitted to *Nature Communications*. (LA-UR-19-31929)

*Kim, T., C. Chien and S. Lin. Reentrant Fulde-Ferrell-Larkin-Ovchinnikov state in small-sized superconductors. 2019. *Physical Review B*. **99** (5): 054509. (LA-UR-18-30667 DOI: 10.1103/PhysRevB.99.054509)

Li, S., Y. Su, Y. Ren and L. He. Realizing valley polarization and valley inversion in graphene by using a valley magnet. Submitted to *Science*. (LA-UR-19-21456)

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)

Su, Y., S. Hayami and S. Lin. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Submitted to *Nature Communications*. (LA-UR-19-25839)

Su, Y., S. Lin and S. Hayami. Anomalous charge transport in magnetic insulators with multiple-Q spin textures. Submitted to *Physical Review Letters*. (LA-UR-19-23218)

*Su, Y. and S. Lin. Nontrivial topology and localization in the double exchange model with possible applications to perovskite manganites. 2018. *Physical Review B*. **98** (23): 235116. (LA-UR-18-29965 DOI: 10.1103/PhysRevB.98.235116)

*Su, Y. and S. Lin. Pairing symmetry and spontaneous vortex-antivortex lattice in superconducting twisted-bilayer graphene: Bogoliubov-de Gennes approach. 2018. *Physical Review B*. **98** (19): 195101. (LA-UR-18-26090 DOI: 10.1103/PhysRevB.98.195101)

Su, Y. and S. Lin. Topological Sliding Moire \xcc\x81 Heterostructure. Submitted to *Physical Review Letters*. (LA-UR-19-30658)

Wang, Z., H. Zhou, M. Guo, L. Zhao, T. Xu, Y. Dong, K. Wu, S. G. Je, W. Chao, M. Im, H. Han, S. Lee, K. Lee, C. Song, H. Wu, S. Lin and W. Jiang. Thermal Generation and Manipulation of Skyrmions. Submitted to *Nature*. (LA-UR-19-25918)

Wang, Z., Y. Su, S. Lin and C. D. Batista. Skyrmion crystal from RKKY interaction mediated by 2D electron gas. Submitted to *Physical Review Letters*. (LA-UR-19-31876)

Presentation Slides

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *Annual Conference on Magnetism and Magnetic Materials*, Las Vegas, Nevada, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31136)

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21986)

Posters

Huang, Z., C. Ting, J. Zhu and S. Lin. Stable Higgs Modes in Fulde-Ferrell-Larkin- Ovchinnikov (FFLO) states. Presented at *CINT annual meeting*, Santa Fe, New Mexico, United States, 2019-09-23 - 2019-09-26. (LA-UR-19-29466)

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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 successfull, 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.

Publications

Posters

Li, M. M. and S. A. Ivanov. Layered Ternary Chalcogenide Nanoparticles towards Supercapacitor Applications. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28807)

McGrath, A. J. and S. A. Ivanov. Magnetic M-Sb and M-Sn2 (M = Mn, Fe, Co) intermetallic nanocrystals from metal amidinate precursors. Presented at *LANL Postdoc Symposium*, Los Alamos, New Mexico, United States, 2018-08-27 - 2018-08-27. (LA-UR-18-27978)

McGrath, A. J. and S. A. Ivanov. Metal amidinates as precursors for transition metal-based intermetallic nanocrystals. Presented at *LANL 2019 Postdoc Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28516)

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 quantites 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

Journal Articles

Klamm, B. E., T. E. Albrecht-Schmitt, R. E. Baumbach, B. S. Billow, F. D. White, S. A. Kozimor, B. L. Scott and A. M. Tondreau. Using Intrinsic Lewis-Acidity in the Generation of Bimetallic Lanthanide Complexes. Submitted to *Inorganic Chemistry*. (LA-UR-20-21131)

Books/Chapters

J. White, F. D. and M. L. Marsh. Recent Advances in Non-aqueous Transuranic Chemistry. (LA-UR-19-23811)

Reports

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

Presentation Slides

Elkin, T. Development of novel MOFs for (CWA) emerging threats. Presented at *IMS Rapid response workshop*, Evanston, Illinois, United States, 2019-09-10 - 2019-09-12. (LA-UR-19-29055)

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.

Publications

Journal Articles

Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Physical Review X*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

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

Journal Articles

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. Van Orden. Imaging of Quantum Dots with Sub-Nanosecond TIme-Resolved Superresolution Microscopy. Submitted to *Applied Physics Letters*. (LA-UR-19-30441)

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. Van Orden. Single Molecule Localization With Four Avalanche Photodiode Detectors. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-20171)

Ryan, D. P., M. K. Dunlap, S. Majumder, C. J. Sheehan, J. H. Werner, J. A. Hollingsworth, M. P. Gelfand and A. K. Van Orden. Dual-color super-resolution imaging for FRET measurements: Energy transfer among donor/acceptor pairs of quantum dots. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-20-20052)

*Ryan, D. P., P. M. Goodwin, C. J. Sheehan, K. J. Whitcomb, M. P. Gelfand and A. Van Orden. Mapping Emission from Clusters of CdSe/ZnS Nanoparticles. 2018. *The Journal of Physical Chemistry C*. **122** (7): 4046-4053. (LA-UR-18-20821 DOI: 10.1021/acs.jpcc.7b10924)

Presentation Slides

Ryan, D. P. Energy Flow through Quantum Dot Networks. . (LA-UR-18-25130)

Ryan, D. P., M. K. Dunlap, P. M. Goodwin, J. H. Werner, J. A. Hollingsworth, S. Majumder, C. J. Sheehan, A. K. Van Orden and M. Gelfand. Dual-color Super-resolution Imaging of Quantum Dot Clusters. Presented at *SPIE Photonic West 2020*, San Francisco, California, United States, 2020-01-31 - 2020-02-06. (LA-UR-20-20728)

Ryan, D. P., M. K. Dunlap, S. Majumder, C. J. Sheehan, J. A. Hollingsworth, M. P. Gelfand, P. M. Goodwin and A. K. Van Orden. Super-resolution Imaging for Energy Transfer: Collective behavior from interacting quantum dots. Presented at *American Chemical Society Annual Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22627)

Ryan, D. P., P. M. Goodwin, J. H. Werner, C. J. Sheehan, J. A. Hollingsworth, S. Majumder, M. K. Dunlap, A. Van Orden and M. Gelfand. Energy Transfer Through Networks of CdSe/CdS Nanoparticles. Presented at *Gordon Research Conference on Colloidal Semiconductor Nanocrystals*, Smithfield, Rhode Island, United States, 2018-07-15 - 2018-07-20. (LA-UR-18-26595)

Posters

Abdollah-nia, F., M. K. Dunlap, J. Gann, D. P. Ryan, P. M. Goodwin, J. A. Hollingsworth, Y. Chen, J. S. Martinez, M. Gelfand and A. Van Orden. Single Molecule Experiments in the Van Orden Resarch Group. Presented at *Colorado State University Chemistry Graduate Student Recruiting Weekend*, Fort Collins, Colorado, United States, 2019-02-15 - 2019-02-15. (LA-UR-19-21376)

Dunlap, M. K., D. P. Ryan, J. H. Werner, J. A. Hollingsworth, M. Gelfand, A. Van Orden and P. M. Goodwin. A Lifetime Imaging Super-Resolution Microscope. Presented at *ACS Spring 2019 National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-03. (LA-UR-19-23084)

Dunlap, M. K., D. P. Ryan, P. M. Goodwin, J. H. Werner, J. A. Hollingsworth, M. Gelfand and A. Van Orden. Sub-Nanosecond Superresolution Imaging of Energy Transfer in CdSe/CdS Quantum Dot Clusters. . (LA-UR-19-24114)

Dunlap, M., D. P. Ryan, M. Gelfand and P. M. Goodwin. Quantum Dot Localization with Time Resolved Super-Resolution Tracking Microscopy. Presented at *Annual Meeting of the APS Four Corners Section*, Fort Collins, New Mexico, United States, 2017-10-20 - 2017-10-21. (LA-UR-17-29934)

Dunlap, M., D. P. Ryan, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand and A. K. Van Orden. Characterizing the Spatial Information of a Superresolution Fluorescence Lifetime Imaging Microscope. Presented at *CINT Annual Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28791)

Ryan, D. P., M. Dunlap, P. M. Goodwin, J. H. Werner, S. Majumder, J. A. Hollingsworth, M. P. Gelfand, A. K. Van Orden and C. J. Sheehan. Energy Transfer Through Networks of CdSe/CdS Nanoparticles. Presented at *Gordon Research Conference on Colloidal Semiconductor Nanocrystals*, Smithfield, Rhode Island, United States, 2018-07-14 - 2018-07-20. (LA-UR-18-25908)

Ryan, D. P., S. Majumder, J. A. Hollingsworth, J. H. Werner, P. M. Goodwin, A. K. Van Orden, M. K. Dunlap and M. P. Gelfand. Emission Dynamics from Clusters of Quantum Dots. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29347)

Ryan, D. P., S. Majumder, J. A. Hollingsworth, P. M. Goodwin, J. H. Werner, M. K. Dunlap, A. K. Van Orden and M. P. Gelfand. Super-resolution Orientation Imaging: A Microscopy Method for Measuring Structure in Biological Samples. Presented at *Biophysical Society Meeting*, San Francisco, California, United States, 2020-02-14 - 2020-02-19. (LA-UR-20-21373)

Improved Biologically Friendly Polymer Drag Reducers From Novel Architectures

Paul Welch
20180220ER

Project Description

The research described in this proposal will directy 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 and 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.

Publications

Journal Articles

J. Welch, P. M. and C. F. Welch. Calculating Dendrimer Titration Curves through Quantum Annealing. Submitted to *ACS Macro Letters*. (LA-UR-19-27637)

Posters

Schmidt, J. G., C. Schein, D. Beasley, M. Braun and D. Weaver. Stabilized PCP-Consensus Peptides for Flavi- and Alphavirus Vaccines and Therapies. Presented at *CBS&T*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-30920)

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

Reports

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

Presentation Slides

Bowlan, P. R., M. S. Powell and S. D. Mcgrane. Ultrafast mid-IR measurements during shock. Presented at *Shocked chemistry LDRD review*, Los Alamos, New Mexico, United States, 2018-02-05 - 2018-02-06. (LA-UR-18-20743)

Bowlan, P. R., T. N. Jones and R. L. Sandberg. Travis' LANL Experience. Presented at *Meeting with Rick Trebino's research group (talk to be given by Travis Jones)*, Atlanta, Georgia, United States, 2019-01-15 - 2019-01-15. (LA-UR-19-20252)

Posters

Jones, T. N., W. K. Peters, R. L. Sandberg and P. R. Bowlan. Measuring Femtosecond Extreme-Ultraviolet Pulses With Slow Visible Cameras. Presented at *LANL Annual Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27709)

Peters, W. K., T. N. Jones, P. R. Bowlan and R. L. Sandberg. Nonlinear Optics with Ionizing Radiation and Ultrafast Lasers: Progress Toward Measuring the Complete Electric Field of XFEL Pulses. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28443)

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

Journal Articles

Berbenni, S., R. A. Lebensohn and V. Taupin. A fast Fourier transform-based mesoscale field dislocation mechanics study of grain size effects and reversible plasticity in polycrystals. 2019. *Journal of the Mechanics and Physics of Solids*. 103808. (LA-UR-19-31410 DOI: 10.1016/j.jmps.2019.103808)

Djaka, K., S. Berbenni, V. Taupin and R. A. Lebensohn. A FFT-based numerical implementation of mesoscale field dislocation mechanics: Application to two-phase laminates. 2019. *International Journal of Solids and Structures*. (LA-UR-18-29918 DOI: 10.1016/j.ijsolstr.2018.12.027)

Genee, J., S. Berbenni, N. Gey, R. A. Lebensohn and F. Bonnet. Particle interspacing effects on the mechanical behavior of a Fe-TiB2 metal matrix composite using FFT-based field dislocation mechanics. Submitted to *Advanced Modeling and Simulation in Engineering Sciences*. (LA-UR-19-31404)

Lebensohn, R. A. and A. D. Rollett. Spectral methods for full-field micromechanical modelling of polycrystalline materials. 2020. *Computational Materials Science*. **173**: 109336. (LA-UR-18-28795 DOI: 10.1016/j.commatsci.2019.109336)

Liu, P., Z. Wang, Y. Xiao, R. A. Lebensohn, Y. Liu, M. F. Horstemeyer, X. Cui and L. Chen. Integration of phase-field model and crystal plasticity for the prediction of process-structure-property relation of additively manufactured metallic materials. Submitted to *International Journal of Plasticity*. (LA-UR-19-31422)

Nagra, J. S., A. Brahme, J. Levesque, R. Mishra, R. A. Lebensohn and K. Inal. A New Micromechanics Based Full Field Numerical Framework to Simulate the Effects of Dynamic Recrystallization on the Formability of HCP Metals. Submitted to *International Journal of Plasticity*. (LA-UR-19-31405)

Presentation Slides

Evans, J. A. Nuclear Reactor Materials and Anisotropy. . (LA-UR-19-32212)

Lebensohn, R. A. and L. Capolungo. Machine learning from physics-based spectral polycrystal plasticity models. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-19 - 2019-02-19. (LA-UR-19-21269)

Tallman, A. E., R. Pokharel and L. Capolungo. Discrete dislocation dynamics-based prediction of dislocation density from diffraction line profiles of Ta. Presented at *TMS Annual Meeting*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21678)

Posters

Christodoulou, P., A. F. Samuel, T. Francis, M. Echeverria, A. Needleman, T. Pollock, R. A. Lebensohn, F. Zok and I. Beyerlein. Mesoscale modeling of two-phase material deformation. Presented at *2019 Stewardship Science Academic Programs (SSAP) Annual Review Symposium*, Albuquerque, New Mexico, United States, 2019-02-19 - 2019-02-19. (LA-UR-19-21415)

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

Journal Articles

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*. **47** (3): 95-100. (LA-UR-18-29738 DOI: 10.9729/AM.2017.47.3.95)

Presentation Slides

T. Mix, L. M., M. C. Lee, K. R. O'Neal, N. S. Sirica, D. Ghosh, J. T. Tisdale, W. Nie, R. P. Prasankumar and D. A. Yarotski. Recombination Dynamics of Chlorine Doped Hybrid Perovskite Single Crystals. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21964)

Yarotski, D. A. Probing and manipulating quantum materials with THz pulses. Presented at *LIGHT ON THE QUANTUM LEAP: XFELS FOR QUANTUM MATERIALS*, tempe, Arizona, United States, 2019-01-16 - 2019-01-19. (LA-UR-19-20432)

Posters

O'Neal, K. R., B. Kuthanazhi, N. H. Jo, S. L. Bud'Ko, P. C. Canfield, J. Zhu, P. Orth, A. J. Taylor, R. P. Prasankumar and D. A. Yarotski. Ultrafast Carrier Dynamics of EuCd2As2. Presented at *CATS EFRC Midterm Review*, Gaithersburg, Maryland, United States, 2020-02-04 - 2020-02-04. (LA-UR-20-20524)

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 breaking 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 (MoS2) 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.

Publications

Journal Articles

Li, M. M. and S. A. Ivanov. 2D nanocrystalline ternary selenides Cu MSe (M = Mo/W). 2019. *Dalton Transactions*. **48** (42): 15795-15801. (LA-UR-19-29655 DOI: 10.1039/C9DT03282G)

Presentation Slides

Li, M. M. and S. A. Ivanov. Syntheses of phase pure ternary layered chalcogenides of Mo and W. Presented at *ACS Fall 2019 National Meeting & Exposition*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-28100)

Li, M. M. and S. A. Ivanov. Syntheses of copper tetrachalcogenide metallate (Mo/W) nanoparticles: Applications towards energy storage. Presented at *ACS Southeastern Regional Meeting*, Savannah, Georgia, United States, 2019-10-19 - 2019-10-23. (LA-UR-19-30075)

Posters

Li, M. M. and S. A. Ivanov. Layered Ternary Chalcogenide Nanoparticles towards Supercapacitor Applications. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28807)

Li, M. M. and S. A. Ivanov. Solutional Nanoparticle Syntheses of Layered Ternary Copper Selenides of Mo/W. Presented at *Materials Research Society 2019 Fall Meeting*, Boston, Massachusetts, United States, 2019-11-30 - 2019-12-05. (LA-UR-19-31366)

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 a 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.

Publications

Journal Articles

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Investigation of Explosive Spin Crossover Complexes for On-Demand Initiation Sensitivity and Energetic Polymers for Additive Manufacturing. Submitted to *AIP Conference Proceedings*. (LA-UR-19-28081)

Nguyen, T. D., J. M. Veauthier, G. F. Angles-Tamayo, D. E. Chavez, E. Lapsheva, T. Myers, T. R. Nelson and E. Schelter. Correlating Mechanical Sensitivity with Spin Transition in the Explosive Spin Crossover Complex [Fe(Htrz)3]n[ClO4]2n. 2020. *Journal of the American Chemical Society*. jacs.9b13835. (LA-UR-19-30677 DOI: 10.1021/jacs.9b13835)

Reports

Nelson, T. R., J. M. Veauthier, G. F. Angles-Tamayo and Y. Zhang. IC Annual Report. Unpublished report. (LA-UR-19-22530)

Presentation Slides

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Investigation of Explosive Spin Crossover Complexes for On-Demand Initiation Sensitivity and Energetic Polymers for Additive Manufacturing. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK19)*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25378)

Veauthier, J. M. Designing Energetic Coordination Complexes to Tune Explosive Initiation and Discover New Routes to Important Materials. Presented at *Inorganic Chemistry Gordon Research Conference*, Biddeford, Maine, United States, 2018-06-19 - 2018-06-19. (LA-UR-18-25262)

Veauthier, J. M. Nitrogen-rich metal coordination complexes for new applications in explosive initiation. Presented at *ACS Fall 2019 National Meeting*, San Diego, California, United States, 2019-08-25 - 2019-08-25. (LA-UR-19-28434)

Posters

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Development of Switchable Explosive Materials for the Additive Manufacturing of Insensitive Munitions. Presented at *Energetic Materials Gordon Research Conference*, Newry, Maine, United States, 2018-06-03 - 2018-06-03. (LA-UR-18-24723)

Nguyen, T. D., D. E. Chavez, A. H. Mueller, B. C. Tappan and J. M. Veauthier. Investigation of an Explosive Spin Crossover Complex for On-Demand Initiation Sensitivity and Energetic Polymers for Additive Manufacturing. Presented at *Agnew National Security and Metropolis Postdoc Fellow Showcase*, Los Alamos, New Mexico, United States, 2019-12-10 - 2019-12-10. (LA-UR-19-32236)

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

Journal Articles

Chen, H., C. Chang, A. J. Taylor, Z. Zhao, S. Fan and D. Li. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. Submitted to *Physical Review Letters*. (LA-UR-18-31108)

*Wang, C., T. G. Habteyes, T. S. Luk, J. F. Klem, I. Brener, H. Chen and O. Mitrofanov. Observation of Intersubband Polaritons in a Single Nanoantenna Using Nano-FTIR Spectroscopy. 2019. *Nano Letters*. **19** (7): 4620-4626. (LA-UR-19-22652 DOI: 10.1021/acs.nanolett.9b01623)

Presentation Slides

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversion. Presented at *The 9th International Symposium on Ultrafast Phenomena and Terahertz Waves (ISUPTW 2018)*, Changsha, China, 2018-04-23 - 2018-04-23. (LA-UR-18-23594)

Chen, H. Broadband Terahertz Linear-to-Circular Polarization Conversion. Presented at *IRMMW-THz 2018*, Nagoya, Japan, 2018-09-10 - 2018-09-10. (LA-UR-18-28683)

Chen, H. Active Metamaterials & Metasurfaces. . (LA-UR-19-24205)

Chen, H. Metasurfaces for Optical Antireflection and Bandpass Filters. Presented at *META 2019*, Lisbon, Portugal, 2019-07-23 - 2019-07-23. (LA-UR-19-27279)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversions. Presented at *MTSA 2019*, Busan, Korea, South, 2019-09-30 - 2019-09-30. (LA-UR-19-29968)

Li, D., C. Chang, Z. Zhao, A. J. Taylor, S. Fan and H. Chen. Broadband Linear-to-Circular Polarization Converter based on Reflective Birefringent Metasurfaces. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21921)

Wang, C. The localized surface plasmonic effects: from far-field to near-field optical measurements. . (LA-UR-19-22548)

Posters

Li, D., C. Chang, A. Singh, J. A. Hollingsworth and H. Chen. Enhancing the Light Emission of Colloidal Quantum Dots with Perfect Absorbers Based on Metasurfaces. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21922)

Wang, C., H. Chen and O. Mitrofanov. Nano-FTIR Spectroscopy of Intersubband Transition in Single Plasmonic Nanoantenna Regime. Presented at *2019 LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-08. (LA-UR-19-27747)

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 the Vienna Ab Initio Simulation Package (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 the National Nuclear Security Administration and has mission relevance to the Stockpile Stewardship Program, Explosives, lithium-ion batteries simulations (Commerce and Transportation and Renewable Energy) and others.

Publications

Journal Articles

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., 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)

*Beir\xc3\xa3o da Veiga, L., G. Manzini and L. Mascotto. A posteriori error estimation and adaptivity in hp virtual elements. 2019. *Numerische Mathematik*. **143** (1): 139-175. (LA-UR-18-23445 DOI: 10.1007/s00211-019-01054-6)

Reports

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)

Certik, O. and J. E. Pask. Why to Use Fortran For New Projects. Unpublished report. (LA-UR-19-24165)

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

Gyrya, V., G. Manzini, S. Naranjo-Alvarez and V. A. Bokil. The virtual element method for resistive magnetohydrodynamics: Design, wellposedness, stability, and preliminary numerical results.. Unpublished report. (LA-UR-19-31726)

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., H. M. Mourad, P. F. Antonietti and M. Verani. The virtual element method for linear elastodynamics models. Design, analysis, and implementation.. Unpublished report. (LA-UR-19-29577)

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)

Presentation Slides

Certik, O., G. Manzini, L. A. Collins, N. Sukumar, J. E. Pask and M. A. Schweitzer. Flat-top Partition of Unity Method for Electronic Structure Calculations. Presented at *WCCM 2018*, New York City, New York, United States, 2018-07-23 - 2018-07-27. (LA-UR-18-26760)

Certik, O., G. Manzini, L. A. Collins, N. Sukumar, J. E. Pask and M. A. Schweitzer. Flat-top Partition of Unity Method for Electronic Structure Calculations. Presented at *WCCM 2018*, New York City, New York, United States, 2018-07-23 - 2018-07-27. (LA-UR-18-26905)

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

Journal Articles

*Bennett, K. C. and D. J. Luscher. Effective Thermoelasticity of Polymer-Bonded Particle Composites with Imperfect Interfaces and Thermally Expansive Interphases. 2019. *Journal of Elasticity*. **136** (1): 55-85. (LA-UR-17-31014 DOI: 10.1007/s10659-018-9688-z)

Berbenni, S., R. A. Lebensohn and V. Taupin. A fast Fourier transform-based mesoscale field dislocation mechanics study of grain size effects and reversible plasticity in polycrystals. 2019. *Journal of the Mechanics and Physics of Solids*. 103808. (LA-UR-19-31410 DOI: 10.1016/j.jmps.2019.103808)

Despr\xc3\xa9s, A., M. Zecevic, R. A. Lebensohn, J. D. Mithieux, F. Chassagne and C. W. Sinclair. Contribution of intragranular misorientations to the cold rolling textures of ferritic stainless steels. 2020. *Acta Materialia*. **182**: 184-196. (LA-UR-19-31386 DOI: 10.1016/j.actamat.2019.10.023)

Genee, J., S. Berbenni, N. Gey, R. A. Lebensohn and F. Bonnet. Particle interspacing effects on the mechanical behavior of a Fe-TiB2 metal matrix composite using FFT-based field dislocation mechanics. Submitted to *Advanced Modeling and Simulation in Engineering Sciences*. (LA-UR-19-31404)

Lebensohn, R. A. Polycrystal plasticity models based on Green's functions: mean-field self-consistent and full-field Fast Fourier Transform formulations. *Handbook of Materials Modeling*. 1-27. (LA-UR-17-31125 DOI: 10.1007/978-3-319-42913-7_15-1)

Lebensohn, R. A. and A. D. Rollett. Spectral methods for full-field micromechanical modelling of polycrystalline materials. 2020. *Computational Materials Science*. **173**: 109336. (LA-UR-18-28795 DOI: 10.1016/j.commatsci.2019.109336)

C. Lieou, C. K. and C. A. Bronkhorst. Thermodynamic theory of crystal plasticity: formulation and application to polycrystal fcc copper. 2020. *Journal of the Mechanics and Physics of Solids*. 103905. (LA-UR-19-31861 DOI: 10.1016/j.jmps.2020.103905)

Liu, P., Z. Wang, Y. Xiao, R. A. Lebensohn, Y. Liu, M. F. Horstemeyer, X. Cui and L. Chen. Integration of phase-field model and crystal plasticity for the prediction of process-structure-property relation of additively manufactured metallic materials. Submitted to *International Journal of Plasticity*. (LA-UR-19-31422)

*Messner, M. C., R. A. Lebensohn, E. Zepeda-Alarcon and N. R. Barton. A method for including diffusive effects in texture evolution. 2019. *Journal of the Mechanics and Physics of Solids*. **125**: 785-804. (LA-UR-18-23915 DOI: 10.1016/j.jmps.2019.01.016)

Nagra, J. S., A. Brahme, J. Levesque, R. Mishra, R. A. Lebensohn and K. Inal. A New Micromechanics Based Full Field Numerical Framework to Simulate the Effects of Dynamic Recrystallization on the Formability of HCP Metals. Submitted to *International Journal of Plasticity*. (LA-UR-19-31405)

*Ran, H., T. de Riese, M. Llorens, M. A. Finch, L. A. Evans, E. Gomez-Rivas, A. Griera, M. W. Jessell, R. A. Lebensohn, S. Piazolo and P. D. Bons. Time for anisotropy: The significance of mechanical anisotropy for the development of deformation structures. 2019. *Journal of Structural*

Geology. **125**: 41-47. (LA-UR-18-23499 DOI: 10.1016/j.jsg.2018.04.019)

*Segurado, J., R. A. Lebensohn and J. LLorca. Computational Homogenization of Polycrystals. *Advances in Applied Mathematics*. **51**: 1-114. (LA-UR-18-23540 DOI: 10.1016/bs.aams.2018.07.001)

Zecevic, M., M. Knezevic, B. A. McWilliams and R. A. Lebensohn. Modeling of the thermo-mechanical response and texture evolution of WE43 Mg alloy in the dynamic recrystallization regime using a viscoplastic self-consistent formulation. 2020. *International Journal of Plasticity*. 102705. (LA-UR-19-28936 DOI: 10.1016/j.ijplas.2020.102705)

*Zecevic, M., R. A. Lebensohn, R. J. McCabe and M. Knezevic. Modeling of intragranular misorientation and grain fragmentation in polycrystalline materials using the viscoplastic self-consistent formulation. 2018. *International Journal of Plasticity*. **109**: 193-211. (LA-UR-18-23679 DOI: 10.1016/j.ijplas.2018.06.004)

*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. 2019. *Acta Materialia*. **164**: 530-546. (LA-UR-18-27030 DOI: 10.1016/j.actamat.2018.11.002)

*Zecevic, M., W. Pantleon, R. A. Lebensohn, R. J. McCabe and M. Knezevic. Predicting intragranular misorientation distributions in polycrystalline metals using the viscoplastic self-consistent formulation. 2017. *Acta Materialia*. **140**: 398-410. (LA-UR-18-22506 DOI: 10.1016/j.actamat.2017.08.056)

Zecevic, M. and R. A. Lebensohn. New Robust Self-Consistent Homogenization Schemes of Elasto-Viscoplastic Polycrystals. Submitted to *International Journal of Solids and Structures*. (LA-UR-20-21794)

Presentation Slides

Alexandrov, B. Unsupervised phase mapping of X-ray diffraction data by nonnegative factorization integrated with custom clustering. Presented at *Computational Data Science Approaches for Materials Conference 2019*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23081)

Bennett, K. Micro-thermomechanical modeling of PBX 9502 & self-consistent homogenization. Presented at *Internal Cross-divisional Research Meeting*, Los Alamos, New Mexico, United States, 2019-11-19 - 2019-11-19. (LA-UR-19-31411)

Zecevic, M., R. A. Lebensohn, R. J. Mccabe and M. Knezevic. PREDICTIONS OF FIELD FLUCTUATIONS IN HETEROGENEOUS MATERIALS. Presented at *TMS2019*, San Antonio, Texas, United States, 2019-03-10 - 2019-03-14. (LA-UR-19-22231)

Zecevic, M. and R. A. Lebensohn. New Robust Self-Consistent Homogenization Schemes of Elasto-Viscoplastic Polycrystals. Presented at *TMS 2020 149th Annual Meeting and Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-27. (LA-UR-20-21848)

Tuning Functionality via Dimensionality in 4f-Based Nanowires

Priscila Ferrari Silveira Rosa
20190076ER

Project Description

This project directly addresses a basic research need for energy and security relevant technology by providing the science required to discover, understand and ultimately control nanostructured forms of matter. Our approach is enabled by the ability to exploit low-dimensional correlated systems to tune functionality. Not only addressing a fundamental problem that is unexplored experimentally, this project also brings a new capability of probing 4f-based nanowires that will enable understanding and control of new materials and new physics that may emerge in the future.

Shockwave Metamaterials: Harnessing Structural Hierarchy for Tailorable Dynamic Response

Dana Dattelbaum
20190084ER

Project Description

Structural materials that function extensively as structural supports and protective components in aerospace and military applications are poised for transformational improvements through an ability to control structure with the advent of additive manufacturing. To date, these advances have been almost entirely related to tailorable mechanical response with only a limited number of studies interrogating the performance of these materials under the high strain rate-deformation, extreme conditions relevant to conventional and nuclear weapons environments. This project aims to lead the development of novel materials through dynamic characterization, materials modeling at high strain rates, along with the high resolution printing capabilities in order to understand the behavior of additively manufactured (AM) materials and their ability to tailor shockwave propagation offering a new class of materials for future stockpile applications.

Publications

Journal Articles

Dattelbaum, D. M., B. Branch, A. Ionita, B. M. Patterson and L. A. Kuettner. Shockwave interactions with additively-manufactured polymer structures. Submitted to *AIP Conference Proceedings*. (LA-UR-19-27099)

Presentation Slides

Dattelbaum, D. M., B. Branch, A. Ionita, B. M. Patterson and L. A. Kuettner. Shockwave interactions with additively-manufactured polymer structures (U). Presented at *2019 American Physical Society Shock Compression of Condensed Matter Topical Group meeting*, Portland, Oregon, United States, 2019-06-16 - 2019-06-22. (LA-UR-19-25436)

Air-Buoyant Vessel

Miles Beaux
20190119ER

Project Description

Remote sensing payloads, suspended from weather balloons for nonproliferation and treaty verification (as well as other surveillance applications), represent a potentially cheaper alternative to orbital satellite payloads. However, these ballooning applications face challenges such as the ever-increasing cost and decreasing supply of helium, the difficulty and cost of transporting helium, and the tendency of payloads to come down in undesirable locations which can be problematic for sensitive surveillance applications. This project aims to produce an air buoyant vacuum vessel (aka a vacuum balloon) as a helium-free alternative to weather balloons for suborbital atmospheric payload deployment. By utilizing a vacuum vessel filled with "nothing" instead of helium, it is expected that more permanent payload deployment can be achieved while greatly reducing the cost and providing better control over targeted location decent. This will be accomplished by developing ultra-light weight super-strong materials to meet the stringent engineering requirements for an air buoyant solid structure to be viable.

Publications

Presentation Slides

Hanson, C. J., S. L. Edwards and C. E. Hamilton. Additive Manufacturing and Novel Drying Methods Increase Accessibility and Decrease Integration Costs for Polyimide Aerogels. Presented at *5th Cross JOWOG on Additive Manufacturing*, Livermore, California, United States, 2020-01-27 - 2020-01-27. (LA-CP-20-20038)

Strongly Interacting Polariton Condensates at Room Temperature

Jinkyoung Yoo
20190224ER

Project Description

Quantum information science and technology will bring disruptive methods of information security, such as quantum computers powerful enough to break current encryption codes and quantum cryptography to prevent eavesdropping. However, the future is speculative because of the absence of suitable physical constituents for quantum information carriers. Current candidates for quantum information carriers do not fulfill the requirements of scalability, controllability, and robustness concurrently. Moreover, a few promising candidates require huge energy consumption due to quantum behaviors at cryogenic temperatures. This project aims at realizing robust and controllable quantum information carriers at room temperature in large scale. The physical constituents of the information carriers are interacting polariton condensates. Interacting polariton condensates will be made in semiconductor micro/nanocavity arrays embedding atomically thin quantum emitters. Interactions between polariton condensates can be controlled by external inputs. Thus, interacting polariton condensates can be used for computation. The system will be scalable due to the solid-state semiconductor platform -- a marked advantage over existing electronic systems. Additionally, polariton condensates are stable at room temperature. The expected deliverables will be breakthroughs in realization and deployment of quantum information systems.

Publications

Journal Articles

Jeong, J., Q. Wang, J. Cha, D. K. Jin, D. H. Shing, S. Kwon, B. K. Kang, J. H. Jang, W. S. Yang, Y. S. Choi, J. Yoo, J. K. Kim, C. Lee, S. W. Lee, A. Zakhidov, S. Hong, M. J. Kim and Y. J. Hong. Remote heteroepitaxy of GaN microrod heterostructures for deformable light-emitting diodes and wafer recycle. Submitted to *Science Advances*. (LA-UR-19-29399)

Presentation Slides

Yoo, J. Two-dimensional Materials Research at LANL. . (LA-UR-19-27080)

Yoo, J. Multi-dimensional van der Waals heterostructures. Presented at *31st Rio Grande Symposium on Advanced Materials*, Albuquerque, New Mexico, United States, 2019-09-16 - 2019-09-16. (LA-UR-19-29194)

Yoo, J. 2D/3D van der Waals heterostructures. Presented at *2019 Materials Research Society Fall Meeting*, Boston, Massachusetts, United States, 2019-12-02 - 2019-12-02. (LA-UR-19-31957)

Posters

Yoo, J. Semiconductor Nano-heterostructures Research at CINT. . (LA-UR-19-24208)

Accelerated Aging of Crystalline Plutonium Compounds

Justin Cross
20190228ER

Project Description

The goal of this project is to provide experimental data on the aging of well-defined, crystalline plutonium (Pu) salts by spiking 238Pu to produce significant radiation self-damage in a short, yet manageable, period of time. These data can then be used to answer the questions: i. What are the mechanisms of atom displacement and final product formation? ii. How resilient are the selected compounds and how long are they still useful? These results can be integrated into current and future efforts in material disposition, storage, and surveillance. Successful investigations can position the Labortaory as a leader in radiation damage of Pu compounds. This project will fill a gap of knowledge in the nuclear material management of the entire DOE complex as there are no studies on the degradation of crystalline salts with Pu as a main constituent. The findings will have high potential to inform a wide variety of unusual legacy residues that must be handled for future repackaging, storage, and/or disposition. This is especially pertinent with the recent resumption of shipments to the WIPP (Waste Isolation Pilot Plant). State-of-the-art radiological facilities, cutting edge spectroscopy, and access 238Pu place Los Alamos in the unique position to undertake this task.

Quantum Dot Sunlight Collectors for Building-Integrated Photovoltaics

Victor Klimov
20190232ER

Project Description

The Department of Energy aims to reduce the energy consumption of buildings by 50% by 2030, identifying building-integrated photovoltaics (BIPV) as an important component of this ongoing effort. The proposed project directly addresses this goal by introducing a new solution to BIPV, which is based on inexpensive luminescent sunlight collectors or luminescent solar concentrators (LSCs) integrated into a building envelope as semitransparent solar windows and/or wall panels coupled to edge-installed PVs. The key innovation in this project is designer semiconductor quantum dots that exhibit close-to-unity emission efficiencies at near-infrared energies, combined with specially tailored optical spectra that feature strong absorptance across the solar spectrum and virtually complete suppression of self-absorption at the emission wavelength. These nearly ideal characteristics, never previously realized with any other fluorophores, will enable large-area sunlight collectors with efficiencies approaching a theoretical limit. The quantum-dot LSC technology developed in this project will become one of the vital elements of ongoing efforts on the realization of net-zero energy consumption buildings.

Publications

Journal Articles

Du, J., R. Singh, I. Fedin, A. S. Fuhr and V. I. Klimov. Spectroscopic insights into high defect tolerance of Zn:CuInSe2 quantum-dot-sensitized solar cells. Submitted to *Nature Energy*. (LA-UR-19-29575)

Klimov, V. I., A. Fuhr, H. Y. Yun and S. A. Crooker. Spectroscopic and Magneto-Optical Signatures of Cu1+ and Cu2+ Defects in Copper Indium Sulfide Quantum Dots. 2020. *ACS Nano*. (LA-UR-20-20156 DOI: 10.1021/acsnano.9b09181)

Klimov, V. I., J. Du, I. Fedin, R. Singh and A. Fuhr. Spectroscopic insights into high defect tolerance of Zn:CuInSe2 quantum-dot-sensitized solar cells. Submitted to *Nature Energy*. (LA-UR-20-20157)

Presentation Slides

Gungor, K., O. Erdem, B. Guzelturk, E. Unal, M. Sak, S. Gaponenko, S. Jun, E. Jang and H. V. Demir. Strongly Polarized Light Generation from Isotropic Colloidal Quantum Dots Coupled to Fano Resonances. Presented at *2019 MRS Spring Meeting & Exhibit*, Phoenix, Arizona, United States, 2019-04-22 - 2019-04-26. (LA-UR-19-22937)

Wavelength-Selectable, Electrically Driven Single-Photon Sources Operating at Room Temperature

Istvan Robel
20190236ER

Project Description

Despite its clear potential to revolutionize secure communications, the implementation of quantum cryptography is stymied by the lack of practical technologies for generating single-photons. To address this, we will develop wavelength-selectable, electrically driven, room-temperature single photon sources that exploit the unique atomic-like yet size-tunable character of electronic states in colloidal semiconductor nanocrystals. This project will leverage our recent advances in demonstrating structure-based control over recombination processes in nanomaterials in the context of electroluminescent devices. Specifically, we will develop single-nanocrystal light-emitting diodes, and use them to demonstrate a new type of room-temperature single-photon source with wavelength-selectable emission as dictated by a particular application. Successful combination of our nanomaterials and device advances, resulting in the first practical single-photon sources, will have a game-changing impact in the field of quantum information by making them as common as blue or white light-emitting diodes (LEDs), ushering in a new era of rigorous cybersecurity and ubiquitous quantum computation.

Thermally Expandable Microspheres for Plastic-bonded Explosive (PBX) Properties Control

Amanda Duque
20190342ER

Project Description

This project aims to develop a high explosive system with shock sensitivity that may be controlled "on-demand". We will incorporate a small fraction (<1 wt%) of thermally expandable microspheres (TEMs) during the manufacturing process of the plastic-bonded explosive (PBX). The remainder of the explosive fabrication process would follow normally (i.e. pressing, casting, machining, etc), and the resulting PBX material would be in the "lower state" of shock sensitivity. That is, it would be less sensitive to insult, in particular an incoming shock wave. After exposure to a thermal stimulus (at a minimum temperature, which may be tuned by the properties of the TEM that is incorporated), either from the environment or electromagnetic energy, the TEMs would expand and decrease the local density. This creates an increase in the size and number of voids in the material, which will ultimately result in an increase in shock sensitivity. Thus, the material remains in a safer configuration until after exposure to the thermal stimulus, resulting in true "on-demand" control of explosives sensitivity.

Publications

Journal Articles

Duque, A. L., B. M. Patterson, L. A. Kuettner, S. R. Robillard, J. T. Mang and W. L. Perry. Novel PBX Formulations Containing Thermally-Expandable Microspheres for On-Demand Control of Explosive Behavior. Submitted to *AIP Conference Proceedings*. (LA-UR-19-26869)

S. Mehana, M. Z. and M. Fahes. Molecular Simulation Study of Low salinity Waterflooding Mechanisms. Submitted to *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. (LA-UR-20-20808)

Presentation Slides

Duque, A. L., B. M. Patterson, L. A. Kuettner, S. R. Robillard, J. T. Mang and W. L. Perry. Novel PBX formulations containing thermally-expandable microspheres for on-demand control of explosive behavior. Presented at *21st Biennial APS Topical Group on Shock Compression*, Portland, Oregon, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25321)

Patterson, B. M., K. C. Henderson, N. L. Cordes, L. A. Kuettner, T. A. Shear, P. M. J. Welch, C. F. Welch, M. J. Herman, J. S. Carpenter, C. J. Montgomery, A. Ionita, N. Chawla, J. J. Williams, K. Fezzaa, T. Sun and X. Xiao. Probing Material Morphology and Deformation as a Response to In situ Loading using X-ray Tomography. Presented at *Microscopy and Microanalysis 2019*, Portland, Oregon, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27238)

Emergent Bogoliubov Fermi Surface in Unconventional Superconductors

Roman Movshovich
20190360ER

Project Description

This research will develop a new tool for superconductivity research, opening a new window into the structure of the superconducting order parameter. This will be relevant to a variety of systems of both fundamental and technological interest, including heavy fermion, iron-based, and high temperature cuprate superconductors.

Organic Molecular Electrocatalysts for Hydrogen Evolution Reaction

Piotr Zelenay
20190420ER

Project Description

This project targets an entirely new class of organic molecular electrocatalysts (OMECs) for hydrogen evolution reaction (HER), an electrochemical process of fundamental importance to the future large-scale hydrogen production and processing, powered by renewable energy. The primary objectives of this work are to understand the underlying HER mechanism at metal-free OMECs, identify the structure-activity relationship for heterocyclic molecules, and enable rational design of future HER catalysts. The proposed research originates from the Laboratory's discovery of the world's first highly active OMEC for hydrogen evolution reaction that, in addition to high activity, exhibits excellent durability in an acidic polymer. In this project, the OMEC performance will be enhanced through a combination of experiments and computational modeling-guided catalyst discovery. This research is expected to conclude in a radical departure from HER electrocatalysis based on metals, either precious or non-precious. It will offer an alternative and cost-effective path to catalyzing hydrogen evolution reaction, which is essential for hydrogen production and purification. This research stands a unique chance of making a significant impact in the fields of electrocatalysis, chemistry, materials science and energy technology, in agreement with Department of Energy goals in energy conversion, including development of materials for clean-energy applications.

Publications

Journal Articles

Yin, X., L. Lin, U. Martinez and P. Zelenay. 2,2#-Dipyridylamine as Heterogeneous Organic Molecular Electrocatalyst for Two-Electron Oxygen Reduction Reaction in Acid Media. 2019. *ACS Applied Energy Materials*. **2** (10): 7272-7278. (LA-UR-18-27879 DOI: 10.1021/acsaem.9b01227)

Presentation Slides

Yin, X. Advancing Electrocatalysts for Energy and Environmental Applications. . (LA-UR-20-20432)

Yin, X., H. Gao, E. F. Holby and P. Zelenay. Structure-Activity Data Mining for Hydrogen Evolution Reaction at Organic Molecular Electrocatalysts. Presented at *235th ECS Meeting*, Dallas, Texas, United States, 2019-05-26 - 2019-05-30. (LA-UR-19-24898)

Posters

Yin, X. Organic Molecular Electrocatalysts for Energy-Water Nexus. Presented at *2019 AIChE Annual Meeting*, Orlando, Florida, United States, 2019-11-10 - 2019-11-15. (LA-UR-19-32632)

Magnetization Fluctuation Spectroscopy as a Dynamic Probe of Emergent Magnetic Phases

Scott Crooker
20190430ER

Project Description

Magnetic materials form the basis for a huge number of essential technological applications -- for example, magnetic information storage (disk drives), certain information processing schemes (magnetic random-access memory), and sensors. New magnetic materials with exotic and potentially useful new properties are continually being developed round the world. Understanding the physics that underpins the behavior of new magnetic materials is essential if a new material is ever to be adopted as a new technology. Traditionally, this physics is revealed using conventional 'perturbative measurements', wherein the material is excited, driven, or otherwise perturbed away from equilibrium, and it's response back to equilibrium is measured. Our project will establish a new and entirely alternative means of revealing the physics of magnetization dynamics -- not based on perturbation, but rather on detecting the intrinsic and ubiquitous fluctuations that naturally exist in every magnetic material. This "magnetization noise" necessarily encodes the same information (as guaranteed by the famous Fluctuation-Dissipation Theorem), and can be used to reveal the underlying magnetization dynamics without ever perturbing the system away from equilibrium, which can be particularly important near magnetic phase transitions.

Publications

Journal Articles

Sinitsyn, N., V. Chernayk, F. Li and C. Sun. Integrable multistate Landau-Zener models with parallel energy levels. Submitted to *Journal of Physics A: Mathematical and Theoretical*. (LA-UR-20-20621)

Yan, B. and N. Sinitsyn. Recovery of damaged information and the out-of-time-ordered correlators. Submitted to *Physical Review Letters*. (LA-UR-20-22064)

Mixed Conductors for Enhanced Fuel Cell Performance

Yu Seung Kim
20190440ER

Project Description

This project addresses energy security issues by improving the performance and reducing the cost of zero-emission energy conversion devices. The goal of the research is to develop improved catalyst supports for fuel cell applications. By enabling the support to conduct electrons and protons at the same time, we will enable higher performance with lower cost, leading to accelerated deployment of fuel cell technology for transportation and defense applications.

Three-dimension (3-D) Printed Hierarchically Porous Heat Pipe Wicks

Matthew Lee
20190463ER

Project Description

This project aims to develop a new class of heat transfer materials with enhanced properties and performance metrics suitable for a wide range of engineering applications. Using three-dimensional (3-D) printing techniques recently pioneered by members of our team, the goal of this project is to generate novel metallic wicking materials for heat pipes with optimized structural geometries and a vastly broadened design space.
Heat pipes are key components in many technologies pertinent to the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) and other government agencies, including waste heat recovery, nuclear energy, space applications and high performance computing. Therefore, this research directly addresses current national security challenges in energy security, aerospace and defense applications. In addition, this research can potentially lead to the large-scale manufacturing of more compact and efficient heat pipe designs with increased capacity to transport thermal energy, thereby broadening the span of their end-use applications and advancing key technologies already used through the DOE complex and beyond. Through our research we aim to identify key parameters governing heat pipe performance, optimize these through the use of 3-D printing, and pave the way toward new heat pipe designs and applications that were not possible until now.

Evaluating and Increasing the Reliability of Supercomputer and Autonomous Vehicles (Rosen Scholar)

Constantine Sinnis
20190499ER

Project Description

This research is focused on the reliability and efficiency of safety-critical computing platforms such as autonomous vehicles (AVs) and High Performance Computing (HPC). As HPC and AVs become more prevalent throughout the National Nuclear Security Administration and the nation, the need for resilience in these systems is ever increasing. Neutron upsets pose a unique and unavoidable threat to these systems. The development of mitigation strategies will increase the reliability and therefore the utility of such systems.

Publications

Conference Papers

Rech, P., F. Fernandes dos Santos, M. Brandalero, P. Basso and M. Shafique. Efficient Duplication With Comparison Strategy for Mixed-Precision Architectures. Presented at *HPCA (The 26th IEEE International Symposium on High-Performance Computer Architecture)*. (San Diego, California, United States, 2020-02-22 - 2020-02-22). (LA-UR-19-28021)

Presentation Slides

Rech, P. Reliability in the Era of Autonomous Vehicles and Supercomputers. Presented at *The Physics and Theoretical Division Colloquium*, los alamos, New Mexico, United States, 2019-10-31 - 2019-10-31. (LA-UR-19-32383)

Rech, P., D. Oliveira and P. Navaux. Increasing the Efficiency and Efficacy of Selective-Hardening for Parallel Applications. Presented at *DFT (The 32nd IEEE Inter)national Symposium on Defect and Fault Tolerance in VLSI and Nanotechnology Systems)*, delft, Netherlands, 2019-10-03 - 2019-10-03. (LA-UR-19-29993)

Posters

Martins Basso, P., F. Fernandes dos Santos and P. Rech. Impact of Tensor Cores and Mixed-Precision on the Reliability of Matrix Multiplication in GPUs. Presented at *RADECS*, Montpellier, France, 2019-09-15 - 2019-09-20. (LA-UR-19-29987)

Interfacial Structure Transfer for Direct Band Gap Wurtzite Group-IV Semiconductors

Jinkyoung 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."

Technical Outcomes

Hexagonal phases of group-IV semiconductors with novel optical characteristics were successfully grown on two-dimensional materials by a conventional semiconductor processing technique. Thorough understanding and universal strategy to control growth behaviors of conventional materials on emerging two-dimensional materials were achieved. The novel heterostructures and growth recipes opened up ways of heterogeneous integration not hindered from materials compatibility.

Publications

Journal Articles

*Jeong, J., K. Min, D. H. Shin, W. S. Yang, J. Yoo, S. W. Lee, S. Hong and Y. J. Hong. Remote homoepitaxy of ZnO microrods across graphene layers. 2018. *Nanoscale*. **10** (48): 22970-22980. (LA-UR-18-28408 DOI: 10.1039/C8NR08084D)

*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. Lee. Enhanced nucleation of germanium on graphene via dipole engineering. *Nanoscale*. **10** (12): 5689-5694. (LA-UR-17-27137 DOI: 10.1039/C7NR06684H)

Books/Chapters

Lopez-Bezanilla, A. Graphene Nanoribbons. (LA-UR-19-20064)

Presentation Slides

Yoo, J. Multi-dimensional semiconductor heterostructures for basic energy sciences. Presented at *CCMR 2017*, Jeju, Korea, South, 2017-06-26 - 2017-06-26. (LA-UR-17-24662)

Yoo, J. Semiconductor quantum structures at CINT. . (LA-UR-17-27196)

Yoo, J. Low-dimensional heterostructures for basic energy sciences. Presented at *Institute for Materials Science Summer School Lecture*, Los Alamos, New Mexico, United States, 2018-06-13 - 2018-06-13. (LA-UR-18-25131)

Yoo, J. Group-IV epitaxy for nanowire heterostructures and van der Waals heterostructures. . (LA-UR-18-29839)

Yoo, J. Growth and characterizations of Si and Ge heterostructures in multi-dimensional architectures. Presented at *TMS meeting*, San Antonio, Texas, United States, 2019-03-10 - 2019-03-10. (LA-UR-19-22060)

Yoo, J. Multi-dimensional van der Waals heterostructures. Presented at *31st Rio Grande Symposium on Advanced*

Materials, Albuquerque, New Mexico, United States, 2019-09-16 - 2019-09-16. (LA-UR-19-29194)

Yoo, J., T. Ahmed, I. Bilgin, R. Chen, A. Chen, S. Krylyuk, S. Kar and A. Davydov. Electrical characteristics and flexible devices of Ge/2D vdW heterostructures. Presented at *Materials Research Society 2017 Fall meeting*, Boston, Massachusetts, United States, 2017-11-26 - 2017-11-26. (LA-UR-17-30698)

Posters

Magginetti, D., Y. Yoon, S. Jeon, J. Yoo and H. Yoon. Nanoscale Surface Properties of MoS2/Ge Heterostructures. . (LA-UR-19-24203)

Yoo, J. Semiconductor Nano-heterostructures Research at CINT. . (LA-UR-19-24208)

Yoo, J., T. Ahmed, I. Bilgin, R. Chen, A. Chen, S. Krylyuk and A. Davydov. General strategy for growth of 2D/3D van der Waals heterostructures. Presented at *Gordon Research Conference: Two dimensional electronics beyond graphene*, Easton, Massachusetts, United States, 2018-06-03 - 2018-06-03. (LA-UR-18-24662)

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, such as magnetic domains in hard disks. Instead artificial materials can contain delocalized monopole charges, which can be seen as mobile degrees of freedom and a possible technological game-changer.

Technical Outcomes

We designed new artificial magnets of exotic behavior, including the first realization of topological order in a classical material. We demonstrated ice rule fragility (breakdown of the rule in spin ices, considered most robust), the first magnetic phase coexistence in an artificial nanomagnet, and the effect of magnetic ensemble on current in artificial spin ices, opening a path toward new memristors. Knowing the different level of frustration, we can exploit them to design desired behaviors.

Publications

Journal Articles

*Lao, Y., F. Caravelli, M. Sheikh, J. Sklenar, D. Gardeazabal, J. D. Watts, A. M. Albrecht, A. Scholl, K. Dahmen, C. Nisoli and P. Schiffer. Classical topological order in the kinetics of artificial spin ice. 2018. *Nature Physics*. **14** (7): 723-727. (LA-UR-17-29552 DOI: 10.1038/s41567-018-0077-0)

*Le, B. L., J. Park, J. Sklenar, G. -. Chern, C. Nisoli, J. D. Watts, M. Manno, D. W. Rench, N. Samarth, C. Leighton and P. Schiffer. Understanding magnetotransport signatures in networks of connected permalloy nanowires. 2017. *Physical Review B*. **95** (6): 060405. (LA-UR-18-29680 DOI: 10.1103/PhysRevB.95.060405)

*Lib\xc3\xa1l, A., C. Nisoli, C. J. O. Reichhardt and C. Reichhardt. Inner Phases of Colloidal Hexagonal Spin Ice. 2018. *Physical Review Letters*. **120** (2): 027204. (LA-UR-18-29684 DOI: 10.1103/PhysRevLett.120.027204)

Libal, A. J., A. Del Campo, C. Nisoli, C. Reichhardt and C. J. Reichhardt. Quenched Dynamics of Artificial Spin Ice: Coarsening vs Kibble-Zurek. Submitted to *Nature Communications*. (LA-UR-19-27840)

*Libal, A., C. Nisoli, C. Reichhardt and C. J. O. Reichhardt. Dynamic Control of Topological Defects in Artificial Colloidal Ice. 2017. *Scientific Reports*. **7** (1): 651. (LA-UR-18-29683 DOI: 10.1038/s41598-017-00452-w)

*Libal, A., D. Y. Lee, A. Ortiz-Ambriz, C. Reichhardt, C. J. O. Reichhardt, P. Tierno and C. Nisoli. Ice rule fragility via topological charge transfer in artificial colloidal ice. 2018. *Nature Communications*. **9** (1): 4146. (LA-UR-18-29641 DOI: 10.1038/s41467-018-06631-1)

*Loreto, R. P., F. S. Nascimento, R. S. Goncalves, J. Borme, J. C. Cezar, C. Nisoli, A. R. Pereira and C. I. L. de Araujo. Experimental and theoretical evidences for the ice regime in planar artificial spin ices. 2019. *Nature Communications*. **31** (2): 025301. (LA-UR-17-29335 DOI: 10.1088/1361-648X/aaeeef)

*Mahault, B., A. Saxena and C. Nisoli. Emergent inequality and self-organized social classes in a network of power and frustration. 2017. *PLOS ONE*. **12** (2). (LA-UR-18-29681 DOI: 10.1371/journal.pone.0171832)

*Nisoli, C. Unexpected Phenomenology in Particle-Based Ice Absent in Magnetic Spin Ice. 2018. *Physical Review Letters*. **120** (16): 167205. (LA-UR-17-29430 DOI: 10.1103/PhysRevLett.120.167205)

*Nisoli, C. Write it as you like it. 2018. *Nature Nanotechnology*. **13** (1): 5-6. (LA-UR-17-29476 DOI: 10.1038/s41565-017-0021-y)

Nisoli, C. Spin Ice vs. Thin Ice. Submitted to *Physical Review Letters*. (LA-UR-18-22142)

*Nisoli, C., V. Kapaklis and P. Schiffer. Deliberate exotic magnetism via frustration and topology. 2017. *Nature*

Physics. **13** (3): 200-203. (LA-UR-18-29682 DOI: 10.1038/nphys4059)

Nisoli, C., X. Zhang, P. Schiffer, J. Sklenar, N. Bingham and C. Leighton. Understanding Thermal Annealing of Articial Spin Ice. Submitted to *Applied Physics Letters*. (LA-UR-19-29694)

Nisoli, C. and A. Duzgun. Skyrmionic Spin Ice in Liquid Crystals. Submitted to *Nature Materials*. (LA-UR-19-29696)

*Nisoli, C. and A. R. Bishop. Attractive Inverse Square Potential, U(1) Gauge, and Winding Transitions. 2014. *Physical Review Letters*. **112** (7): 070401. (LA-UR-18-29685 DOI: 10.1103/PhysRevLett.112.070401)

Ortiz, A., C. Nisoli, C. J. Reichhardt, C. Reichhardt and P. Tierno. Colloquium: Ice rule in soft condensed matter. Submitted to *Reviews of Modern Physics*. (LA-UR-19-25339)

Reichhardt, C., C. J. Reichhardt, A. Duzgun and C. Nisoli. Commensurate states and pattern switching via liqued crystal skyrmions trapped in a square lattice.. Submitted to *Soft Matter*. (LA-UR-19-31800)

Reichhardt, C., C. J. Reichhardt, A. Libal and T. Balazs. Colloidal Dynamics on a Choreographic Time Crsyatl. Submitted to *Physical Review Letters*. (LA-UR-19-31969)

Reichhardt, C., C. J. Reichhardt, K. Li, K. Wang, F. Yan and M. S. Murillo. Depinning dynamics of two-dimensional dusty plasmas on a one-dimensional periodic substate. Submitted to *Physical Review E*. (LA-UR-19-25157)

Reichhardt, C., C. J. Reichhardt, M. Olszewski and M. Eskildsen. Rotational transition, domain formation, dislocations and defects in vortex systems with combined six and 12 fold anistropic inteactins. Submitted to *Physical Review B*. (LA-UR-19-30148)

Reichhardt, C., C. J. Reichhardt, M. S. Murillo, W. Li and Y. Feng. Oscillation-like diffusion of two-dimensional liquid dusty plasmas on one-dimensional periodic substrates with varied widths. Submitted to *Physics of Plasmas*. (LA-UR-20-20139)

Reichhardt, C., C. J. Reichhardt, M. S. Murillo, W. li, K. Wang and F. Yan. Depinning dynamics of of two-dimensional dusty plasmas on a one-dimensional periodic substrate.. Submitted to *Physical Review E*. (LA-UR-19-25838)

Reichhardt, C., C. J. Reichhardt, N. Porto Vizarim and P. Venegas. Shapiro Steps and Nonlinear Skyrmion Hall Angles for dc and ac Driven Skyrmions on a Two Dimensional Periodic Substrate. Submitted to *Physical Review B*. (LA-UR-20-22228)

Reichhardt, C., C. J. Reichhardt, N. Porto Vizarim and P. Venegas. Skyrmion Dynamics and Transverse Mobility: Skyrmion Hall Angle Reversal on 2D Periodic Substrates with dc and Biharmonic ac Drives. Submitted to *European Physical Journal B. Condensed Matter and Complex Systems*. (LA-UR-20-22293)

Reichhardt, C., C. J. Reichhardt and D. McDermott. Detecting Depinning and Nonequilibrium Transitions with Unsupervised Machine Learning. Submitted to *Physical Review E*. (LA-UR-19-28836)

Reichhardt, C., C. J. Reichhardt and X. Ma. Braiding Majorana Fermions and Creating Quantum Logic Gates with Vortices on a Periodic Pinning Structure. Submitted to *Physical Review B*. (LA-UR-19-30449)

Reichhardt, C. and C. J. Reichhardt. Reetrant pinning, dynamic row reduction and skyrmion accumulation for driven skyrmion in inhomogenous pinning arrays. Submitted to *EPL*. (LA-UR-19-28203)

Reichhardt, C. and C. J. Reichhardt. Vortex Shear Banding Transitions in Superconductors with Inhomogeneous Pinnng Array. Submitted to *New Journal of Physics*. (LA-UR-19-28414)

Reichhardt, C. and C. J. Reichhardt. Chiral Edge Currents for ac Driven Skyrmions in Confined Pinning Geometries. Submitted to *Physical Review B*. (LA-UR-19-29754)

Reichhardt, C. and C. J. Reichhardt. Shear Banding, Intermittency, Jamming and Dynamic Phases for Skyrmions in Inhomogeneous Pinning Arrays. Submitted to *Physical Review B*. (LA-UR-19-31466)

Reichhardt, C. and C. J. Reichhardt. Plastic Flow and the Skyrmion Hall Effect. Submitted to *Nature Communications*. (LA-UR-19-31805)

Reichhardt, C. and C. J. Reichhardt. Vortex guidance and transport in channeled pinning arrays. Submitted to *Low Temperature Physics*. (LA-UR-19-32592)

*Sklenar, J., Y. Lao, A. Albrecht, J. D. Watts, C. Nisoli, G. Chern and P. Schiffer. Field-induced phase coexistence in an artificial spin ice. 2019. *Nature Physics*. **15** (2): 191-195. (LA-UR-18-29639 DOI: 10.1038/s41567-018-0348-9)

Books/Chapters

Nisoli, C. Topology by Design in Magnetic Nano-materials: Artificial Spin Ice. (LA-UR-18-29640)

Nisoli, C. FRUSTRATION(S) AND THE ICE RULE: FROM NATURAL MATERIALS TO THE DELIBERATE DESIGN OF EXOTIC BEHAVIORS. (LA-UR-18-29642)

Presentation Slides

Duzgun, A. Liquid crystal skyrmions as building blocks for material by design. Presented at *Gordon Research Conference: Exploiting the Functionality of Soft Materials*, Ventura, California, United States, 2019-01-27 - 2019-01-27. (LA-UR-19-20926)

Nisoli, C. Deliberate exotic magnetism via frustration and topology. Presented at *Loch Lomond Workshop on Artificial Spin Ice*, Luss, United Kingdom, 2017-06-26 - 2017-06-26. (LA-UR-17-23536)

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 Department of Energy 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.

Technical Outcomes

1. Developed a capability for performing nuclear magnetic resonance (NMR) measurements under applied strain of 1%. 2. Investigated a number of materials with our strain-NMR measurements to provide the most impactful demonstration of our capability. 3. Determined the nature of superconductivity in strontium ruthenate, a prototypical correlated electron material. We have completely changed the way the scientific community understands this archetypal compound, turning 30 years of research on its head with our NMR-strain capability.

Publications

Journal Articles

*Luo, Y., A. Pustogow, P. Guzman, A. P. Dioguardi, S. M. Thomas, F. Ronning, N. Kikugawa, D. A. Sokolov, F. Jerzembeck, A. P. Mackenzie, C. W. Hicks, E. D. Bauer, I. I. Mazin and S. E. Brown. Normal State NMR Studies of under Uniaxial Stress. 2019. *Physical Review X*. **9** (2): 021044. (LA-UR-18-30163 DOI: 10.1103/PhysRevX.9.021044)

Pustogow, A., Y. Luo, A. Chronister, Y. Su, D. Sokolov, F. Jerzembeck, A. P. Mackenzie, C. Hicks, N. Kikugawa, S. Raghu, E. D. Bauer and S. E. Brown. Constraints on the superconducting order parameter in Sr2RuO4 from 17^O NMR. Submitted to *Nature*. (LA-UR-19-26179)

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.

Technical Outcomes

Phase transitions are defined through equilibrium properties of systems such as scaling of correlation length and time near the critical point where transitions occur. Renormalization theory classifies transitions into universality classes by these scalings. Our aim was to develop non-equilibrium theory for when transition happens at a finite rate. We have verified (both numerically and in the laboratory, in liquid crystal experiments) the Kibble-Zurek mechanism that uses equilibrium universality to make non-equilibrium predictions.

Publications

Journal Articles

Zurek, W. H. Quantum jumps, Born's rule, and objective classical reality via quantum Darwinism. Submitted to *Quantum jumps, Born's rule, and objective classical reality via quantum Darwinism*. (LA-UR-19-23643)

Zurek, W. H., M. M. Rams and J. P. Dziarmaga. Symmetry breaking bias in the dynamics of a quantum phase transition: a shortcut to adiabaticity?. Submitted to *Symmetry breaking bias in the dynamics of a quantum phase transition: a shortcut to adiabaticity?*. (LA-UR-19-23644)

Conference Papers

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

Presentation Slides

Bowlan, J. M., V. Zapf, R. L. Sandberg, S. Lin, B. A. Pound, C. S. Walker, C. Mazzoli, a. barbour, w. hu, s. wilkins, n. lee and j. c. young. Dynamics of Incommensurate Antiferromagnetic Domains with Coherent Soft X-ray Scattering. Presented at *APS March Meeting*, Boston, Massachusetts, United States, 2019-03-05 - 2019-03-05. (LA-UR-19-21818)

Posters

Bowlan, J. M., V. Zapf, R. L. Sandberg, B. Li, W. H. Zurek, C. Mazzoli, S. Wilkins and O. Lavrentovich. Universal Dynamics of Quenched Phase Transitions in Liquid Crystals and Antiferromagnets. Presented at *Non-equilibrium Dynamics of Condensed Matter in the Time Domain*, Kerkrade, Netherlands, 2018-09-03 - 2018-09-07. (LA-UR-18-28340)

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.

Technical Outcomes

Our study of covalently-introduced carbon nanotube (CNT) defect states has led to a fundamental understanding of their electronic structure and origins of defect-state photoluminescence. We have also established chemical control of defects for manipulation of energies and to facilitate integration with other materials. Finally, we have established CNTs as a tunable single photon source at telecom wavelengths and integrated them to functioning devices capable of photon indistinguishability for quantum information processing applications.

Publications

Journal Articles

*Danne, N., M. Kim, A. G. Godin, H. Kwon, Z. Gao, X. Wu, N. F. Hartmann, S. K. Doorn, B. Lounis, Y. Wang and L. Cognet. Ultrashort Carbon Nanotubes That Fluoresce Brightly in the Near-Infrared. 2018. *ACS Nano*. **12** (6): 6059-6065. (LA-UR-18-20557 DOI: 10.1021/acsnano.8b02307)

*Dervishi, E., Z. Ji, H. Htoon, M. Sykora and S. K. Doorn. Raman spectroscopy of bottom-up synthesized graphene quantum dots: size and structure dependence. 2019. *Nanoscale*. **11** (35): 16571-16581. (LA-UR-19-24729 DOI: 10.1039/C9NR05345J)

Doorn, S. K., S. Ozden, A. Saha, Y. Kim, K. Thurman, J. L. Blackburn and H. Htoon. Route to sp3 Functionalization of Polyfluorene Polymer-Wrapped Single-Wall Carbon Nanotubes. Submitted to *Journal of the American Chemical Society*. (LA-UR-19-26407)

*Gifford, B. J., A. E. Sifain, H. Htoon, S. K. Doorn, S. Kilina and S. Tretiak. Correction Scheme for Comparison of Computed and Experimental Optical Transition Energies in Functionalized Single-Walled Carbon Nanotubes. 2018. *The Journal of Physical Chemistry Letters*. **9** (10): 2460-2468. (LA-UR-18-21776 DOI: 10.1021/acs.jpclett.8b00653)

Gifford, B. J., A. Saha, B. M. Weight, X. He, G. Ao, M. Zheng, H. Htoon, S. Kilina, S. K. Doorn and S. Tretiak. Mod(n-m,3) Dependence of Defect-State Emission Bands in Aryl Functionalized Carbon Nanotubes. Submitted to *Nature Communications*. (LA-UR-19-26231)

*Gifford, B. J., S. Kilina, H. Htoon, S. K. Doorn and S. Tretiak. Exciton Localization and Optical Emission in Aryl-Functionalized Carbon Nanotubes. 2018. *The Journal of Physical Chemistry C*. **122** (3): 1828-1838. (LA-UR-17-28653 DOI: 10.1021/acs.jpcc.7b09558)

*Gifford, B. J., X. He, M. Kim, H. Kwon, A. Saha, A. E. Sifain, Y. Wang, H. Htoon, S. Kilina, S. K. Doorn and S. Tretiak. Optical Effects of Divalent Functionalization of Carbon Nanotubes. 2019. *Chemistry of Materials*. **31** (17): 6950-6961. (LA-UR-18-31887 DOI: 10.1021/acs.chemmater.9b01438)

Gifford, B. J. and S. Kilina. Contribution of Alkyl Side Chains to Chirality Sensitive Interactions between Single Walled Carbon Nanotubes and Polyfluorenes. Submitted to *Carbon*. (LA-UR-19-23831)

Hartmann, N. F., K. A. Velizhanin, E. H. Haroz, M. Kim, X. Ma, Y. Wang, H. Htoon and S. K. Doorn. Photoluminescence Dynamics of Aryl sp3 Defect States in Single-Walled Carbon Nanotubes. 2016. *ACS Nano*. **10** (9): 8355-8365. (LA-UR-17-24661 DOI: 10.1021/acsnano.6b02986)

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Luo, Y., X. He, Y. Kim, J. L. Blackburn, S. K. Doorn, H. Htoon and S. Strauf. Indistinguishable Single Photons at Telecom O-Band from sp3 Functionalized Carbon Nanotubes Coupled to Plasmonic Nanocavities. Submitted to *Science*. (LA-UR-19-21707)

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Presentation Slides

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Velizhanin, K. A. Final 2016 IC report for w15_cnanostruct. . (LA-UR-17-21066)

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Posters

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"Zero-Threshold Gain" and Continuous-Wave Lasing Using Charged Quantum Dots

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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.

Technical Outcomes

Colloidal semiconductor quantum dots are attractive materials for realizing highly flexible optical gain media, but are difficult to use in lasing due to multiexcitonic nature of optical gain leading to high lasing thresholds. Here we demonstrate that by combining compositional grading of quantum dots for impeding charged-exciton decay with post-synthetic photodoping for suppressing parasitic absorption, we can reduce the lasing threshold to unprecedented values of less than one exciton per dot on average.

Publications

Journal Articles

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Lim, J., Y. Park and V. I. Klimov. Optical gain in colloidal quantum dots achieved with direct-current electrical pumping. Submitted to *Nature Materials*. (LA-UR-19-29402)

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Singh, R., W. Liu, J. Lim, I. Robel and V. I. Klimov. Hot-Electron Dynamics in Quantum Dots Manipulated by Spin-Exchange Auger Interactions. Submitted to *Nature Physics*. (LA-UR-19-20385)

Wu, K., Y. 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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Presentation Slides

Klimov, V. I. Quantum Dot Lasing: From Prehistoric Times until Now. Presented at *5th\xc2\xa0International Workshop on Nanotechnology, Renewable Energy & Sustainability (Xian). Invited talks at Peking University, Beijing Institute of Technology, and Shanghai Jiaotong University*, Beijing, Xian, Shanghai, China, 2017-09-19 - 2017-09-19. (LA-UR-17-31370)

Posters

Kozlov, O. V., R. Singh, B. Ai, J. Zhang, C. Liu and V. I. Klimov. Transient Spectroscopy of Glass-Embedded Perovskite Quantum Dots: Novel Structures in an Old Wrapping. Presented at *Excited State Processes in Electronic and Bio Nanomaterials (ESP-2018)*, Santa Fe, New Mexico, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-24781)

Roh, J., J. Lim, Y. Park and V. I. Klimov. Nano-Patterning by Interferometric Lithography for Optoelectronic Devices. Presented at *Center for Advanced Solar Photophysics*

2017 Workshop, Los Alamos, New Mexico, United States, 2017-08-01 - 2017-08-04. (LA-UR-17-26610)

Hetero-Interfaces of Novel 2-Dimensional Dirac Semiconductors

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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 photovaltaics and other optoelectronic and energy efficient applications.

Technical Outcomes

Results of the project exceeded our expectations. We produced multi-layer TMD materials and performed characterization of excitons and spin characteristics using LANL's unique capabilities in 100T magnetic field and spin noise spectroscopy. We obtained detailed absorption spectrum of TMD excitons in strong magnetic field and in the absence of unwanted substrate effects. We also performed first successful measurements of valley noise and relaxation in monolayer TMD. Theory predicted a new effect called dynamic spin localization.

Publications

Journal Articles

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Reports

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Sinitsyn, N. Topological phases of quantum matter with decoherence. Unpublished report. (LA-UR-18-24545)

Presentation Slides

Crooker, S. A. Excitons, Electrons, & Holes in Atomically Thin 2D Semiconductors. Presented at *MCR 2017*, Los ALamos, New Mexico, United States, 2017-05-02 - 2017-05-02. (LA-UR-17-22703)

Sinitsyn, N. Origin of Decoherence. Presented at *LANL Fellows Prize Ceremony*, Los Alamos, New Mexico, United States, 2017-11-06 - 2017-11-06. (LA-UR-17-30127)

Posters

Crooker, S. A. Excitons, Electrons, & Holes in Atomically Thin 2D Semiconductors. Presented at *Materials Capability Review review 2017*, Los ALamos, New Mexico, United States, 2017-05-02 - 2017-05-02. (LA-UR-17-22702)

Chemical Approaches to Stable, Narrow-Bandgap Perovskite Materials

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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 onto 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.

Technical Outcomes

We focused on sulfide and selenide perovskite materials as it was anticipated that they would be more suited to visible light absorption than their oxide analogues and would be more stable than the more commonly studied lead-halide perovskite materials. Using complementary theoretical approaches, we narrowed down thousands of potential formulations to five that are predicted to have advantageous thermodynamic and photophysical properties and attempted synthesis via solid-state methodologies in order to verify the calculated properties.

Publications

Journal Articles

Gonzales, I., N. C. Smythe, J. C. Gordon and M. Sykora. Screening Sulfide and Selenide Perovskites as Stable Photovoltaic Materials. Submitted to *Chemistry of Materials*. (LA-UR-19-31076)

Posters

Sykora, M., S. K. Doorn and Z. Ji. Graphene Molecules: Synthesis, Electronic Structure and Potential in Applications. . (LA-CP-17-20163)

Quantum Molecular Dynamics of Strongly Correlated Materials

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Project Description

Molecular dynamics (MD) simulations have become a powerful and widely used predictive tool in computational materials science, chemistry and biology. MD is a 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.

Technical Outcomes

We achieved linear-scaling molecular dynamics with near-complete quantum accuracy. This was enabled by our development of new machine learning methodologies. Specifically, we have developed an active learning framework to collect quantum mechanical reference data, from which we train neural network models. We have applied this framework to study the molecular dynamics of a model with strong electron correlations, within the context of the Gutzwiller approximation. The method will generalize to other types of reference data.

Publications

Journal Articles

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Chern, G., K. M. Barros, Z. Wang, H. Suwa and C. D. Batista. Semiclassical dynamics of spin density waves. Submitted to *Physical Review B*. (LA-UR-18-31199)

*Chern, G. and K. Barros. Nonequilibrium dynamics of superconductivity in the attractive Hubbard model. 2019. *Physical Review B*. **99** (3): 035162. (LA-UR-18-31201 DOI: 10.1103/PhysRevB.99.035162)

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Hao, L., Z. Wang, J. Yang, D. Meyers, J. Sanchez, G. Fabbris, Y. Choi, J. Kim, D. Haskel, P. J. Ryan, K. M. Barros, J. Chu, M. P. M. Dean, C. D. Batista and J. Liu. Anomalous Magnetoresistance in an Antiferromagnetic Mott Semiconductor. Submitted to *Science*. (LA-UR-18-31200)

*Lubbers, N., J. S. Smith and K. Barros. Hierarchical modeling of molecular energies using a deep neural network. 2018. *The Journal of Chemical Physics*. **148** (24): 241715. (LA-UR-17-28890 DOI: 10.1063/1.5011181)

Samarakoon, A. M., K. M. Barros, Y. W. Li, M. Eisenbach, Q. Zhang, F. Ye, Z. L. Dun, H. Zhou, S. A. Grigera, C. D. Batista and A. D. Tennant. Machine Learning Assisted Insight to Spin Ice Dy2Ti2O7. Submitted to *Nature Communications*. (LA-UR-19-30738)

*Smith, J. S., B. T. Nebgen, R. Zubatyuk, N. Lubbers, C. Devereux, K. Barros, S. Tretiak, O. Isayev and A. E. Roitberg. Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. 2019. *Nature Communications*. **10** (1): 2903. (LA-UR-18-25687 DOI: 10.1038/s41467-019-10827-4)

Smith, J. S., R. Zubatyuk, B. T. Nebgen, N. E. Lubbers, K. M. Barros, A. E. Roitberg, O. Isayev and S. Tretiak. The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for organic molecules. Submitted to *Nature - Scientific Data*. (LA-UR-19-29769)

*Suwa, H., J. S. Smith, N. Lubbers, C. D. Batista, G. Chern and K. Barros. Machine learning for molecular dynamics with strongly correlated electrons. 2019. *Physical Review B*. **99** (16): 161107. (LA-UR-18-31198 DOI: 10.1103/PhysRevB.99.161107)

*Wang, Z., K. Barros, G. Chern, D. L. Maslov and C. D. Batista. Resistivity Minimum in Highly Frustrated Itinerant

Magnets. 2016. *Physical Review Letters*. **117** (20): 206601. (LA-UR-18-31202 DOI: 10.1103/PhysRevLett.117.206601)

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Presentation Slides

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Barros, K. M. Active Learning for Molecular Dynamics Potentials. Presented at *XXXI IUPAP Conference on Computational Physics*, Hong Kong, China, 2019-07-28 - 2019-08-01. (LA-UR-19-27187)

Smith, J. S., A. E. Sifain, S. Tretiak, B. T. Nebgen, N. E. Lubbers, L. A. Lystrom, K. M. Barros, O. Isayev, R. Zubatiuk, A. Roitberg, C. Devereux and K. Ranasinghe. Machine Learning for Molecular Properties. Presented at *Excited State Properties 2018*, Santa Fe, New Mexico, United States, 2018-06-03 - 2018-06-07. (LA-UR-18-24818)

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Smith, J. S., K. M. Barros, B. T. Nebgen, N. E. Lubbers and S. Tretiak. Opening the black box: the anatomy of a deep learning atomistic potential. Presented at *deep learning for science*, berkeley, California, United States, 2019-07-15 - 2019-07-19. (LA-UR-19-26488)

Smith, J. S., K. M. Barros, N. E. Lubbers, S. Tretiak, A. E. Sifain and B. T. Nebgen. Applications of ANI Deep Learning Potentials to General Computational Chemistry Problems. Presented at *255th American chemical society national meeting and exposition*, New orleans, Louisiana, United States, 2018-03-18 - 2018-03-22. (LA-UR-18-22212)

Smith, J. S., K. M. Barros, S. Tretiak, S. J. Fensin, N. Mathew, T. C. Germann, L. Burakovsky, B. T. Nebgen and N. E. Lubbers. The importance of sampling for machine learning potentials. Presented at *American Chemical Society Conference*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-28758)

Smith, J. S., N. E. Lubbers, K. M. Barros, B. T. Nebgen, S. Tretiak, T. C. Germann, S. J. Fensin, A. E. Roitberg, O. Isayev, r. zubatyuk, L. Burakovsky, C. Devereux, K. Ranashingha, H. Suwa, C. Batista and G. Chern. Accelerated modeling of atomistic physics with machine learning. Presented at *Machine Learning for Computational Fluid and Solid Dynamics*, Santa Fe, New Mexico, United States, 2019-02-19 - 2019-02-21. (LA-UR-19-21274)

Smith, J. S., S. Tretiak, K. M. Barros, B. T. Nebgen, N. E. Lubbers, S. J. Fensin, T. C. Germann, O. Isayev, r. zubatyuk, A. Roitberg, C. Devereux, K. Ranashingha, H. Suwa, C. Batista and G. W. Chern. Accelerated Modeling of Atomistic Physics with Machine Learning. Presented at *American Chemical Society*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22830)

Posters

Smith, J. S., K. M. Barros, S. Tretiak, N. Mathew, N. E. Lubbers and B. T. Nebgen. Atomistic Potentials for molecules and materials from machine learning. . (LA-UR-19-24846)

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.

Technical Outcomes

We investigated fundamental properties of quantum dynamics from the perspective of quantum information. Our analysis suggested that such information is compressible. We exemplified this compressibility in topological information crucial for topology based device engineering and quantum computing platforms, and proposed an experimental protocol for its dynamical extraction. We generalized these ideas to study quench dynamics of Dirac Materials, the result of which hints at potential dynamic control of entanglement switch and entanglement memory.

Publications

Journal Articles

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

Scalable Dielectric Technology for Very Low Frequency (VLF) Antennas

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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.

Technical Outcomes

After detailed simulations, the two most promising designs were selected and 1/1000 scale models working at 10-20 MHz were built and are being tested using protocols derived in consultation with a leading US VLF propagation expert. Based on the modeling work, it appears that two of the designs achieve a significant improvement in efficiency/size/complexity compared to current VLF technology. Though at an early stage, tests of the demonstrator antennas offer support for this view.

Materials Informatics for Actinide-Based 2D Materials

Alejandro Lopez-Bezanilla
20190636ER

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 research activities. This proposal is in line with the work supported by the Lab's Nuclear Deterrence and Energy Security mission areas as well as 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 more than 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.

Technical Outcomes

Principles of design to create dynamically stable transition metal, lanthanide, and actinide based low-dimensional borides were investigated. Applicable guidelines to predict physical stability of nanometer-thick covalent heterostructures were based on phonon spectra analysis. These borides exhibit promising features to integrate a new generation of two-dimensional materials.

Publications

Journal Articles

Lopez-Bezanilla, A. f-Orbital based Dirac states in a two-dimensional uranium compound. 2020. *Physical Review Research*. **3** (2): 024002. (LA-UR-19-25995 DOI: 10.1088/2515-7639/ab69af)

Lopez-Bezanilla, A. and P. B. Littlewood. The growing field of materials informatics: databases and artificial intelligence.. Submitted to *MRS Communications*. (LA-UR-19-28933)

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.

Publications

Journal Articles

*Lystrom, L., Y. Zhang, S. Tretiak and T. Nelson. Site-Specific Photodecomposition in Conjugated Energetic Materials. 2018. *The Journal of Physical Chemistry A*. **122** (29): 6055-6061. (LA-UR-18-24161 DOI: 10.1021/acs.jpca.8b04381)

Nelson, T. R., A. J. White, J. A. Bjorgaard, A. E. Sifain, Y. Zhang, B. T. Nebgen, S. Fernandez-Alberti, D. V. Mozyrsky, S. Tretiak and A. E. Roitberg. Non-adiabatic Excited State Molecular Dynamics: theory and applications for modeling photophysics in extended molecular materials. Submitted to *Chemical Reviews*. (LA-UR-19-25569)

Nelson, T. R., B. T. Nebgen, A. J. White, Y. Zhang, H. Song, J. A. Bjorgaard, A. E. Sifain, B. Rodriguez-Hernandez, V. M. Freixas, S. Fernandez-Alberti, A. Roitberg, W. F. I. Malone and S. Tretiak. NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-20-22362)

*Nelson, T. R., D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. F. Galindo, V. D. Kleiman, S. Fernandez-Alberti, A. E. Roitberg and S. Tretiak. Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. 2018. *Nature Communications*. **9** (1): 2316. (LA-UR-17-30143 DOI: 10.1038/s41467-018-04694-8)

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., S. Fernandez-Alberti, A. E. Roitberg and S. Tretiak. Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. 2017. *The Journal of Physical Chemistry Letters*. **8** (13): 3020-3031. (LA-UR-17-23765 DOI: 10.1021/acs.jpclett.7b00790)

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)

Zhang, Y., T. Nelson and S. Tretiak. Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. 2019. *Journal of Chemical Theory and Computation*. **151** (15): 154109. (LA-UR-19-24300 DOI: 10.1063/1.5116550)

Zhang, Y., T. R. Nelson and S. Tretiak. Non-Adiabatic Excited-State Molecular Dynamics for Open-Shell Systems. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-19-29917)

Reports

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

Presentation Slides

Nelson, T. R. 20180552ECR: Excited State Dynamics for Spin Systems. . (LA-UR-19-28487)

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.

Publications

Presentation Slides

Hollebon, P. J. and T. Sjostrom. High temperatures Density Functional Theory Calculations. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-22002)

Sjostrom, T. Hybrid Density Functional Theory: Combining Kohn-Sham and orbital-free DFT. Presented at *CECAM: Fundamentals of Density Functional Theory for T> 0 : Quantum meets Classical*, Lausanne, Switzerland, 2019-05-20 - 2019-05-23. (LA-UR-19-24617)

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

Journal Articles

*Piva, M. M., S. M. Thomas, Z. Fisk, J. -. X. Zhu, J. D. Thompson, P. G. Pagliuso and P. F. S. Rosa. Putative hybridization gap in CaMn2Bi2 under applied pressure. 2019. *Physical Review B*. **100** (4): 045108. (LA-UR-19-28476 DOI: 10.1103/PhysRevB.100.045108)

*S. Rosa, P. F., S. M. Thomas, F. F. Balakirev, E. D. Bauer, R. M. Fernandes, J. D. Thompson, F. Ronning and M. Jaime. Enhanced Hybridization Sets the Stage for Electronic Nematicity in CeRhIn5. 2019. *Physical Review Letters*. **122** (1): 016402. (LA-UR-18-30371 DOI: 10.1103/PhysRevLett.122.016402)

Ferrari Silveira Rosa, P., P. J. Robinson, M. E. Valentine, A. Granmoe, N. Drichko, J. R. Chamorro, T. M. McQueen and A. N. Alexandrova. Dynamical Bonding Driving Mixed Valency in a Metal Boride. Submitted to *Nature Materials*. (LA-UR-19-30421)

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

Journal Articles

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)

Conference Papers

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)

Reports

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

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

Presentation Slides

Brown, K. E. Picosecond to Nanosecond Spectroscopy of Shocked Reactive Materials. Presented at *Seminars at Cornell and Coe Colleges*, Mount Vernon, Iowa, United States, 2019-02-21 - 2019-02-21. (LA-UR-19-21400)

Brown, K. E. Probing the Chemistry of Shocked Energetic Materials at Picosecond to Nanosecond Timescales. Presented at *Invited seminar at University of Missouri*, Columbia, Missouri, United States, 2019-09-27 - 2019-09-27. (LA-UR-19-29634)

Moore, D. S. Dynamic compression induced chemistry. Presented at *Dynamic Compression Summer School*, Chicago, Illinois, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-26654)

Electronic Transport in Atomically Thin Materials at Far from Mechanical Equilibrium Conditions

Michael Pettes
20190516ECR

Project Description

Transition metal dichalcogenides (TMDs) are particularly sensitive to mechanical strain as they are capable of experiencing high strains without nucleating defects to release excess energy. As both the effective mass and optical phonon energies in these materials decrease with strain, and since the electron lifetime is inversely proportional to the phonon energy and occupation, an increase of electron mobility is hypothesized to occur with tensile elastic strain. This is significant as the drift velocity directly determines the switching speed in ultra-fast transistors as well as excitonic recombination dynamics in nano photonic devices. This research will address the fundamental question of how the variable of strain influences electronic performance in 2-dimensional materials, so that it can be fully accounted for in the design of next-generation nano electronic devices. Upon completion of this project, the PI will have established a globally unique in situ TEM-based structure-property characterization capability to quantify and correlate atomic-level strain experienced by a suspended nano material with electronic transport properties, a technique currently not possible and very relevant to structure-processing-property testing of other thin films including actinide-based materials required for advanced weapons and sensor applications.

Publications

Journal Articles

*Wei, W., C. K. Dass, J. R. Hendrickson, R. D. Montano, R. E. Fischer, Z. Xiaotian, T. H. Choudhury, J. M. Redwing, W. Yongqiang and M. T. Pettes. Locally defined quantum emission from epitaxial few-layer tungsten diselenide. 2019. *Applied Physics Letters*. **114** (21): 213102. (LA-UR-18-27142 DOI: 10.1063/1.5091779)

Presentation Slides

Pettes, M. T. Deterministic Defect Emission from Epitaxial TMD Thin Films. Presented at *2D Crystal Consortium-Materials Innovation Platform NSF Site Visit Year 4*, University Park, Pennsylvania, United States, 2019-05-21 - 2019-05-21. (LA-UR-19-24535)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. Presented at *Invited presentation to the UC Merced Mechanical Engineering Seminar Series*, Merced, California, United States, 2019-09-27 - 2019-09-27. (LA-UR-19-29644)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. . (LA-UR-19-30501)

Pettes, M. T. Deterministic Quantum Emission in an Epitaxial 2D Material. . (LA-UR-19-25907)

Pettes, M. T. Strain and Isotopic Effects in Two-Dimensional WSe2. . (LA-UR-19-27328)

Pettes, M. T. Strain and Defect Induced Phenomena in van der Waals Materials: WSe2 and Te. Presented at *Invited Seminar at Rice University Materials Science Department*, Houston, Texas, United States, 2020-01-16 - 2020-01-16. (LA-UR-20-20408)

Posters

Pettes, M. T. Intrinsic and Extrinsic Control over Physical Properties in a Representative Atomically Thin Semiconductor. Presented at *2019 National Academy of Engineering EU-US Frontiers of Engineering symposium*, Stockholm, Sweden, 2019-11-18 - 2019-11-20. (LA-UR-19-31073)

Pettes, M. T., A. Londono Calderon and D. J. Williams. Crystallographic Orientation of 1D & 2D Tellurium from 4D Scanning Transmission Electron Microscopy. . (LA-UR-19-32519)

Adaptive Framework for Enabling Real-time Feedback During Three-dimensional Mesoscale Microstructure Evolution Measurements

Reeju Pokharel
20190571ECR

Project Description

This project will develop a data analysis framework that will revolutionize experiments and data analysis at current and future light sources. This project will combine state-of-the-art measurement techniques, machine learning based data analysis tools, measurement informed mechanics simulations, and adaptive model independent optimization methods to enable real-time feedback during microstructure evolution studies at light sources. The ability to provide real-time feedback during a beam line experiment will be crucial for guiding experiments that can provide information that will be crucial for influencing predictive model development. The framework will maximize the productivity and impact of a beam time and will have broad programmatic and mission impacts. Results will also be of significant interest to the light source user community and numerous collaborations will emerge as an outcome.

Publications

Presentation Slides

R. Castillo, J. A. HEDM Reconstruction Problem. Presented at *Weekly meeting*, Los Alamos, New Mexico, United States, 2019-06-18 - 2019-06-18. (LA-UR-19-25507)

R. Castillo, J. A. Fourier Dictionary Approach for HEDM reconstruction. Presented at *weekly meeting with advisor*, Los Alamos, New Mexico, United States, 2019-07-23 - 2019-07-24. (LA-UR-19-27031)

Pokharel, R. Data analysis framework for enabling real-time feedback during microstructure evolution. Presented at *IMS Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-08. (LA-UR-19-23306)

Pokharel, R. 3D microstructure characterization using high-energy X-rays. Presented at *3D Summer School*, Pittsburgh, Pennsylvania, United States, 2019-08-19 - 2019-08-19. (LA-UR-19-28333)

Nonlinear Photonics of Topological Phase Transitions in the Graphene Family

Wilton Junior de Melo Kort-Kamp
20190574ECR

Project Description

Topology studies the properties of space that are preserved under continuous deformations. Distinct topologies are mathematically characterized by integers called topological invariants; topologically equivalent objects, such as a donut and a coffee cup, share the same invariant (the number of "holes"). An object undergoes a topological phase transition whenever an abrupt transformation changes the topological invariant. Over the past few decades, notions of topology have become ubiquitous in materials science, culminating in the 2016 Nobel Prizes in Physics and Chemistry. The topological nature of electronic states is a pivotal concept in various recent advances in low dimensional quantum systems. This project aims to investigate ultrafast nonlinear photonic phenomena in newly discovered two-dimensional materials of the graphene family supporting topological phase transitions. The project focuses on discovery and application of fundamental material properties for controlled functionality and performance prediction beyond the linear response regime, and it will significantly advance the country's initiatives in nanotechnology and nanophotonics. Investigations on the interplay between topological chiral edge states and nonreciprocal behavior arising from nonlinearities will unveil the potential of the graphene family materials as a reliable platform for information transport, with implications for quantum computing.

Publications

Journal Articles

Muniz, Y., A. Manjavacas, C. Farina, D. A. R. Dalvit and W. J. de Melo Kort-Kamp. Unraveling the decay mechanisms of two-quanta spontaneous photonic transitions. Submitted to *Nature Photonics*. (LA-UR-20-20456)

Presentation Slides

Malla, R. K. and W. J. de Melo Kort-Kamp. Nonlinear optical response of graphene family materials near topological phase transitions. Presented at *2020 APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-02. (LA-UR-20-21863)

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.

Technical Outcomes

To summarize, we have investigated the magnetic properties of heavy fermion materials. The results have been published in prestigious international scientific journals. Our work has gained lots of visibility as evidenced by several invited talks in international conferences. The new capability developed in this project will enable us to tackle more challenging problems in strongly correlated quantum materials and to seek funding opportunities in the near future.

Publications

Journal Articles

*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. W. Cai and B. Shen. Evolution of topological skyrmions across the spin reorientation transition in Pt/Co/Ta multilayers. 2018. *Physical Review B*. **97** (17): 174419. (LA-UR-18-24332 DOI: 10.1103/PhysRevB.97.174419)

*Kim, T., C. Chien and S. Lin. Reentrant Fulde-Ferrell-Larkin-Ovchinnikov state in small-sized superconductors. 2019. *Physical Review B*. **99** (5): 054509. (LA-UR-18-30667 DOI: 10.1103/PhysRevB.99.054509)

Li, S., Y. Su, Y. Ren and L. He. Realizing valley polarization and valley inversion in graphene by using a valley magnet. Submitted to *Science*. (LA-UR-19-21456)

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)

Su, Y., S. Hayami and S. Lin. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Submitted to *Nature Communications*. (LA-UR-19-25839)

Su, Y., S. Lin and S. Hayami. Anomalous charge transport in magnetic insulators with multiple-Q spin textures. Submitted to *Physical Review Letters*. (LA-UR-19-23218)

*Su, Y. and S. Lin. Nontrivial topology and localization in the double exchange model with possible applications to perovskite manganites. 2018. *Physical Review B*. **98** (23): 235116. (LA-UR-18-29965 DOI: 10.1103/PhysRevB.98.235116)

*Su, Y. and S. Lin. Pairing symmetry and spontaneous vortex-antivortex lattice in superconducting twisted-bilayer graphene: Bogoliubov-de Gennes approach. 2018. *Physical Review B*. **98** (19): 195101. (LA-UR-18-26090 DOI: 10.1103/PhysRevB.98.195101)

Reports

Lin, S. Annual reports for IC projects. Unpublished report. (LA-UR-18-21212)

Lin, S., S. M. Thomas and P. Ferrari Silveira Rosa. Design principles for skyrmions in f-electron materials. Unpublished report. (LA-UR-19-21423)

Presentation Slides

Lin, S. Annual Report on Numerical Study of Emergent magnetic particles in Rare earth magnets. . (LA-UR-19-22442)

Lin, S. Annual Report on Numerical simulations of magnetic and superconducting order in twisted bilayer graphene. . (LA-UR-19-21420)

Su, Y. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures. Presented at *Annual Conference on Magnetism and Magnetic Materials*, Las Vegas, Nevada, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31136)

Posters

Su, Y. and S. Lin. Switching of Valley Polarization by Electric Current in Twisted Bilayer Graphene. Presented at

2020 Theory Winter School: Quantum Matter Without Quasiparticles, Tallahassee, Florida, United States, 2020-01-06 - 2020-01-10. (LA-UR-20-20140)

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.

Technical Outcomes

With this 2-year Early Career Project we developed the technology and methods to increase the measurement resolution of both Photonic Doppler Velocimetry (PDV) and Broadband Laser Ranging (BLR). We successfully built and tested prototype systems, and published our results at a conference. We demonstrated an increase in the velocity resolution of PDV by a factor of 3x and the position resolution of BLR by 6x.

Publications

Presentation Slides

Azad, A. K. Metasurfaces Enable Flat Lenses. Presented at *Progress In Electromagnetics Research Symposium*, Singapore, Singapore, 2017-11-19 - 2017-11-19. (LA-UR-17-30712)

Briggs, M. E., A. Albert and P. Younk. Simultaneous Green and Infrared PDV. Presented at *2019 Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25399)

Younk, P. PDV at 532 nm. Presented at *Photonic Doppler Velocimetry Workshop*, Santa Fe, New Mexico, United States, 2018-05-16 - 2018-05-17. (LA-UR-18-24003)

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.

Technical Outcomes

This project focused on the synthesis and characterization of a variety of functional thin films materials for flexible electronic applications. Functional oxides have tremendous potential electronic and spintronic applications. However, these materials often exhibit poor mechanical properties and could change properties due to bending. This proposal investigated electric, optical and magnetic properties of oxide thin films under bending and developed new oxide/metal superlattice films for future flexible electronic devices.

Publications

Journal Articles

*Chen, A., Q. Su, H. Han, E. Enriquez and Q. Jia. Metal Oxide Nanocomposites: A Perspective from Strain, Defect, and Interface. 2019. *Advanced Materials*. **31** (4): 1803241. (LA-UR-18-28283 DOI: 10.1002/adma.201803241)

*Chen, A., Q. Su, H. Han, E. Enriquez and Q. Jia. Metal Oxide Nanocomposites: A Perspective from Strain, Defect, and Interface. 2019. *Advanced Materials*. **31** (4): 1803241. (LA-UR-19-29397 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*. **115** (32): 8119-8124. (LA-UR-18-28365 DOI: 10.1073/pnas.1805832115)

Lu, X., A. Chen, Y. DAI, B. Wei, H. Xu, J. Wen, N. Li, E. M. Enriquez, Z. Wang, P. C. Dowden, W. Yang, Y. Zhao and Q. Jia. Metallic interface induced by electronic reconstruction in crystalline-amorphous bilayer oxide films. Submitted to *Science Bulletin*. (LA-UR-19-29647)

*Wang, Q., A. P. Chen, E. J. Guo, M. A. Roldan, Q. X. Jia and M. R. Fitzsimmons. Upper limit for the effect of elastic bending stress on the saturation magnetization of. 2018. *Physical Review B*. **97** (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, C. You, A. Chen, C. Huang, L. Chen, M. Alexe and C. Jia. Flexible Quasi-Two-Dimensional CoFe O Epitaxial Thin Films for Continuous Strain Tuning of Magnetic Properties. 2017. *ACS Nano*. **11** (8): 8002-8009. (LA-UR-18-28697 DOI: 10.1021/acsnano.7b02637)

Presentation Slides

Chen, A. Energy Storage in Sn Doped Ba0.7Ca0.3TiO3-Ba(Zr0.2Ti0.8)O3(BCT-BZT)Thin Films. Presented at *The 6th International Workshop on Relaxor Ferroelectrics*, Vancouver, Canada, 2018-07-17 - 2018-07-17. (LA-UR-18-26743)

Chen, A. Controlling functionality via strain, defects and interface in epitaxial thin films. . (LA-UR-18-23204)

Chen, A. Anomalous Exchange Bias Induced by Hidden Interface in Oxide Heterostructures. Presented at *MRS 2019*, phoenix, Arizona, United States, 2019-04-22 - 2019-04-22. (LA-UR-19-23694)

Chen, A. Size Controlled Functionalities in Ferroic Nanocomposites. Presented at *Electronic Materials and Applications 2019(EMA 2019)*, Orlando, Florida, United States, 2019-01-23 - 2019-01-23. (LA-UR-19-20513)

Enriquez, E. M., P. C. Dowden, Q. Jia and A. Chen. Functional Thin Film Synthesis and Characterization at CINT. Presented at *CINT USERS MEETING*, SANTA FE, New Mexico, United States, 2017-09-25 - 2017-09-26. (LA-UR-17-28524)

Posters

Chen, A., E. M. Enriquez, P. C. Dowden, R. P. Prasankumar, D. A. Yarotski, A. J. Taylor, T. Lookman, J. Zhu, Q. Jia, J. L. MacManus-Driscoll and M. Fitzsimmons. Strain and Interfaces Enabled Multifunctionalities in Heteroepitaxial Thin Films. Presented at *LANL MCR 2018*, Los Alamos, New Mexico, United States, 2018-04-09 - 2018-04-11. (LA-UR-18-21888)

enriquez, E., Q. Li, P. R. Bowlan, P. Lu, B. Zhang, L. Li, H. WANG, B. P. Uberuaga, D. A. Yarotski, R. P. Prasankumar, S. V. Kalinin, Q. JIA and A. Chen. Controlled Functionalities in Vertical Nanocomposites via Strain and Defect Engineering. . (LA-UR-19-24312)

enriquez, e., H. Han, P. C. Dowden and A. Chen. Advanced Thin Film Synthesis and Functionality Design Capabilities at CINT. . (LA-UR-19-24301)

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.

Technical Outcomes

This project developed a new experimental capability that allows the use of strain gauges under pressure to measure the thermal expansion of materials of interest. The good performance of this project is evidenced by six manuscripts (three already published in prestigious journals and three to be submitted soon) as well as four oral presentations. This project not only impacts existing DOE/BES programs, but also has stimulated proposals that are relevant to the Laboratory's mission.

Publications

Journal Articles

*Jung, S., S. Seo, S. Lee, E. D. Bauer, H. Lee and T. Park. A peak in the critical current for quantum critical superconductors. 2018. *Nature Communications*. **9** (1): 434. (LA-UR-18-26340 DOI: 10.1038/s41467-018-02899-5)

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)

Seo, S., X. Wang, S. M. Thomas, M. C. Rahn, D. Carmo, F. Ronning, E. D. Bauer, R. D. dos Reis, M. Janoschek, J. D. Thompson, R. M. Fernandes and P. Ferrari Silveira Rosa. Nematic state in CeAuSb2. Submitted to *Physical Review X*. (LA-UR-19-27666)

Toward Controlled Synthesis of Actinide Oxide Nanocrystals: A Theoretical Perspective

Gaoxue Wang
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

Journal Articles

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. *Physical Chemistry Chemical Physics*. **20** (26): 17563-17573. (LA-UR-17-31042 DOI: 10.1039/C8CP00240A)

*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*. **2** (1): 17. (LA-UR-17-26824 DOI: 10.1038/s41699-018-0062-6)

Wang, G., P. Yang and E. R. Batista. Computational screening of 2D coatings for semiconducting photocathodes. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-29869)

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.

Technical Outcomes

We successfully measured the intrinsic relaxation times of electrons in these 2D semiconductors. Timescales of order 1 microsecond were determined, which is encouragingly long and suggests these materials as a viable basis for so-called "valleytronic" applications. This work was published in Science Advances.

Publications

Journal Articles

*Goryca, M., J. Li, A. V. Stier, T. Taniguchi, K. Watanabe, E. Courtade, S. Shree, C. Robert, B. Urbaszek, X. Marie and S. A. Crooker. Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields. 2019. *Nature Communications*. **10** (1): 4172. (LA-UR-19-23579 DOI: 10.1038/s41467-019-12180-y)

*Goryca, M., N. P. Wilson, P. Dey, X. Xu and S. A. Crooker. Detection of thermodynamic “valley noise” in monolayer semiconductors: Access to intrinsic valley relaxation time scales. 2019. *Science Advances*. **5** (3). (LA-UR-18-27841 DOI: 10.1126/sciadv.aau4899)

Presentation Slides

Goryca, M. M., A. Lopion, K. Nogajewski, M. Potemski and P. Kossacki. Temperature dependence of photoluminescence lifetimes of WSe2 monolayer. Presented at *APS March Meeting*, Los Angeles, Colorado, United States, 2018-03-04 - 2018-03-04. (LA-UR-18-21719)

Goryca, M. M., T. Kazimierczuk, M. Koperski, T. Smolenski, W. Pacuski, A. Golnik, P. Kossacki, P. Wojnar and G. Karczewski. Single magnetic ion in a quantum dot as a memory device. Presented at *XII Symposium of the Institute of Theoretical Physics, University of Warsaw*, Warsaq, Poland, 2017-12-08 - 2017-12-09. (LA-UR-18-22488)

Posters

Goryca, M. M. Detection of thermodynamic “valley noise” in monolayer semiconductors: access to intrinsic valley relaxation timescales. Presented at *46th Conference on the Physics and Chemistry of Surfaces and Interfaces (PCSI-46)*, Santa Fe, New Mexico, United States, 2019-01-13 - 2019-01-17. (LA-UR-19-20396)

Goryca, M. M., J. Li, A. V. Stier, E. Courtade, S. Shree, C. Robert, B. Urbaszek, X. Marie and S. A. Crooker. Revealing exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields.. Presented at *NSF site visit*, Tallahassee, Florida, United States, 2019-09-05 - 2019-09-05. (LA-UR-19-28676)

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

Journal Articles

*Chen, Y., M. L. Phipps, J. H. Werner, S. Chakraborty and J. S. Martinez. DNA Templated Metal Nanoclusters: From Emergent Properties to Unique Applications. 2018. *Accounts of Chemical Research*. **51** (11): 2756-2763. (LA-UR-18-25907 DOI: 10.1021/acs.accounts.8b00366)

Presentation Slides

Chen, Y. Pathogen lights: Fast-testing for food safety. . (LA-UR-19-23194)

Chen, Y. Pathogen Light: Fluorescent Probe for Rapid Foodborne Bacteria Detection. . (LA-UR-19-23193)

Chen, Y. and J. Martinez. NanoCluster Beacons: A Spotlight on DNA Targets. . (LA-UR-18-23524)

Accelerated Discovery of New Nanocomposites for Energy Applications

Aiping Chen
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.

Technical Outcomes

This project investigated the synthesis of oxide nanocomposites and explored their energy applications. Using the well-defined carbon dots (CDs) arrays loaded zeolitic imidazolate framework-8 anchored on ZnO 1D nanocomposites, significantly enhanced photoelectrochemical (PEC) water splitting properties were reported. In addition, we also explored the synthesis of SrTiO3:MgO nanocomposites. Via chemical etching, obtained novel STO nanostructures showed enhanced PEC properties. Simple extension of such strategies is expected to synthesize different oxide nanocomposites for energy applications.

Publications

Journal Articles

*Han, H., S. Kment, F. Karlicky, L. Wang, A. Naldoni, P. Schmuki and R. Zboril. Sb-Doped SnO2 Nanorods Underlayer Effect to the \xce\xb1-Fe2O3 Nanorods Sheathed with TiO2 for Enhanced Photoelectrochemical Water Splitting. 2018. *Small*. **14** (19): 1703860. (LA-UR-18-21360 DOI: 10.1002/smll.201703860)

Presentation Slides

Han, H. Morphological Control Effect of Hierarchical Heterostructure Fe2O3/TiO2 for Photoelectrochemical Water Splitting. Presented at *ECS conference 2018*, Seattle, Washington, United States, 2018-05-12 - 2018-05-12. (LA-UR-18-24154)

Han, H. The synthesis of one dimensional nanostructure for energy storage application. . (LA-UR-19-25579)

Excited State Dynamics for Photochemistry and Light-Matter Interactions

Yu Zhang
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.

Publications

Journal Articles

*Jiang, H. and Y. Zhang. Preferred states of open electronic systems. 2019. *Physics Letters A*. **383** (24): 2878-2882. (LA-UR-19-26160 DOI: 10.1016/j.physleta.2019.06.035)

*Lystrom, L., Y. Zhang, S. Tretiak and T. Nelson. Site-Specific Photodecomposition in Conjugated Energetic Materials. 2018. *The Journal of Physical Chemistry A*. **122** (29): 6055-6061. (LA-UR-18-24161 DOI: 10.1021/acs.jpca.8b04381)

Nelson, T. R., A. J. White, J. A. Bjorgaard, A. E. Sifain, Y. Zhang, B. T. Nebgen, S. Fernandez-Alberti, D. V. Mozyrsky, S. Tretiak and A. E. Roitberg. Non-adiabatic Excited State Molecular Dynamics: theory and applications for modeling photophysics in extended molecular materials. Submitted to *Chemical Reviews*. (LA-UR-19-25569)

*Wu, X., R. Wang, Y. Zhang, B. Song and C. Yam. Controllable Single-Molecule Light Emission by Selective Charge Injection in Scanning Tunneling Microscopy. 2019. *The Journal of Physical Chemistry C*. **123** (25): 15761-15768. (LA-UR-19-25118 DOI: 10.1021/acs.jpcc.9b02198)

*Zhang, Y., T. Nelson, S. Tretiak, H. Guo and G. C. Schatz. Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. 2018. *ACS Nano*. **12** (8): 8415-8422. (LA-UR-18-24121 DOI: 10.1021/acsnano.8b03830)

Zhang, Y., T. Nelson and S. Tretiak. Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. 2019. *Journal of Chemical Theory and Computation*. **151** (15): 154109. (LA-UR-19-24300 DOI: 10.1063/1.5116550)

Zhang, Y., T. R. Nelson and S. Tretiak. Non-Adiabatic Excited-State Molecular Dynamics for Open-Shell Systems. Submitted to *Journal of Chemical Theory and Computation*. (LA-UR-19-29917)

Conference Papers

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)

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)

Books/Chapters

Zhang, Y., T. R. Nelson and S. Tretiak. Atomistic Simulations of Plasmon Mediated Photochemistry. (LA-UR-19-22815)

Reports

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

Zhang, Y. and T. R. Nelson. Non-adiabatic Excited State Molecular Dynamics Modeling of Photochemistry and Polariton Chemistry. Unpublished report. (LA-UR-19-28554)

Presentation Slides

Zhang, Y. Non-Adiabatic Molecular Dynamics for Strong Light-Matter Interaction. Presented at *257th ACS National Meeting, Orlando 2019*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22862)

Zhang, Y. Plasmonic Hot-Carriers for Solar Energy Conversion & Photochemical Reactions. Presented at *META 2019, the 10th International Conference on Metamaterials, Photonic Crystals and Plasmonics*, Lisbon, Portugal, 2019-07-23 - 2019-07-23. (LA-UR-19-26864)

Zhang, Y. Theory and Modeling of Non-Equilibrium Electron Transport and Energy Conversion. . (LA-UR-19-25320)

Conformal Field Theories with the Bootstrap

Emil Mottola
20180709PRD1

Project Description

The ultimate goal of this project is to help the development of new materials with properties suitable for applications in high-performance electrical circuits and quantum computing. This pursuit is extremely relevant for national security, for it holds the promise of significant technological and computational advances. Through the theoretical study of newly discovered critical theories with promising properties, the project aims to provide a solid framework for further theoretical developments, and to guide the experimental effort for the development of new materials.

Publications

Journal Articles

Kousvos, S. and A. Stergiou. Bootstrapping Mixed Correlators in Three-Dimensional Cubic Theories II. Submitted to *SciPost*. (LA-UR-19-30978)

Lin, Y., D. Meltzer, S. Shao and A. Stergiou. Bounds on Triangle Anomalies in (3+1)d. Submitted to *Journal of High Energy Physics*. (LA-UR-19-30323)

Manenti, A., A. Vichi and A. Stergiou. Implications of ANEC for SCFTs in four dimensions. 2020. *Journal of High Energy Physics*. **2020**: 93. (LA-UR-19-25902 DOI: 10.1007/JHEP01(2020)093)

*Stergiou, A. Bootstrapping MN and tetragonal CFTs in three dimensions. 2019. *SciPost Physics*. **7** (1): 010. (LA-UR-19-25903 DOI: 10.21468/SciPostPhys.7.1.010)

*Stergiou, A. and S. Kousvos. Bootstrapping mixed correlators in three-dimensional cubic theories. 2019. *SciPost Physics*. **6** (3): 035. (LA-UR-19-25906 DOI: 10.21468/SciPostPhys.6.3.035)

*Stergiou, A. and S. Rychkov. General properties of multiscalar RG Flows in d=4−\xce\xb5. 2019. *SciPost Physics*. **6** (1): 008. (LA-UR-19-25904 DOI: 10.21468/SciPostPhys.6.1.008)

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.

Technical Outcomes

High temperature polymer electrolyte membrane fuel cells that operate above 100C without humidification offer advantages in enhanced catalytic activity and CO tolerance. However lack of ionomeric electrode binder for controlled, balanced proton conductivity and hydrophobicity have limited the performance of such membrane electrode assemblies. Through development of novel ion conducting electrode materials, high temperature polymer electrolyte membrane fuel cell power performance was doubled compared to current commercially available materials.

Publications

Journal Articles

Kim, Y. S., E. J. Park, A. S. S. Lee, D. P. Leonard, D. Li, J. Y. Jeon and C. S. Bae. How does a small structural change of anode ionomer make a big difference in alkaline membrane fuel cell performance?. Submitted to *Journal of Materials Chemistry A*. (LA-UR-20-21325)

*Langlois, D. A., A. S. Lee, N. Macauley, S. Maurya, M. E. Hawley, S. D. Yim and Y. S. Kim. A rejuvenation process to enhance the durability of low Pt loaded polymer electrolyte membrane fuel cells. 2018. *Journal of Power Sources*. **396**: 345-354. (LA-UR-17-30764 DOI: 10.1016/j.jpowsour.2018.06.013)

*Lee, A. S., Y. Choe, I. Matanovic and Y. S. Kim. The energetics of phosphoric acid interactions reveals a new acid loss mechanism. 2019. *Journal of Materials Chemistry A*. **7** (16): 9867-9876. (LA-UR-18-31799 DOI: 10.1039/C9TA01756A)

Maurya, S., A. S. Lee, D. Li, E. J. Park, D. P. Leonard, S. Noh, C. Bae and Y. S. Kim. On the origin of permanent performance loss of anion exchange membrane fuel cells: Electrochemical oxidation of phenyl group. 2019. *Journal of Power Sources*. **436**: 226866. (LA-UR-19-23575 DOI: 10.1016/j.jpowsour.2019.226866)

Posters

S. Lee, A. S., E. J. Park, S. Maurya, V. Atanasov, J. Kerres, H. Jia and Y. S. Kim. Towards Optimization of High Temperature PEMFC Performance with Phosphonated Ionomer Electrodes and Ion-Pair Coordinated Electrolytes. Presented at *Gordon Conference*, Providence, Rhode Island, United States, 2018-07-29 - 2018-08-03. (LA-UR-18-26900)

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

Journal Articles

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)

*Cai, S., J. Guo, V. A. Sidorov, Y. Zhou, H. Wang, G. Lin, X. Li, Y. Li, K. Yang, A. Li, Q. Wu, J. Hu, S. K. Kushwaha, R. J. Cava and L. Sun. Independence of topological surface state and bulk conductance in three-dimensional topological insulators. 2018. *npj Quantum Materials*. **3** (1): 62. (LA-UR-19-26035 DOI: 10.1038/s41535-018-0134-z)

*Cai, S., S. K. Kushwaha, J. Guo, V. A. Sidorov, C. Le, Y. Zhou, H. Wang, G. Lin, X. Li, Y. Li, K. Yang, A. Li, Q. Wu, J. Hu, R. J. Cava and L. Sun. Universal superconductivity phase diagram for pressurized tetradymite topological insulators. 2018. *Physical Review Materials*. **2** (11): 114203. (LA-UR-19-26036 DOI: 10.1103/PhysRevMaterials.2.114203)

Kushwaha, S. K., M. K. Chan, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning, P. Ferrari Silveira Rosa and N. Harrison. Magnetic field-tuned Fermi liquid in a Kondo insulator. 2019. *Physical Review X*. **10** (1): 5487. (LA-UR-19-25216 DOI: 10.1038/s41467-019-13421-w)

Ferrari Silveira Rosa, P., Y. Xu, S. K. Kushwaha, J. C. Souza, M. C. Rahn, L. S. Veiga, A. Bombardi, S. M. Thomas, M. Janoschek, E. D. Bauer, M. K. Chan, Z. Wang, J. D. Thompson, P. G. Pagliuso, N. Harrison, B. A. Bernevig and F. Ronning. Colossal magnetoresistance in a nonsymmorphic antiferromagnetic insulator. Submitted to *npj Quantum Materials*. (LA-UR-20-20098)

Presentation Slides

Kushwaha, S. K. Development and study of the novel topological quantum materials. Presented at *Invited Colloquium*, Kalamazoo, Michigan, United States, 2020-03-16 - 2020-03-17. (LA-UR-20-22457)

Kushwaha, S. K., M. K. Chan, N. Harrison, P. Ferrari Silveira Rosa, S. M. Thomas, E. D. Bauer, F. Ronning, J. Park and J. D. Thompson. Magnetic field induced Fermi liquid in a candidate topological Kondo insulator. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-22244)

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, E. D. Bauer, J. D. Thompson, J. Zhu, C. Cao, F. Ronning and N. Harrison. Insulator/metal transition in a Topological Kondo Insulator at 60 T. Presented at *NSF meeting*, Tallahassee, Florida, United States, 2018-11-14 - 2018-11-14. (LA-UR-18-30652)

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, E. D. Bauer, J. D. Thompson, J. Zhu, F. Ronning, N. Harrison and C. Chao. Transport and magnetic properties of correlated Ce3Bi4Pd3 at high magnetic fields. Presented at *APS March Meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-08. (LA-UR-19-23573)

Posters

Kushwaha, S. K., M. K. Chan, P. Ferrari Silveira Rosa, J. Park, S. M. Thomas, E. D. Bauer, J. D. Thompson, F. Ronning and N. Harrison. Field induced metallic state in Ce3Bi4Pd3 Correlated Kondo material. Presented at *CNLS 39th Annual Conference - Strongly Correlated Quantum Materials*, Santa Fe, New Mexico, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-23792)

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

Journal Articles

Gigax, J. G., A. J. Torrez, Q. Mcculloch, H. Kim, S. A. Maloy and N. Li. Sizing up mechanical testing: Comparison of microscale and mesoscale mechanical testing techniques on a FeCrAl tube assembly. Submitted to *Journal of Nuclear Materials*. (LA-UR-19-32551)

*Gigax, J. G., H. Vo, Q. McCulloch, M. 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. 2019. *Scripta Materialia*. **170**: 145-149. (LA-UR-19-21957 DOI: 10.1016/j.scriptamat.2019.05.004)

*Gigax, J. G., J. K. 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. 2019. *Journal of Materials Research*. **34** (9): 1574-1583. (LA-UR-19-21222 DOI: 10.1557/jmr.2019.104)

Gigax, J. G., O. El Atwani, Q. Mcculloch, B. Aytuna, M. Efe, S. J. Fensin, S. A. Maloy and N. Li. Micro- and mesoscale mechanical properties of an ultra-fine grained FeCrMnNi high entropy alloy produced by large strain machining. Submitted to *Scripta Materialia*. (LA-UR-19-29789)

Mcculloch, Q., J. G. Gigax and P. Hosemann. Femtosecond laser ablation for mesoscale specimen evaluation. Submitted to *JOM*. (LA-UR-19-27649)

Presentation Slides

Gigax, J. G., O. El Atwani, M. R. Chancey, J. K. S. Baldwin and S. A. Maloy. Nanomechanical Properties of Pristine and Heavy Ion Irradiation Nanocrystalline Tungsten. Presented at *TMS 2020*, San Diego, California, United States, 2020-02-23 - 2020-02-28. (LA-UR-20-21593)

Gigax, J. G., Q. Mcculloch, S. A. Maloy, P. Hosemann and N. Li. Femtosecond laser ablation techniques for mesoscale specimen analysis. Presented at *University of California Berkeley Mechanics Workshop*, Berkeley, California, United States, 2020-03-02 - 2020-03-03. (LA-UR-20-21927)

Posters

Gigax, J. G., O. El Atwani, Q. Mcculloch, B. Aytuna, M. Efe, S. J. Fensin, S. A. Maloy and N. Li. Micro- and mesoscale mechanical properties of an ultra-fine grained CrFeMnNi high entropy alloy produced by large strain machining. Presented at *TMS 202*, San Diego, California, United States, 2020-02-23 - 2020-02-28. (LA-UR-20-21399)

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).

Publications

Posters

Li, J. and J. Zhu. Probing Quantum Hall and Quantum Valley Hall Effect in Bilayer Graphene Nanostructures. Presented at *The 46th Conference on the Physics and Chemistry of Surfaces and Interfaces (PCSI-46)*, Santa Fe, Minnesota, United States, 2019-01-13 - 2019-01-17. (LA-UR-19-20395)

Doped Carbon Dots for Enhanced Fuel Cell Catalysis

Piotr Zelenay
20180754PRD4

Project Description

This project will use sonochemistry to develop carbon dots-based fuel cell catalysts. The work will focus on dual metallic/nonmetallic-doping as a way of imparting enhanced oxygen reduction reaction activity in carbon dots. This approach is directly aligned with the Laboratory's mission and goals in the area of energy security, and has potential for the development of a new research program at Los Alamos National Laboratory.

Publications

Journal Articles

Kumar, V. B. AS101-Loaded PLGA–PEG Nanoparticles for Autoimmune Regulation and Chemosensitization. 2019. *ACS Applied Bio Materials*. **2** (5): 2246-2251. (LA-UR-19-23090 DOI: 10.1021/acsabm.9b00200)

Books/Chapters

Kumar, V. B. Synthesis of Micro and Nanoparticles of Lignin. (LA-UR-19-23396)

Overcoming the Curse of Dimensionality to Predict Chemical Reactivity

Beth Lindquist
20180758PRD4

Project Description

This project aims to provide a critical component of an equation of state (EOS) that is typically missing from atomistic modeling. Such work will be directly applied to high explosives (HE) equation of state modeling. This can be used to understand many important issues confronting the stockpile, such as understanding and predicting the behavior and performance of HE. This will be critical for new formulations or aged HE materials.

Publications

Journal Articles

*Howard, M. P., R. B. Jadrich, B. A. Lindquist, F. Khabaz, R. T. Bonnecaze, D. J. Milliron and T. M. Truskett. Structure and phase behavior of polymer-linked colloidal gels. 2019. *Journal of Chemical Physics*. **151** (12): 124901. (LA-UR-19-26202 DOI: 10.1063/1.5119359)

Lindquist, B. A. Connecting Inverse Design with Experimentally Relevant Models. Submitted to *Journal of Physics: Conference Series*. (LA-UR-20-21571)

*Lindquist, B. A., R. B. Jadrich, M. P. Howard and T. M. Truskett. The role of pressure in inverse design for assembly. 2019. *The Journal of Chemical Physics*. **151** (10): 104104. (LA-UR-19-25001 DOI: 10.1063/1.5112766)

Sherman, Z. M., M. P. Howard, B. A. Lindquist, R. B. Jadrich and T. M. Truskett. Inverse methods for design of soft materials. Submitted to *Journal of Chemical Physics*. (LA-UR-20-20466)

Presentation Slides

Lindquist, B. A. Using Statistical Inference to Discover Interactions for Colloidal Self-Assembly. Presented at *Computational Data Science Approaches for Materials 2019 Conference*, Los Alamos, New Mexico, United States, 2019-04-08 - 2019-04-10. (LA-UR-19-23041)

Lindquist, B. A. Statistical Inference of Equilibrium Statistical Mechanical Models. Presented at *33rd Annual CSP Workshop: Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, Georgia, United States, 2020-02-17 - 2020-02-21. (LA-UR-20-21358)

Perovskite-type Metal-Organic Framework with Strong Magnetoelectric Coupling

Hsinhan Tsai
20190613PRD1

Project Description

The project ties closely with Laboratory mission-relevant projects to address challenges in national energy security. The obtained material can be potentially used in low energy consuming devices for information processing. The magnetic based materials offer unique physical properties where the magnetic-electric and optical properties are coupled together, which allows full control over these properties. The full control of these properties is acheived through external triggering, which offers possibility for greatly enhancing the information security.

Publications

Journal Articles

Kinigstein, E. D., H. Tsai, W. Nie, J. C. Blancon, K. G. Yager, K. Appavoo, J. Even, M. G. Kanatzidis, A. D. Mohite and M. Y. Sfeir. Edge States Drive Exciton Dissociation in Hot Cast Ruddlesden-Popper Lead Halide Perovskite Thin Films. Submitted to *ACS Nano*. (LA-UR-20-21239)

Liu, F., M. D. Yoho, H. Tsai, K. Fernando, J. T. Tisdale, S. Shrestha, J. K. S. Baldwin, A. Mohite, S. Tretiak, D. T. Vo and W. Nie. The Working Principle of Hybrid Perovskite Single Crystal Detector for Gamma-Ray Photon Counting. Submitted to *Nature Communications*. (LA-UR-19-25920)

Tsai, H., C. Liu, E. Kinigstein, M. Li, S. Tretiak, M. Cotlet, X. Ma, X. Zhang and W. Nie. The Origin for Bright Light Emitting Diodes Using 2D Layered Perovskites. Submitted to *Nature Communications*. (LA-UR-19-25919)

Tsai, H., E. Kinigstein, C. C. Stoumpos, L. Mao, O. Durand, S. Tretiak, P. M. Ajayan, M. Y. Sfeir, M. G. Kanatzidis, A. Mohite and W. Nie. Molecular design principles for Ruddlesden-Popper hybrid perovskites for bright light emission devices. Submitted to *Advanced Materials*. (LA-UR-19-20440)

Tsai, H., F. Liu, K. Fernando, B. L. Scott, S. Tretiak, D. T. Vo, J. Strzalka and W. Nie. Highly Sensitive, Self-powered Thin Film X-ray Detector Using 2D Layered Perovskite Diodes. Submitted to *Nature*. (LA-UR-19-22971)

Posters

Tsai, H., F. Liu, S. Shrestha, K. Fernando, S. Tretiak, B. L. Scott, D. T. Vo, J. Strzalka and W. Nie. Highly Sensitive, Self-powered Thin Film X-ray Detector Using Ruddlesden-Popper Phase Layered Perovskite Diodes. Presented at *LANL Post-Doc Research Day*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28484)

A Novel “Three-in-One” Metal Organic Framework-Based Platform For Nanoparticle Encapsulation and Organization

Jennifer Hollingsworth
20190620PRD1

Project Description

New and improved light-emitting, light-directing and light-transmitting materials are needed to support advanced technologies that underpin economic competitiveness, e.g., Information Science and Technology, as well as global security, e.g., via enabling new tools for improved Remote Sensing for Nuclear Nonproliferation and Counterproliferation, new materials for scintillation and radiation detection for Nuclear Nonproliferation and Counterproliferation, new strategies for Information Collection, Surveillance, and Reconnaissance, and new sensors/detectors for Chemical and Biological Weapons and Defense.

Publications

Presentation Slides

Dolgopolova, E. and J. A. Hollingsworth. Alternative plasmonic nanomaterials as building blocks for Purcell-enhanced emission in the infrared. Presented at *2020 Spring ACS National Meeting, COLL Virtual Technical Symposium*, Los Alamos, New Mexico, United States, 2020-03-22 - 2020-03-24. (LA-UR-20-22500)

Posters

Dolgopolova, E., J. S. Mohar, Y. Kim, G. Pilania, R. Bose, A. V. Malko, H. Htoon and J. A. Hollingsworth. Semiconductors Helping Semiconductors: Alternative Plasmonic Nanomaterials as Building Blocks for Purcell-enhanced Emission. Presented at *CINT Annual User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29475)

Novel X-ray Imaging to Unlock the Potential of Antiferromagnetic Materials

Vivien Zapf
20190623PRD2

Project Description

This research will help to develop techniques critical to understanding how materials structure at the nanometer scale controls its magnetic and electronic behavior. Understanding this critical information is key to unlocking the potential for new magnetic materials that could have broad impact in information systems technology (computers, cell phones, sensors, etc). Understanding how our information systems behave is critical to all aspects of our modern life including commerce and national security.

Publications

Posters

Burdet, N. G., A. V. Carr, J. M. Bowlan, K. M. Mertes, J. D. Nguyen, R. Tobey, X. Ding, S. Lin, C. S. Walker, B. A. Pound, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins , V. Zapf, C. Mazzoli and R. L. Sandberg. Towards spatially mapping domain dynamics in Antiferromagnetic materials with soft x-ray scattering at NSLS-II. Presented at *SLAC Users Meeting*, Standford, California, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-25092)

In Situ Mesoscale Response under Combined Pressure-Shear Dynamic Loading

Darby Luscher
20190639PRD2

Project Description

A combined experiment and theory approach will be developed to perform in situ measurements of materials under pressure-shear shock loading. This work will result in better understanding of the mesoscale material deformation mechanisms and a computational model for simulating the material response. This work directly addresses the national security challenges related to the dynamic behavior of materials. The ability to understand and simulate pressure-shear shock conditions in low symmetry materials will be immediately useful to the mission areas of Dynamic Mesoscale Materials Science and to Stockpile Stewardship.

Publications

Posters

Zuanetti, B., C. A. Bolme, K. J. Ramos and D. J. Luscher. Investigation of the Mesoscale Response of Anisotropic Crystals under Combined Pressure-Shear Dynamic Loading. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27842)

Synthesis of Platinum-Rare Earth Intermetallic Fuel Cell Catalysts

Jacob Spendelow
20190640PRD3

Project Description

The project seeks to develop improved fuel cell catalysts. Fuel cells are relevant and important to multiple Department of Energy missions related to energy security, as well as fuel cells for National Nuclear Security Administration-specific national security applications. If successful, we expect that catalysts developed through this project could have transformative impact on fuel cell technology, providing near-term as well as long-term benefits for energy security and national security applications.

Publications

Presentation Slides

Wang, C., D. Li, Y. S. Kim and J. S. Spendelow. Carbon Effect on the Synthesis and MEA Performances of L10 CoPt Intermetallic Catalysts. Presented at *236th Electrochemical Society Meeting*, Atlanta, Georgia, United States, 2019-10-13 - 2019-10-18. (LA-UR-19-30298)

Wang, C., Z. Qiao, V. B. Kumar, D. A. Cullen, D. Li, K. L. More, G. Wu, Y. S. Kim and J. S. Spendelow. Size-Controlled Synthesis of L10-CoPt Intermetallic Fuel Cell Catalysts on Nitrogen-Doped Mesoporous Graphitized Carbon Support. Presented at *237th Electrochemical Society Meeting*, Montreal, Canada, 2020-05-10 - 2020-05-15. (LA-UR-19-32027)

Ex Machina Hamiltonians for Next-Generation Molecular Simulations

Sergei Tretiak
20190642PRD3

Project Description

The project will apply advanced computer simulation methods to examine the molecular mechanisms underlying electrical and thermal conduction processes in emerging energy nanotechnologies with direct applications to sustainable energy initiatives. The two specific applications to be explored are electronic conduction in molecular nanodevices that operate at the human-machine interface and heat conduction in complex molecular devices. This proposal will advance the current understanding of molecular-level functionality in several energy nanotechnologies and could significantly impact DOE missions related to energy independence.

Publications

Journal Articles

Craven, G. T., N. E. Lubbers, K. M. Barros and S. Tretiak. Ex machina determination of structural correlation functions. Submitted to *Physical Review Letters*. (LA-UR-19-32446)

Designing New Ferroelectric Materials with Spin Crossover Transitions

Wanyi Nie
20190647PRD3

Project Description

The successful demonstration in this project will provide materials for quantum information processing and energy efficient device operation. It will provide new solution for enhancing the information security and energy security missions. Since we are expecting new physical principles in the new material systems, the outcome can lead to high impact results that push the quantum information processing forward under practical operational conditions.

The Optoelectronic Device Applications of 2-Dimensional Interlayer Moiré Excitons

Han Htoon
20190648PRD3

Project Description

Light emitting diodes (LEDs) and lasers lie at the heart of almost all modern technologies. They make high speed internet possible and can be found inside of your television set. This project aims toward developing a new class of ultra-compact and efficient light emitting diodes and lasers by exploiting a novel phenomenon called Moire inter-layer exciton emerged at the interface of two atomically thin semiconductor layers. The devices that could be as thin as 4 atomic layers, can be fabricated by simply stacking different type of atomically thin metallic (graphene) and semiconductor layers in a way similar to Lego blocks. They can also be integrated into existing Silicon-based electronic and photonic integrated circuits. This project therefore has a potential to revolutionize telecommunication, display and flexible electronic industries.

Exploration of Colossal Thermoelectric Power in 4f and 5f Topological Magnets

Filip Ronning
20190654PRD4

Project Description

This research project is well aligned with the Laboratory agenda on quantum information science. Topological materials are widely believed to provide a route to harnessing new functionality in quantum materials in the future. This research is designed to understand the origin of large topological effects in strongly correlated magnetic metals, which are particularly strong in actinide-based materials. The Berry curvature of a wavefunction creates an anomalous velocity, which produces large transverse voltages in topological materials. The large transverse voltage response has potential interest for spintronic applications, as well as developing fundamentally new states of matter. Here we will study how this large response varies as a function of alloying various actinide materials. This research will help elucidate the origin of large responses in materials, and hopefully demonstrate how to control their effects.

Publications

Journal Articles

Asaba, T., S. M. Thomas, M. T. Curtis, J. D. Thompson, E. D. Bauer and F. Ronning. Anomalous Hall Effect in Kagome Ferrimagnet GdMn6Sn6. Submitted to *Physical Review B*. (LA-UR-20-20100)

Hamann, D. M., S. P. Rudin, F. Ronning, T. Asaba, D. L. M. Cordova, P. Lu and D. C. Johnson. Emergent Structures and Properties in Interface Stabilized 2D-Layers. Submitted to *Science*. (LA-UR-19-31418)

Defect tolerant scintillators: Linking structure and performance via machine learning (ML)

Blas Uberuaga
20190656PRD4

Project Description

Nuclear processes are associated with the emission of high energy particles capable of ionizing atoms, and detecting this ionization enables the observation of the nuclear process itself and is critical for identifying nuclear materials. One such detection technique is the use of scintillators - materials that convert the energy deposited by incident radiation into visible or ultraviolet photons. However, this irradiation introduces damage in the material, lowering efficiency. This proposal aims to minimize the detrimental effect of defects by tailoring the chemistry of scintillator materials, allowing one to design defect tolerant scintillators that can absorb and nullify the adverse consequences of defects. This will be facilitated via atomistic calculations and machine learning (ML). This work will integrate first-principle calculations, experimental data and ML in line with the Materials Genome Initiative and the laboratory's Science of Signatures and Materials for the Future Science Pillars. Concomitantly, we will develop a fundamental understanding of the relationship between defects and the performance of scintillators which will be applicable to other optical materials as well. New defect-tolerant detector materials will enhance the mission-driven science at both current and future facilities and also impact other arenas such as global security, non-destructive testing and medical imaging.

Publications

Presentation Slides

Talapatra, A. A. A Machine-Learning based Hierarchical Screening Strategy to Expedite Search of Novel Scintillator Chemistries. Presented at *MRS Fall Meeting, 2019*, Boston, Massachusetts, United States, 2019-12-01 - 2019-12-06. (LA-UR-19-31946)

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.

Technical Outcomes

An ab initio molecular dynamics study of the oxide transport properties of newly discovered, efficient solid-oxide fuel cell membranes was undertaken to understand the mechanism for this and facilitate the design of similar membranes. The study could rule out certain mechanisms, but could not definitely identify the controlling features of these new materials. The interfacial properties of the composite structure were clearly of significance.

Publications

Journal Articles

*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*. **122** (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. Fluctuations of Kinetically Constrained States from Multinomial Probability Theory. Submitted to *Physical Review Letters*. (LA-UR-18-24746)

Francis, M. F., E. F. Holby and A. W. Richards. A first principles evaluation of the structure, stiffness, and low index traction curves of \xce\xb1U, UC, \xce\xb1UH3, and \xce\xb2UH3. Submitted to *Journal of Nuclear Materials*. (LA-UR-19-21867)

Presentation Slides

Francis, M. F. Microkinetic Rate Theory: Generalization, Application to Catalysis, Prospects as Basis for Continuum Rate Theory. Presented at *Energy Materials Nanotechnology*, Orlando,, Florida, United States, 2017-12-04 - 2017-12-08. (LA-UR-17-26606)

Francis, M. F. Microkinetic Rate Theory: Formalization, Current Limitations, a Possible Basis for Continuum Rate Theory. Presented at *Global Conference on Catalysis and Reaction Engineering*, Las Vegas, Nevada, United States, 2017-10-19 - 2017-10-21. (LA-UR-17-28693)

Francis, M. F. Probing Colossal Ion Conductivity Hypotheses: Structure and Operando Mechanism. Presented at *Electrochemical Society (ECS)*, Cancun, Mexico, 2018-10-02 - 2018-10-02. (LA-UR-18-29311)

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.

Technical Outcomes

This project developed, tested and understood the morphology and mechanical response of different tungsten material grades (including tungsten based nanocrystalline high entropy alloys, ultrafine tungsten, nanocrystalline tungsten, and tungsten alloys) to different extreme environments including heavy ion irradiation and low energy helium irradiation at RT and high temperature. The project included multiscale material response investigation and characterization and fundamental understanding of the materials responses through correlation of phenomena across different scales.

Publications

Journal Articles

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*. **7** (1): 1836. (LA-UR-17-30505 DOI: 10.1038/s41598-017-01744-x)

El Atwani, O., K. C. Unal, W. S. Cunningham, S. J. Fensin, J. Hinks, G. Greaves and S. A. Maloy. In-situ TEM/Implantation Investigation of Radiation Tolerance to Bubble Damage in Nanocrystalline Tungsten and Ultrafine Tungsten-TiC Alloy. Submitted to *Scripta Materialia*. (LA-UR-19-30601)

El Atwani, O., W. S. Cunningham, D. Perez, E. Martinez Saez, J. Trelewicz, M. Li and S. A. Maloy. Temperature Threshold for Preferential Bubble Formation on Grain Boundaries in Tungsten Under in-situ Helium Irradiation. Submitted to *Materials Research Letters*. (LA-UR-19-29529)

El Atwani, O., W. S. Cunningham, J. R. Trelewicz, M. Li, B. D. Wirth and S. A. Maloy. Revealing the Synergistic Effects of Sequential and Simultaneous Dual Beam Irradiations in Tungsten via In-situ TEM. Submitted to *Acta Materialia*. (LA-UR-19-30538)

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., J. M. Gentile, O. El-Atwani, C. N. Taylor, M. Efe, S. A. Maloy and J. R. Trelewicz. Softening due to Grain Boundary Cavity Formation and its Competition with Hardening in Helium Implanted Nanocrystalline Tungsten. 2018. *Scientific Reports*. **8** (1): 2897. (LA-UR-17-26895 DOI: 10.1038/s41598-018-20990-1)

*El-Atwani, O., C. N. Taylor, J. Frishkoff, W. Harlow, E. Esquivel, S. A. Maloy and M. L. Taheri. Thermal desorption spectroscopy of high fluence irradiated ultrafine and nanocrystalline tungsten: helium trapping and desorption correlated with morphology. 2018. *Nuclear Fusion*. **58** (1): 016020. (LA-UR-17-24924 DOI: 10.1088/1741-4326/aa86cf)

*El-Atwani, O., E. Aydogan, E. Esquivel, M. Efe, Y. Q. Wang and S. A. Maloy. Detailed transmission electron microscopy study on the mechanism of dislocation loop rafting in tungsten. 2018. *Acta Materialia*. **147**: 277-283. (LA-UR-17-27884 DOI: 10.1016/j.actamat.2018.01.003)

*El-Atwani, O., E. Esquivel, E. Aydogan, E. Martinez, J. K. Baldwin, M. Li, B. P. Uberuaga and S. A. Maloy. Unprecedented irradiation resistance of nanocrystalline tungsten with equiaxed nanocrystalline grains to dislocation loop accumulation. 2019. *Acta Materialia*. **165**: 118-128. (LA-UR-18-26832 DOI: 10.1016/j.actamat.2018.11.024)

*El-Atwani, O., E. Esquivel, M. Efe, E. Aydogan, Y. Q. Wang, E. Martinez and S. A. Maloy. 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*. **149**: 206-219. (LA-UR-17-31237 DOI: 10.1016/j.actamat.2018.02.035)

*El-Atwani, O., E. Martinez, E. Esquivel, M. Efe, C. Taylor, Y. Q. Wang, B. P. Uberuaga and S. A. Matoy. Does sink efficiency unequivocally characterize how grain boundaries impact radiation damage?. 2018. *Physical Review Materials*. **2** (11): 113604. (LA-UR-18-26334 DOI: 10.1103/PhysRevMaterials.2.113604)

*El-Atwani, O., J. A. 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*. **5** (5): 343-349. (LA-UR-16-28940 DOI: 10.1080/21663831.2017.1292326)

*El-Atwani, O., J. E. Nathaniel, A. C. Leff, B. R. Muntifering, J. K. Baldwin, K. Hattar and M. L. Taheri. The role of grain size in He bubble formation: Implications for swelling resistance. 2017. *Journal of Nuclear Materials*. **484**: 236-244. (LA-UR-17-31194 DOI: 10.1016/j.jnucmat.2016.12.003)

*El-Atwani, O., J. E. Nathaniel, A. C. Leff, J. K. Baldwin, K. Hattar and M. L. 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. Gigax, M. Chancey, J. K. S. Baldwin and S. A. Maloy. Nanomechanical properties of pristine and heavy ion irradiated nanocrystalline tungsten. 2019. *Scripta Materialia*. **166**: 159-163. (LA-UR-18-31796 DOI: 10.1016/j.scriptamat.2019.03.014)

*El-Atwani, O., N. Li, M. Li, A. Devaraj, J. K. S. Baldwin, M. M. Schneider, D. Sobieraj, J. S. Wrobel, D. Nguyen-Manh, S. A. Maloy and E. Martinez. Outstanding radiation resistance of tungsten-based high-entropy alloys. 2019. *Science Advances*. **5** (3). (LA-UR-18-27481 DOI: 10.1126/sciadv.aav2002)

*El-Atwani, O., N. Li, M. Li, A. Devaraj, J. K. S. Baldwin, M. M. Schneider, D. Sobieraj, J. S. Wrobel, D. Nguyen-Manh, S. A. Maloy and E. Martinez. Outstanding radiation resistance of tungsten-based high-entropy alloys. 2019. *Science Advances*. **5** (3): eaav2002. (LA-UR-19-29986 DOI: 10.1126/sciadv.aav2002)

*El-Atwani, O., W. S. Cunningham, E. Esquivel, M. Li, J. R. Trelewicz, B. P. Uberuaga and S. A. Maloy. In-situ irradiation tolerance investigation of high strength ultrafine tungsten-titanium carbide alloy. 2019. *Acta Materialia*. **164**: 547-559. (LA-UR-18-27540 DOI: 10.1016/j.actamat.2018.10.038)

Nathaniel, J. E., A. C. Lang, O. El-Atwani, P. K. Suri, J. K. Baldwin, M. A. Kirk, Y. Wang and M. L. Taheri. Toward high-throughput defect density quantification: A comparison of techniques for irradiated samples. 2019. *Ultramicroscopy*. **206**: 112820. (LA-UR-19-21178 DOI: 10.1016/j.ultramic.2019.112820)

Presentation Slides

El Atwani, O. Advanced multiscale material studies for future fusion power. . (LA-UR-18-24862)

El Atwani, O., E. Aydogan, E. V. Esquivel, J. K. S. Baldwin, E. Martinez Saez, S. A. Maloy and M. Li. Multiscale irradiation effects of tungsten based materials for nuclear power. Presented at *TMS-2018*, Phoenix, Arizona, United States, 2018-03-10 - 2018-03-10. (LA-UR-18-22198)

El Atwani, O., E. Martinez Saez, J. K. S. Baldwin, S. A. Maloy, M. Li and A. Devaraj. On the radiation tolerance of nanocrystalline tungsten materials. Presented at *Ion beam modification of materials (IBMM) 2018*, San Antonio, New Mexico, United States, 2018-06-24 - 2018-06-30. (LA-UR-18-25643)

El Atwani, O., E. Martinez Saez, Y. Wang, B. P. Uberuaga and S. A. Maloy. New Insights on Denuded Zone Formation in Polycrystalline Materials. Presented at *Ion Beam Modification of Materials (IBMM) 2018*, San Antonio, Texas, United States, 2018-06-24 - 2018-06-24. (LA-UR-18-25284)

El Atwani, O., E. V. Esquivel, S. A. Maloy, J. Weaver, N. Mara, J. Trelewicz and M. Efe. Mechanical Properties, Damage and Morphology Details of Nanocrystalline and Ultrafine Tungsten \xc2\xa0Exposed to Low Energy Helium and Heavy Ion Irradiation. Presented at *TMS-2018*, Phoenix, Arizona, United States, 2018-03-10 - 2018-03-10. (LA-UR-18-21865)

El Atwani, O., J. Gentile, C. Taylor, S. A. Maloy and J. Trelewicz. Detrimental Effects of Bubble-loaded Grain Boundaries in Nanocrystalline and Coarse-grained Tungsten via Nanoindentation. Presented at *24th Conference on Application of Accelerators in Research and Industry*, Fort worth, Texas, United States, 2016-10-30 - 2016-11-04. (LA-UR-16-28926)

El Atwani, O., S. A. Maloy, B. D. Wirth, W. S. Cunningham, J. R. Trelewicz, M. Li and W. Chen. Dual Beam Irradiation of Tungsten Materials: Synergistic Effects and Comparison with Sequential and Single Beam Irradiation. Presented at *TMS 2020 Annual Meeting and Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-21761)

El Atwani, O. and S. A. Maloy. Defect Evolution and Radiation Resistance of Advanced Fusion Materials Under Heavy Ion and Low Energy Helium Irradiation. Presented at *TMS 2020 Annual Meeting and Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-21759)

El Atwani, O. and S. A. Maloy. In Situ Transmission Electron Microscopy Characterization of Advanced Nuclear Materials During Single and Dual Beam Irradiation. Presented at *TMS 2020 Annual Meeting and Exhibition*, San Diego, California, United States, 2020-02-23 - 2020-02-23. (LA-UR-20-21760)

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.

Technical Outcomes

CVD growth of hybrid perovskites was explored. The postdoc, while in MPA-11, also investigated 3D-carbon nanotube solid networks and 3D-interconnected molybdenum carbide nanoflakes. During his brief period in MPA-CINT, he split his efforts between quantum-dot and carbon-nanotube projects. He worked toward synthesizing size/shape-controlled Au nanocrystals for assembly with emitters and targeting defect emission from metal-ligand interactions. Progress was made in both, with latter demonstrating promising single-emitter-photoluminescence. Doped-single-walled-carbon-nanotube efforts focused on improving the chemistry of emissive-defect-introduction.

Publications

Journal Articles

*Koizumi, R., S. Ozden, A. Samanta, 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*. **5** (6): 1701113. (LA-UR-17-27486 DOI: 10.1002/admi.201701113)

Owuor, P. S., O. 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. Galv\xc3\xa3o, C. S. Tiwary and P. M. Ajayan. Lightweight Hexagonal Boron Nitride Foam for CO2 Absorption. 2017. *ACS Nano*. **11** (9): 8944-8952. (LA-UR-18-26004 DOI: 10.1021/acsnano.7b03291)

*Owuor, P. S., T. Tsafack, H. Y. Hwang, O. 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. 2017. *ACS Nano*. **11** (1): 806-813. (LA-UR-18-26024 DOI: 10.1021/acsnano.6b07249)

*Ozden, S., I. G. MacWan, P. S. Owuor, S. Kosolwattana, P. A. S. Autreto, S. Silwal, R. Vajtai, C. S. Tiwary, A. D. Mohite, P. K. Patra and P. M. Ajayan. Bacteria as Bio-Template for 3D Carbon Nanotube Architectures. 2017. *Scientific Reports*. **7** (1): 9855. (LA-UR-17-21459 DOI: 10.1038/s41598-017-09692-2)

*Ozden, S., T. Tsafack, P. S. Owuor, Y. Li, A. S. Jalilov, R. Vajtai, C. S. Tiwary, J. Lou, J. M. Tour, A. D. Mohite and P. M. Ajayan. Chemically interconnected light-weight 3D-carbon nanotube solid network. 2017. *Carbon*. **119**: 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. 2018. *Advanced Materials Interfaces*. **5** (2): 1700657. (LA-UR-18-25996 DOI: 10.1002/admi.201700657)

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.

Technical Outcomes

This project provides a better theoretical understanding of the electronic states and magnetic states in various quantum materials, ranging from topological insulators to quantum spin liquids. The underlying studies address some fundamental issues, such as the nature of quantum phase transitions and quantum critical points. In addition, this project provides a strong theoretical support for the ongoing research of heavy fermion and actinide materials at Los Alamos National Laboratory.

Publications

Journal Articles

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. N. Sheng and K. Yang. Global phase diagram and quantum spin liquids in a spin-1/2 triangular antiferromagnet. 2017. *Physical Review B*. **96** (7): 075116. (LA-UR-17-23332 DOI: 10.1103/PhysRevB.96.075116)

*Huang, Z., W. Zhu, D. P. Arovas, J. Zhu and A. V. Balatsky. Invariance of Topological Indices Under Hilbert Space Truncation. 2018. *Physical Review Letters*. **120** (1): 016403. (LA-UR-17-24060 DOI: 10.1103/PhysRevLett.120.016403)

Ren, Y., W. Zhu, T. 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)

*Tian-Sheng, Z., W. Zhu and D. N. Sheng. Two-component quantum Hall effects in topological flat bands. 2017. *Physical Review B*. **95** (12): 125134. (LA-UR-17-20075 DOI: 10.1103/PhysRevB.95.125134)

*Wang, L., N. Chepiga, D. Ki, L. Li, F. Li, W. Zhu, Y. Kato, O. S. Ovchinnikova, F. Mila, I. Martin, D. Mandrus and A. F. Morpurgo. Controlling the Topological Sector of Magnetic Solitons in Exfoliated Cr1/3NbS2 Crystals. 2017. *Physical Review Letters*. **118** (25): 257203. (LA-UR-17-22951 DOI: 10.1103/PhysRevLett.118.257203)

*Wang, Z., A. E. Feiguin, W. Zhu, O. A. Starykh, A. V. Chubukov and C. D. Batista. Chiral liquid phase of simple quantum magnets. 2017. *Physical Review B*. **96** (18): 184409. (LA-UR-17-22905 DOI: 10.1103/PhysRevB.96.184409)

*Zhang, S., W. Zhu and C. D. Batista. Pairing from strong repulsion in triangular lattice Hubbard model. 2018. *Physical Review B*. **97** (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. 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 in the \xce\xbd=5/2 Fractional Quantum Hall Effect. 2019.

Physical Review Letters. **123** (5): 056804. (LA-UR-18-28368 DOI: 10.1103/PhysRevLett.123.056804)

Zhu, W. and J. Zhu. Local quantum criticality of a one-dimensional Kondo insulator model. 2018. *Physical Review B*. **97** (24): 245119. (LA-UR-18-20364 DOI: 10.1103/PhysRevB.97.245119)

Presentation Slides

Zhu, W. Detection of Topological Phases and related Transitions via High Harmonic Generation. Presented at *Emergent Topological Orders in Classical Systems*, Santa Fe, New Mexico, United States, 2018-08-20 - 2018-08-23. (LA-UR-18-27883)

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.

Technical Outcomes

We demonstrated that Resonant Inelastic X-ray Scattering could probe the low energy electronic structure of intermediate valence compounds. It highlighted a deficiency of the current state-of-the-art electronic structure calculations done by dynamical mean field theory.

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.

Technical Outcomes

The postdoctoral fellow has successfully accomplished the research as proposed. The work conducted during the project addressed two distinct sub-projects: 1) Theoretical design of novel electronic functionalities of two-dimensional materials. Here studies have suggested a new family of 2D double-metal-layered carbides with unique interlayer-decoupled optoelectronic properties; and 2) Modeling of charge dynamics and polarons in halide perovskites. Here detailed properties of polaronic states were determined and compared to experimental data.

Publications

Journal Articles

*Li, W., L. Zhou, O. V. Prezhdo and A. V. Akimov. Spin–Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. 2018. *ACS Energy Letters*. **3** (9): 2159-2166. (LA-UR-18-26702 DOI: 10.1021/acsenergylett.8b01226)

Liu, J., Y. Li, Y. Xuan, L. Zhou, H. Lin, Q. Zhang, S. Tretiak, H. Wang, Y. Gu, Z. Guo, L. Wang, L. Wang and S. Feng. Exploiting multifunctional cellulose nanocrystals as high efficiency immobilizer for long-life Li-S batteries. Submitted to *Angewandte Chemie - International Edition*. (LA-UR-19-23417)

*Sun, Y., Z. Zhou, Z. Huang, 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. 2019. *Advanced Materials*. **31** (17): 1806562. (LA-UR-18-31375 DOI: 10.1002/adma.201806562)

*Zhang, J., J. Zhang, L. Zhou, C. Cheng, C. Lian, 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*. **57** (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*. **3** (4): 787-793. (LA-UR-18-20635 DOI: 10.1021/acsenergylett.8b00166)

Zhou, L., C. Katan, W. Nie, H. Tsai, L. Pedesseau, J. J. Crochet, J. Even, A. Mohite, S. Tretiak and A. J. Neukirch. Cation Alloying Destabilizes Polarons in Lead-halide Perovskites. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-20075)

Zhou, L., Y. Zhang, Z. Zhuo, A. J. Neukirch and S. Tretiak. Interlayer-decoupled Sc-based Mxene with High Carrier Mobility and Strong Light-harvesting Ability. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-24534)

Presentation Slides

Zhou, L. Computational Design and Modeling on Optoelectronic (Nano) devices. . (LA-UR-18-23124)

Zhou, L. Promises for photocatlysis and light-harvesting in transition-metal based 2D material. Presented at *Telluride workshop "Electronic and Structural Dynamics in Hybrid Perovskites: Theory Meets Experiment"*, Telluride, Colorado, United States, 2018-07-17 - 2018-07-21. (LA-UR-18-26615)

Zhou, L., A. J. Neukirch, C. Katan, J. Even and S. Tretiak. Tuning the Polaronic Properties of Lead Halide Perovskites by Mixing Cation. Presented at *APS March Meeting 2018*,

Los Angeles, California, United States, 2018-03-05 - 2018-03-09. (LA-UR-18-21687)

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.

Technical Outcomes

We have developed robust experimental methods to arrange photonic nanoparticles within block copolymer nanostructures, dramatically increasing the morphological uniformity of the nanoparticle-copolymer composites. We have also developed and experimentally verified machine learning strategies for design of a second photonic materials templated by a biopolymer: DNA-stabilized silver clusters. These methods learn from experimental observations to enable informed design of silver clusters with desired optical properties, and our methods are directly applicable to other materials systems.

Publications

Journal Articles

*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. 2019. *ACS Nano*. **12** (8): 8240-8247. (LA-UR-18-29957 DOI: 10.1021/acsnano.8b03404)

Copp, S. M., S. M. Swasey, A. Gorovits, P. Bogdanov and E. G. Gwinn. Towards Universal Machine Learning-Aided Design of DNA-Stabilized Silver Clusters. Submitted to *Chemistry of Materials*. (LA-UR-19-24854)

*Swasey, S. M., S. M. Copp, H. C. Nicholson, A. Gorovits, P. Bogdanov and E. G. Gwinn. High throughput near infrared screening discovers DNA-templated silver clusters with peak fluorescence beyond 950 nm. 2018. *Nanoscale*. **10** (42): 19701-19705. (LA-UR-18-29958 DOI: 10.1039/C8NR05781H)

Conference Papers

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)

Posters

Copp, S. M., A. Gorovits, S. Swasey, S. A. Ivanov, P. Bogdanov and E. G. Gwinn. Machine learning-aided design of soft photonic materials. Presented at *2018 CINT User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-28913)

Hamblin, R. L. Characterization Techniques for Nanoscale Structures of Soft Matter. Presented at *LANL Student Symposium 2018*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-26449)

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.

Technical Outcomes

Using multiscale modeling approaches, this project examined multiple aspects associated with mass transport in materials relevant for nuclear energy systems, focused on the context of corrosion of those materials. These included the effects of electrical charge on the transport of radiation induced defects in ionic materials and the transport of hydrogen and oxygen in complex metal alloys. These results provide new insights into the evolution of these materials in a nuclear environment.

Publications

Journal Articles

*Samin, A. J. A review of radiation-induced demagnetization of permanent magnets. 2018. *Journal of Nuclear Materials*. **503**: 42-55. (LA-UR-18-28395 DOI: 10.1016/j.jnucmat.2018.02.029)

*Samin, A. J., D. A. Andersson, E. F. Holby and B. P. Uberuaga. On the role of electro-migration in the evolution of radiation damage in nanostructured ionic materials. 2018. *Electrochemistry Communications*. **96**: 47-52. (LA-UR-18-25848 DOI: 10.1016/j.elecom.2018.09.010)

*Samin, A. J., D. A. Andersson, E. F. Holby and B. P. Uberuaga. First-principles localized cluster expansion study of the kinetics of hydrogen diffusion in homogeneous and heterogeneous Fe-Cr alloys. 2019. *Physical Review B*. **99** (1): 014110. (LA-UR-19-21216 DOI: 10.1103/PhysRevB.99.014110)

*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. *Journal of The Electrochemical Society*. **165** (7): C302-C309. (LA-UR-18-28387 DOI: 10.1149/2.0031807jes)

Presentation Slides

Uberuaga, B. P. Highlights performed on LANL IC on the project w17_amdoxides. . (LA-UR-19-21674)

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.

Technical Outcomes

In this project, we developed an ultrafast white-light microscopy system and used it to study a variety of phenomena, including carrier dynamics in metal nanoparticles, polarization-dependent exciton dynamics in group-VII TMDs, and exciton diffusion in lateral 2D-TMD heterostructures. Our work contributes to the use of 2D-TMDs as building blocks in “ultra-high” speed optoelectronic systems, while also expands our knowledge of low-dimensional quantum systems, revealing new phenomena unique to anisotropic 2D excitons.

Publications

Journal Articles

Sim, S., A. Bierle, P. Mantos, S. McCrory, R. P. Prasankumar and S. Chowdhury. Ultrafast relaxation dynamics in bimetallic plasmonic catalysts. Submitted to *Nanoscale*. (LA-UR-20-20520)

Sim, S., D. Lee, J. Lee, M. Cha, S. Cha, H. Bae, S. Cho, W. Shim, K. Lee, J. Yoo, R. P. Prasankumar, H. Choi and M. Jo. Layer-number-dependent ultrafast exciton-exciton interaction in mono-, bi-, and tri-layer ReS2. Submitted to *ACS Photonics*. (LA-UR-20-20522)

Presentation Slides

Sim, S. Ultrafast dynamics of excitons and spin carriers in 2D semiconductors and 3D Rashba materials. . (LA-UR-18-29033)

Posters

Sim, S. Ultrafast dynamics of excitons and spin carriers in 2D semiconductors and 3D Rashba materials. Presented at *CINT user meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-24. (LA-UR-18-28862)

Nuclear and Particle Futures

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

Journal Articles

*Alvis, S. I., I. J. Arnquist, F. T. I. Avignone, A. S. Barabash, C. J. Barton, V. Basu, F. E. Bertrand, B. Bos, V. Brudanin, M. Busch, M. Buuck, T. S. Caldwell, Y. Chan, C. D. Christofferson, P. Chu, C. Cuesta, J. A. Detwiler, Y. Efremenko, H. Ejiri, S. R. Elliott, T. Gilliss, G. K. Giovanetti, M. P. Green, J. Gruszko, I. S. Guinn, V. E. Guiseppe, C. R. Haufe, R. J. Hegedus, L. Hehn, R. Henning, D. H. Aguilar, E. W. Hoppe, M. A. Howe, K. J. Keeter, M. F. Kidd, S. I. Konovalov, R. T. Kouzes, A. M. Lopez, R. D. Martin, R. Massarczyk, S. J. Meijer, S. Mertens, J. Myslik, G. Othman, W. Pettus, A. Piliounis, A. W. P. Poon, D. C. Radford, J. Rager, A. L. Reine, K. Rielage, N. W. Ruof, B. Shanks, M. Shirchenko, D. Tedeschi, R. L. Varner, S. Vasilyev, B. R. White, J. F. Wilkerson, C. Wiseman, W. Xu, E. Yakushev, C. Yu, V. Yumatov, I. Zhitnikov and B. X. Zhu. Search for trinucleon decay in the Majorana Demonstrator. 2019. *Physical Review D*. **99** (7): 072004. (LA-UR-18-31257 DOI: 10.1103/PhysRevD.99.072004)

*I. Avignone, F. T. and S. R. Elliott. The Search for Double Beta Decay With Germanium Detectors: Past, Present, and Future. 2019. *Frontiers in Physics*. **7**: 6. (LA-UR-18-30325 DOI: 10.3389/fphy.2019.00006)

Chu, P., S. R. Elliott, I. w. Kim, R. Massarczyk, S. J. Meijer, K. R. Rielage, B. White, X. B. Zhu and M. J. Stortini. ADC Nonlinearity Correction for the Majorana Demonstrator. Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-20-21663)

Elliott, S. R., P. Chu, B. White, K. R. Rielage, R. Massarczyk and X. B. Zhu. A Search for Neutrinoless Double-Beta Decay in 76Ge 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, X. B. Zhu and B. White. Multi-site event discrimination for the Majorana Demonstrator. Submitted to *Physical Review C*. (LA-UR-19-20305)

Gupta, R., Y. Jang, T. Bhattacharya and B. Yoon. Axial Vector Form Factors from Lattice QCD that Satisfy the PCAC Relation. Submitted to *Physics Letters. Section B: Nuclear, Elementary Particle and High-Energy Physics*. (LA-UR-19-29302)

Mereghetti, E., V. Cirigliano, W. G. Dekens, J. de Vries, M. L. Graesser, S. Pastore, M. Piarulli, U. Van Kolck and R. B. Wiringa. A renormalized approach to neutrinoless double beta decay. Submitted to *Physical Review C*. (LA-UR-19-26002)

Wang, X. B., A. C. Hayes, J. Carlson, G. X. Dong, E. Mereghetti, S. Pastore and R. B. Wiringa. Comparison between variational Monte Carlo and shell model calculations of neutrinoless double beta decay matrix elements in light nuclei. 2019. *Physics Letters B*. **798**: 134974. (LA-UR-19-25587 DOI: 10.1016/j.physletb.2019.134974)

Conference Papers

Gupta, R., S. Park, T. Bhattacharya, Y. Jang, J. Bailey, B. Choi, H. Jeong, S. Jwa, S. Lee, W. Lee, J. Pak and J. Leem. Update on B \xe2\x86\x92 D\xe2\x88\x97l\xce\xbd form factor at zero-recoil using the Oktay-Kronfeld action. Presented at *The 36th Annual International Symposium on Lattice Field Theory - LATTICE2018*. (East Lansing, Michigan, United States, 2018-07-22 - 2018-07-28). (LA-UR-19-20196)

Presentation Slides

Elliott, S. R. Future of Double Beta Decay. Presented at *3rd Conference on Science at the Sanford Underground Research Facility*, Rapid City, South Dakota, United States, 2019-05-15 - 2019-05-17. (LA-UR-19-24356)

Elliott, S. R. LEGEND: The Large Enriched Germanium Experiment for Neutrinoless Double-Beta Decay. Presented at *APS April Meeting*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23033)

Elliott, S. R. Future Double Beta Experiments. Presented at *Heraeus Seminat*, Bad Honnef, Germany, 2019-07-08 - 2019-07-11. (LA-UR-19-26621)

Elliott, S. R. LEGEND. Presented at *SNOLAB Future Projects Workshop*, Sudbury, Canada, 2019-07-15 - 2019-07-17. (LA-UR-19-26849)

Massarczyk, R. The Large Enriched Germanium Experiment for Neutrinoless \xce\xb2\xce\xb2 Decay. Presented at *Neutrino 2018 - XXVIII International Conference on Neutrino Physics and Astrophysics*, Heidelberg, Germany, 2018-06-04 - 2018-06-09. (LA-UR-18-24464)

Massarczyk, R. LEGEND. Presented at *"Double beta decay and underground science" (DBD18)"*, Hawaii Island, Hawaii, United States, 2018-10-21 - 2018-10-21. (LA-UR-18-29731)

Massarczyk, R. From MAJORANA to LEGEND. Presented at *Neutrino Nuclear Responses 2019 (NNR19) for Double Beta Decays and Astro Neutrinos*, Osaka, Japan, 2019-05-08 - 2019-05-08. (LA-UR-19-24026)

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

Journal Articles

Li, H. Signatures of Alfv \xcc\x81en-mode and Slow-mode Waves and Non-Propagating Structures in 3D Compressive MHD Turbulence. Submitted to *Astrophysical Journal*. (LA-UR-18-30429)

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Rasmus, A. M. Shock driven discrete vortex growth on oblique interfaces. Unpublished report. (LA-UR-18-26572)

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Barnak, D. H., K. A. Flippo, C. Y. Fiedler Kawaguchi, K. V. Kelso, H. Li, S. Li, E. N. Loomis, Y. Lu, N. N. Vazirani, A. Birkel, B. Lahmann and C. Li. Impact of self-generated B-fields on HED experiments. Presented at *49th Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-10 - 2019-06-14. (LA-UR-19-25392)

Barnak, D. H., K. A. Flippo, C. Y. Fiedler Kawaguchi, K. V. Kelso, H. Li, S. Li, E. N. Loomis, Y. Lu, N. N. Vazirani, A. Birkel, B. Lahmann and C. Li. Impact of self-generated B-fields on HED experiments. Presented at *61st American Physical Society Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30709)

Flippo, K. A. Shock-driven magnetic field generation in ICF relevant plasmas. Presented at *Kinetic Effects in ICF Workshop*, Santa Fe, New Mexico, United States, 2018-05-22 - 2018-05-25. (LA-UR-18-24503)

Flippo, K. A. High Energy Density Hydrodynamics and ICF Experiments at Los Alamos National Lab. . (LA-UR-19-26212)

Flippo, K. A., A. M. Rasmus, C. Y. Fiedler Kawaguchi, B. J. Tobias, T. Desjardins, E. C. Merritt, C. Di Stefano, F. W. Doss, S. Palaniyappan, J. P. Sauppe, T. N. Archuleta, R. P. Gonzales, V. A. Garcia, D. W. Schmidt, A. Strickland, D. H. Barnak and C. C. Kuranz. Developing New X-ray Diagnostic Methods for HED Hydrodynamic Experiments. Presented at *61st American Physical Society Division of Plasma Physics Meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30706)

Flippo, K. A., H. Li, B. J. Albright, A. S. Liao, S. Li, Y. Lu, D. H. Barnak, A. M. Rasmus, C. Y. Fiedler Kawaguchi, K. V. Kelso, T. Weber, E. N. Loomis, Y. H. Kim, T. J. Murphy, A. Zylstra, C. C. Kuranz, S. R. Klein, A. Angulo, J. Levesque, C. Li and P. Tzeferacos. Self-Generated Magnetic Fields in High Energy Density Laboratory Experiments. Presented at *American Physical Society Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30589)

Li, H. Turbulent Dynamo Modeling and Experiments. . (LA-UR-18-30403)

Li, H. Energy Evolution and Particle Energization in Different Turbulent Environments. . (LA-UR-18-30384)

Li, H. Modeling and Experiments of Turbulent Flows with Applications to Astrophysics and Space Physics. . (LA-UR-18-30383)

Li, H. Dynamics of Dust-Gas Interactions in Protoplanetary Disks and Implications for Planetesimal Formation. . (LA-UR-18-30388)

Li, S. Understanding Asymmetry Formation in Dusty Proto-Planetary Disks with Dust-Growth Model. . (LA-UR-19-22495)

Lu, Y., E. Liang, L. Gao, P. Tzeferacos, R. Follett, A. Birkel, D. Froula, D. Lamb, C. Li, H. Sio, R. Petrasso, M. Wei, W. Fu and H. Ji. Creating Magnetized Jets Using a Ring of Laser Beams. Presented at *Z Fundamental Science Program Workshop*, Albuquerque, New Mexico, United States, 2018-07-30 - 2018-08-01. (LA-UR-18-30100)

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Chien, A., L. Gao, H. Ji, K. Hill, J. Fuchs, S. Chen, A. Fazzini, B. Bleotu, R. Takizawa, A. M. Rasmus, X. Yuan and H. Chen. Magnetically-Driven Reconnection using Laser-Powered Capacitor Coils on the Titan Laser. Presented at *NIF and JLF User Group Meeting 2020*, Livermore, California, United States, 2020-02-03 - 2020-02-05. (LA-UR-20-21800)

Flippo, K. A., D. H. Barnak, H. Li, S. Li, C. L. Rousculp, T. A. Gianakon, A. M. Rasmus, A. S. Liao, C. Y. Fiedler Kawaguchi, K. V. Kelso, Y. H. Kim, E. N. Loomis, Y. Lu, C. C. Kuranz, A. Angulo, J. Levesque, C. Li, A. Birkel and B. Lahmann. Self-generated Magnetic Fields in HED Shock Tubes. . (LA-UR-19-25456)

Fiedler Kawaguchi, C., B. Tobias, S. Palaniyappan, J. P. Sauppe, K. A. Flippo, E. N. Loomis, C. C. Kuranz, J. L. Kline and S. H. Batha. Using the Bayes Inference Engine to study the deceleration-phase of Rayleigh-Taylor growth rates in laser-driven cylindrical implosions. Presented at *OMEGA user group meeting*, Rochester, New York, United States, 2019-04-24 - 2019-04-26. (LA-UR-19-23632)

Kelso, K. V., K. A. Flippo, Y. Lu, K. D. Meaney, A. S. Liao, S. Li, C. W. Wilburn, H. Li, C. Y. Fiedler Kawaguchi and J. T. Laune. Proton Radiography Utilizing MCNP. Presented at *60th Annual Meeting of the APS Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30350)

Lu, Y., H. Li, S. Li, D. H. Barnak, K. A. Flippo, C. Li, A. Birkel and B. Lahmann. Characterizing shock and shear-flow generated magnetic fields for ICF relevant configurations. Presented at *Omega Laser Facility Users Group Workshop*, Rochester, New York, United States, 2019-04-24 - 2019-04-26. (LA-UR-19-27358)

Sadler, J. D., C. Arran, H. Li and K. A. Flippo. Overcoming wakefield dephasing using multiple laser pulses. Presented at *APS DPP conference 2019*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30472)

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New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-29416)

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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

Journal Articles

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*Scheiner, B. and M. Schmitt. The role of incidence angle in the laser ablation of a planar target. 2019. *Physics of Plasmas*. **26** (2): 24502. (LA-UR-18-29321 DOI: 10.1063/1.5085122)

Vinyard, N. S., M. J. Schmitt, S. C. Hsu, B. S. Scheiner, D. W. Schmidt, V. Geppert-Kleinrath, P. W. McKenty, D. T. Michel, D. H. Edgell, F. J. Marshall and H. Huang. Development of a directly driven multi-shell platform: laser drive energetics. Submitted to *Physics of Plasmas*. (LA-UR-19-23347)

Presentation Slides

Kyrala, G. A., T. J. Murphy, N. S. Vinyard and M. J. Schmitt. Comparing Backlighter Images at NIF to calculations. Presented at *Anomalous Absorption ZCOnference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-09. (LA-UR-19-25366)

Molvig, K., M. J. Schmitt, R. Betti, E. M. Campbell and P. McKenty. The Revolver Ignition Capsule: Persistent stagnation and high efficiency burn. . (LA-UR-17-31342)

Molvig, K. and M. J. Schmitt. Pointing scheme for the NIF laser with "perfect" low mode uniformity. Presented at *The 61st Annual Meeting of the APS Division of Plasma Physics*, Ft. Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30763)

Scheiner, B. S. Revolver 19A Omega Results. . (LA-UR-19-21123)

Scheiner, B. S., M. J. Schmitt, D. W. Schmidt, F. Marshall, C. H. Wilde and P. Adrian. Revolver-20A Campaign Preview. . (LA-UR-19-32065)

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Schmidt, D. W., T. Cardenas, T. H. Day, P. M. Donovan, F. Fierro, L. A. Goodwin, M. J. Herman, J. C. Lamar, L. A. Kuettner, B. M. Patterson, T. E. Quintana, R. B. Randolph, B. S. Scheiner, M. J. Schmitt, O. C. Trautschold, D. R. Vodnik, C. T. Wilson, H. Huang, C. Shuldberg and T. Drake. Target Fabrication Efforts for Multi-Shell Direct Drive. Presented at *Target Fabrication Speacilists*, Anapolis, Massachusetts, United States, 2019-04-23 - 2019-04-26. (LA-UR-19-23462)

Schmitt, M. J., K. Molvig, B. S. Scheiner, C. H. Wilde, N. S. Vinyard, D. W. Schmidt, S. C. Hsu, T. A. Gianakon, L. Kot, M. J. Rosenberg, F. J. Marshall, D. Edgell, P. W. McKenty, D. N. Polsin, R. S. Craxton and H. Huang. Progress in advancing the Revolver triple-shell direct-drive ignition concept. Presented at *American Physical Society Division of Plasma Physics Conference*, Ft Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30727)

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Schmitt, M. J., K. Molvig, B. S. Scheiner, N. S. Vinyard, P. McKenty, D. Edgell, T. Michel and F. Marshall. 2-Dimensional simulations of the Revolver direct-drive multi-shell ignition concept. Presented at *48th Annual Anomalous Absorption Conference*, Bar Harbor, Maine, United States, 2018-07-09 - 2018-07-13. (LA-UR-18-26304)

Schmitt, M. J., K. Molvig, B. S. Scheiner, N. S. Vinyard, S. C. Hsu, T. A. Gianakon and D. W. Schmidt. A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility. . (LA-UR-18-31102)

Schmitt, M. J., K. Molvig, D. W. Schmidt, B. S. Scheiner, C. H. Wilde, T. A. Gianakon, B. Keenan and A. N. Black. LDRD-DR Project Appraisal: A Low Fuel Convergence Path to Inertial Confinement Fusion on the National Ignition Facility. . (LA-UR-20-21789)

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Schmitt, M. J., N. S. Vinyard, B. S. Scheiner, K. Molvig, A. Zylstra, C. H. Wilde, D. W. Schmidt, P. McKenty, M. Rosenberg, D. Turnbull, J. Di Nicola, G. Guruangan, M. Hohenberger, P. Di Nicola, B. MacGowan, T. Zobrist, H. Huang and M. Schoff. Multi-Shell Direct-Drive Ablator Energetics Campaign: P-000428. Presented at *HED/ICF Council & PRP Meeting*, Livermore, California, United States, 2018-08-28 - 2018-08-30. (LA-UR-18-27730)

Schmitt, M. J., N. S. Vinyard, B. S. Scheiner, K. Molvig, C. H. Wilde, D. W. Schmidt, P. W. McKenty, M. Rosenberg, D. Turnbull, M. Hohenberger, H. Huang and L. Kot. Direct-Drive Multi-Shell (DDMS) Collision Energetics: ABLE P-000515. Presented at *ICF Council Meeting for NIF shots*, Livermore, California, United States, 2019-03-05 - 2019-03-05. (LA-UR-19-21451)

Schmitt, M. J. and C. H. Wilde. Multi-Shell Direct-Drive Ablator Energetics (ABLE). . (LA-UR-20-21770)

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I. Magrogan, W. R., B. S. Scheiner and M. J. Schmitt. Performance impacts of Beam Width on Direct Drive ICF. Presented at *60th Annual Meeting of the APS Division of Plasma Physics Co-Located with the 71st Annual Gaseous Electronics Conference*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30401)

Scheiner, B. S. and M. J. Schmitt. Understanding the role of incidence angle in PDD. Presented at *Omega Laser Users Group Workshop*, Rochester, New York, United States, 2018-04-25 - 2018-04-25. (LA-UR-18-23461)

Scheiner, B. S. and M. J. Schmitt. The Role of Incidence Angle in the Laser Ablation of ICF Targets. Presented at *Anomalous Absorption Conference*, Bar Harbor, Maine, United States, 2018-07-08 - 2018-07-08. (LA-UR-18-26080)

Scheiner, B. S. and M. J. Schmitt. The Role of Incidence Angle in the Laser Ablation of ICF Targets. Presented at *APS DPP meeting*, Portland, Oregon, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30399)

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Nucleosynthesis Probes of Cosmic Explosions

Christopher Fryer
20190021DR

Project Description

Multi-physics modeling, combining transport, nuclear physics, and hydrodynamics all play an important role in a range of problems of national interest. This project brings together both physics experts and computational scientists to study the multi-physics problem surrounding the emission of from the merger of two neutron stars. The physics components and the numerical methods used to combine these physics components will develop techniques Los Alamos scientists will be able to use throughout the Advanced Simulation and Computing (ASC) program.

Publications

Journal Articles

Banerjee, S., K. Belczynski, C. L. Fryer, P. Berczik, J. Hurley, R. Spurzem and L. Wang. BSE versus StarTrack: implementations of new wind, remnant-formation, and natal-kick schemes in NBODY7 and their astrophysical consequences. Submitted to *Astronomy and Astrophysics*. (LA-UR-20-22131)

Belczynski, K., T. Bulik, A. Olejak, M. Chru\xc5\x9bli \xc5\x84ska, N. Singh, N. Pol, L. Zdunik, R. O'Shaughnessy, M. McLaughlin, D. Lorimer, O. Korobkin, E. van den Heuvel, M. B. Davies and D. E. Holz. Binary neutron star formation and the origin of GW170817. Submitted to *Astronomy and Astrophysics*. (LA-UR-19-20692)

Braun, C., S. Safi-Harb and C. L. Fryer. Chandra and XMM–Newton Study of the Supernova Remnant RCW 103 (G332.4–0.4) Containing the Peculiar Central Compact Object 1E 161348–5055. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-18-31702)

Braun, C., S. Safi-Harb and C. L. Fryer. Progenitors and explosion properties of supernova remnants hosting central compact objects: I. RCW \xe2\x80\x89103 associated with the peculiar source 1E \xe2\x80\x89161348–5055. 2019. *Monthly Notices of the Royal Astronomical Society*. **489** (3): 4444-4463. (LA-UR-19-24543 DOI: 10.1093/mnras/stz2437)

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*Chatzopoulos, E., M. S. Gilmer, R. T. Wollaeger, C. Frohlich and W. P. Even. Synthetic Spectra of Pair-instability Supernovae in 3D. 2019. *The Astrophysical Journal*. **875** (2): 140. (LA-UR-19-21458 DOI: 10.3847/1538-4357/ab1082)

Couture, A. J., R. Casten and R. B. Cakirli. Improved Predictions for r-process Cross Sections. Submitted to *Nuclear Physics News International*. (LA-UR-19-25512)

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The Neutron Electric Dipole Moment as a Gateway to New Physics

Takeyasu Ito
20190041DR

Project Description

The research supported by this project addresses the question "Why does the Universe that we live in have so much more matter than antimatter", one of the biggest questions in present day science. This project, on completion, will have demonstrated a capability to perform next generation experiments looking for neutron electric dipole moment, have controlled systematics important for all such experiments, and have developed a theory to use results from these experiments to constrain theories of new physics. Collectively, this research will have a profound impact on our understanding of the interaction among the fundamental building blocks of our world and the history of the Universe. The methods of precision measurements and computation will benefit other researches performed at the Laboratory and elsewhere. The theory employs the tools of Lattice Quantum ChromoDynamics, which have consistently driven the development of novel computer architectures for a long time. The theoretical work done as part of this project will not only enhance the laboratory's stature among theoretical physicists, thus benefiting in hire and retention of personnel, but will also develop and maintain the capability of employing high performance computing architectures in service of simulating challenging scientific problems.

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Park, S., T. Bhattacharya, R. Gupta, B. Yoon, Y. C. Jang, H. W. Lin, K. Orginos, D. Richards and B. Joo. Nucleon Charges and Form Factors using Clover Fermions. Presented at *the 37th international conference on lattice field theory*. (Wuhan, China, 2019-06-16 - 2019-06-22). (LA-UR-19-31873)

Reports

Cirigliano, V., T. Bhattacharya, Z. Davoudi, T. Izubuchi, P. Shanahan, M. Wagman and S. Syritsin. The Role of Lattice QCD in Searches for Violations of Fundamental Symmetries and Signals for New Physics. Unpublished report. (LA-UR-19-22184)

Presentation Slides

Bhattacharya, T. nEDM Theory. Presented at *Workshop on Fundamental Physics at the Second Target Station (FPSTS19)*, Oak Ridge, Tennessee, United States, 2019-07-26 - 2019-07-27. (LA-UR-19-27343)

Bhattacharya, T. Gradient Flow. Presented at *Workshop on Lattice QCD*, Santa Fe, New Mexico, United States, 2019-08-26 - 2019-08-30. (LA-UR-19-28608)

Bhattacharya, T. Neutron Electric Dipole Moments. Presented at *Workshop on Lattice QCD*, Santa Fe, New Mexico, United States, 2019-08-26 - 2019-08-30. (LA-UR-19-28747)

Bhattacharya, T. Neutron Electric Dipole Moment & QFT on quantum computers. . (LA-UR-20-22412)

Ito, T. A New Experiment to Search for the Neutron's Electric Dipole Moment at LANSCE. Presented at *LANSCE Users' Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-07. (LA-UR-18-30605)

Ito, T. nEDM Experiment at Los Alamos National Laboratory. Presented at *Workshop on "Particle Physics with Neutrons at the ESS"*, Stockholm, Sweden, 2018-12-10 - 2018-12-14. (LA-UR-18-31385)

Ito, T. nEDM — North American Efforts. Presented at *ACFI Workshop on "Theoretical Issues and Experimental Opportunities in Searches for Time Reversal Invariance Violation Using Neutrons"*, Amherst, Massachusetts, United States, 2018-12-06 - 2018-12-08. (LA-UR-18-31384)

Ito, T. LANL nEDM Overview and requirements. Presented at *Meeting at PTB Berlin*, Berlin, Germany, 2019-09-17 - 2019-09-17. (LA-UR-19-29478)

Ito, T. Neutron Electric Dipole Moment Search Experiments in the US. Presented at *Atomic nuclei as laboratories for BSM physics*, Trento, Italy, 2019-04-15 - 2019-04-18. (LA-UR-19-23340)

Park, S., T. Bhattacharya, R. Gupta, B. Yoon, Y. Jang, K. Orginos, D. Richards, H. Lin and B. Joo. Nucleon Charges and Form Factors on clover lattices. Presented at *the 37th international conference on lattice field theory*, Wuhan, China, 2019-06-16 - 2019-06-22. (LA-UR-19-25549)

Yoon, B., T. Bhattacharya, R. Gupta and V. Cirigliano. Neutron Electric Dipole Moment from QCD and BSM using Clover-on-HISQ. Presented at *Lattice 2019*, Wuhan, China, 2019-06-16 - 2019-06-22. (LA-UR-19-25441)

Posters

Yoon, B., N. T. T. Nguyen, T. Bhattacharya, G. Kenyon and R. Gupta. Quantum Machine Learning for Lattice QCD. Presented at *2019 Quantum Information Science (QIS) Kick Off Principal Investigators' Meeting*, Rockville, Maryland, United States, 2019-01-31 - 2019-01-31. (LA-UR-19-20388)

Yoon, B., N. T. T. Nguyen-Fotiadis, T. Bhattacharya, R. Gupta and G. Kenyon. Quantum Machine Learning for Lattice QCD. Presented at *Quantum Information Science (QIS) Principal Investigator (PI) Meeting*, Washington, District Of Columbia, United States, 2020-03-12 - 2020-03-13. (LA-UR-20-22302)

Convincing Search for Sterile Neutrinos at Lujan

Richard Van De Water
20190098DR

Project Description

This project will have a significant impact on the Laboratory, as it brings experimental neutrino physics back to the place it started in the 1950's with the Nobel Prize winning discovery of the neutrino by Cowen and Reines. High profile Research & Development attracts the brightest and best students, with most of our postdocs going on to successful careers at Los Alamos and at other national labs and universities. We are developing a significant external collaboration of world leading researchers in neutrino physics, who will bring talented students and postdocs to work on the experiment. Fermi National Accelerator Laboratory (FNAL) has expressed support for the project and is allowing a staff scientist to participate. The long-term goal is to develop a robust and flexible neutrino facility to attract new National Science Foundation/Department of Energy basic science funding to support novel neutrino experiments and to test technologies for future short- and long- baseline programs. These element are all important to Los Alamos for producing a stronger scientific base, and hence by extension, to DOE/National Nuclear Security Administration, and the nation.

Publications

Journal Articles

Van De Water, R. G. and W. C. I. Louis. Sterile Neutrinos. Submitted to *Scientific American*. (LA-UR-19-32514)

Presentation Slides

Van De Water, R. G. Searching for Sterile Neutrinos with the Coherent CAPTAIN-Mills Detector at the Los Alamos Neutron Science Center. Presented at *APS April Meeting 2019*, Denver, Colorado, United States, 2019-04-13 - 2019-04-13. (LA-UR-19-24037)

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.

Technical Outcomes

The LDRD team addressed the project proposal across a wide variety of fronts. Legacy design tools were updated for modern codes and fundamentally new design methodologies were developed and exercised. The design process of interest was expanded to include engineering and experiments including a hydrodynamic test of a novel design. This LDRD is directly driving the decisions being made for the Stockpile Responsiveness Program and all future system design efforts.

Publications

Journal Articles

*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*. **43** (1): 62-68. (LA-UR-17-27057 DOI: 10.1002/prep.201700197)

Conference Papers

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, 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, Minnesota, United States, 2016-10-06 - 2016-10-07). (LA-UR-16-29501)

Reports

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)

Presentation Slides

Bowden, P. R., B. C. Tappan, M. M. Schmitt, J. P. Lichthardt, E. G. Francois and L. G. Hill. Performance Evaluation of Reduced Sensitivity Explosvies. Presented at *20th Biennial International Conference of the APS Topical Group on Shock Compression of Condensed Matter (SCCM-2017)*, St. Louis, Missouri, United States, 2017-07-10 - 2017-07-14. (LA-UR-17-25370)

Bowen, C. M. How to Get that Funding: Writing Successful Scholarship Applications. Presented at *Women in Statistics and Data Science Conference*, Cincinnati, Ohio, United States, 2018-10-18 - 2018-10-20. (LA-UR-18-29742)

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 Detonation Symposium, 16th*, Cambridge, Maryland, United States, 2018-07-15 - 2018-07-15. (LA-UR-18-26331)

Tappan, B. C., P. R. Bowden, V. W. Manner, S. F. Son, J. P. Lichthardt, E. G. Francois 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 in Energetic Materials*, Pardubice, Czech Republic, 2018-04-17 - 2018-04-17. (LA-UR-18-23162)

Wendelberger, J. R. Understanding Today's Complex World. Presented at *2016 Fall Technical Conference*, Minneapolis, Minnesota, United States, 2016-10-06 - 2016-10-07. (LA-UR-16-27620)

Wendelberger, J. R. May All Your Errors Be Small And Normal. Presented at *Fall Technical Conference Statistics: Powering a Revolution in Quality Improvement*, Philadelphia, Pennsylvania, United States, 2017-10-04 - 2017-10-06. (LA-UR-17-29008)

Wendelberger, J. R. Statistical Thinking and Analysis for Large and Complex Data. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-27 - 2019-08-01. (LA-UR-19-27126)

Wendelberger, J. R. Statistical Thinking and Analysis for Large and Complex Data. Presented at *Joint Statistical Meetings*, Denver, Colorado, United States, 2019-07-28 - 2019-08-01. (LA-UR-19-24601)

Wendelberger, J. R. and C. M. Bowen. Scientific Modeling with Functional Data. Presented at *Spring Research Conference*, Blacksburg, Virginia, United States, 2019-05-22 - 2019-05-24. (LA-UR-19-24600)

Wendelberger, J. R. and C. M. Bowen. Iterative Modeling with Functional Data. Presented at *2019 Fall Technical Conference*, Gaithersburg, Maryland, United States, 2019-09-25 - 2019-09-27. (LA-UR-19-29532)

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.

Technical Outcomes

This project completed over 90% of its scope, including demonstration of the ultra-short electron bunches produced by the strong field photoemission from diamond field emitter cathodes and development of the high refractive index printable polymers. The project left behind test stands that became important additions to LANL's established capability to study advanced cathodes.The polymer science part of the project developed a unique technology proprietary to LANL on production of the high refractive index printable materials.

Publications

Journal Articles

*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. 2019. *Journal of Applied Physics*. **125** (16): 164501. (LA-UR-18-31776 DOI: 10.1063/1.5086292)

Kim, D., H. L. Andrews, B. K. Choi, R. L. Fleming, C. Huang, T. J. T. Kwan, J. W. I. Lewellen, K. Nichols, V. Pavlenko and E. I. Simakov. A Divergence Study for the Electron Beam Emitted from a Diamond Pyramid. Submitted to *Physical Review Accelerators and Beams*. (LA-UR-19-24005)

*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*. **8** (1): 9258. (LA-UR-18-20571 DOI: 10.1038/s41598-018-27572-1)

*Piryatinski, A., C. Huang and T. J. T. Kwan. Theory of electron transport and emission from a semiconductor nanotip. 2019. *Journal of Applied Physics*. **125** (21): 214301. (LA-UR-19-20009 DOI: 10.1063/1.5088518)

*Piryatinski, A., C. Huang and T. J. T. Kwan. Theory of electron transport and emission from a semiconductor nanotip. 2019. *Journal of Applied Physics*. **125** (21): 214301. (LA-UR-19-20009 DOI: 10.1063/1.5088518)

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)

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)

Conference Papers

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. Focusing Studies Of An Electron Beam In Diamond Field Emitter Array Cathodes. Presented at *NAPAC*. (Lansing, Michigan, United States, 2019-09-01 - 2019-09-01). (LA-UR-19-28736)

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, V. Pavlenko, A. Piryatinski and E. I. Simakov. Physics of electron beam generation and dynamics from diamond field emitter arrays. Presented at *10th International Particle Accelerator Conference*. (Melbourne, Australia, 2019-05-19 - 2019-05-24). (LA-UR-19-24417)

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. Aragonez 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)

Pavlenko, V., K. J. Leedle, H. L. Andrews, D. V. Gorelov, D. Kim, R. L. Fleming, E. I. Simakov and D. S. Black. Characterization of Femtosecond-Laser-Induced Electron Emission from Diamond Nano-Tips. Presented at *2019 North American Particle Accelerator Conference (NAPAC2019)*. (Lansing, Michigan, United States, 2019-09-02 - 2019-09-02). (LA-UR-19-28710)

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, 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., H. L. Andrews, R. L. Fleming, D. Kim, V. Pavlenko, D. Black and K. Leedle. OBSERVATION OF THE FEMTOSECOND LASER-INDUCED EMISSION FROM THE DIAMOND FIELD EMITTER TIPS. Presented at *International Particle Accelerator Conference (IPAC 2019)*. (Melbourne, Australia, 2019-05-20 - 2019-05-20). (LA-UR-19-24441)

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)

Presentation Slides

Baker, R. C. Calculating the Electron Emission of Diamond Field Emitters with Nanotips. . (LA-UR-18-27026)

Fleming, R. L. A Simple Variable Focus Lens For Field-Emitter Cathodes. Presented at *18th Advanced Accelerators Concepts Workshop*, Breckenridge, Colorado, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27618)

Fleming, R. L., V. Pavlenko, D. Kim, H. L. Andrews, C. Huang, T. J. T. Kwan, A. Piryatinski, R. J. Aragonez and E. I. Simakov. Studies of the field assisted photoemission from nanocrystalline diamond and diamond field emitter arrays. Presented at *Advanced Accelerator Concepts*, Breckenridge, Colorado, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27723)

Huang, C. Particle accelerators: present, future and the enabling computational modeling. . (LA-UR-19-31915)

Huang, C., T. J. T. Kwan, A. Piryatinski, R. C. Baker, D. Kim, R. L. Fleming, V. Pavlenko, H. L. Andrews and E. I. Simakov. Emission models and beam dynamics for diamond emitters in a compact source of high brightness beams. Presented at *2018 Photocathode Physics for Photoinjectors (P3) Conference*, Santa Fe, New Mexico, United States, 2018-10-15 - 2018-10-17. (LA-UR-18-29868)

Huang, C., T. J. T. Kwan, A. Piryatinski, R. C. Baker, D. Kim, R. L. Fleming, V. Pavlenko, H. L. Andrews and E. I. Simakov. Modeling of Electron Emission from Diamond Field Emitters. Presented at *Nanomaterials: Computation,*

Theory, and Experiment, Telluride, Colorado, United States, 2019-07-16 - 2019-07-19. (LA-UR-19-26879)

Huang, C., T. J. T. Kwan, A. Piryatinski, R. C. Baker, H. L. Andrews, D. Kim, B. K. Choi, R. L. Fleming, K. Nichols, V. Pavlenko, D. Shchegolkov and E. I. Simakov. Emission models and beam dynamics for diamond emitters in a compact source of high brightness beams. Presented at *18th Advanced Accelerator Concepts Workshop*, Breckenridge, Colorado, United States, 2018-08-13 - 2018-08-17. (LA-UR-18-27768)

Kim, D. Current DFEA Cathode Research at LANL. Presented at *8th ACHIP Collaboration Meeting*, Palo Alto, California, United States, 2019-03-27 - 2019-03-29. (LA-UR-19-22583)

Kim, D., H. L. Andrews, B. K. Choi, E. I. Simakov and R. L. Fleming. Fabrication and Characterization of Diamond Field Emitter Array Cathodes. Presented at *PPPS 2019 (2019 IEEE Pulsed Power and Plasma Science Conference)*, orlando, Florida, United States, 2019-06-23 - 2019-06-28. (LA-UR-19-25821)

Nichols, K., H. L. Andrews, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. E. Wisniewski, S. Antipov and G. Chen. Shaped beams from Diamond Field-Emitter Array Cathodes. Presented at *AWA NOW*, Lemont, Illinois, United States, 2019-08-21 - 2019-08-21. (LA-UR-19-28620)

Simakov, E. I. Update on the dielectric laser accelerator project at LANL. Presented at *Accelerator on a chip collaboration meeting*, Menlo Park, California, United States, 2017-09-13 - 2017-09-13. (LA-UR-17-28183)

Simakov, E. I. Additive manufacturing of dielectric laser accelerating structures. Presented at *MST University Outreach Workshop*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-27275)

Simakov, E. I., D. Kim, H. L. Andrews, R. L. Fleming, J. W. I. Lewellen, V. Pavlenko and D. Shchegolkov. Study of the Beam Divergence in Diamond Field Emitter Array Cathodes. Presented at *Advanced Accelerator Concepts Workshop 2018*, Breckenridge, Colorado, United States, 2018-08-12 - 2018-08-12. (LA-UR-18-27633)

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 *Advanced Accelerator Concepts Workshop 2018*, Breckenridge,, Colorado, United States, 2018-08-12 - 2018-08-12. (LA-UR-18-27624)

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Simakov, E. I., H. L. Andrews, D. Kim, V. Pavlenko, K. Leedle and D. Black. Observations of the laser-induced emission from the diamond field emitter tips. Presented at *Photocathode Physics for Photoinjectors Workshop*, Santa Fe, New Mexico, United States, 2018-10-15 - 2018-10-15. (LA-UR-18-29733)

Walker, E. M. High-Dielectric 3-D Printable Materials for Laser Accelerators. Presented at *Advanced Accelerator Concepts*, Breckenridge, Colorado, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27785)

Walker, E. M., R. D. Gilbertson, E. I. Simakov, C. J. Hanson and M. J. Herman. DEVELOPING NEW MATERIALS FOR ADDITIVE MANUFACTURE OF DIELECTRIC LASER ACCELERATOR STRUCTURES. Presented at *International Particle Accelerator Conference 2019*, Melbourne, Australia, 2019-05-19 - 2019-05-24. (LA-UR-19-24348)

Weis, E., K. M. Hubbard, M. J. Herman, R. J. Peterson, G. Pilania, D. Shchegolkov, T. S. Luk, A. V. Efimov, E. I. Simakov and B. M. Patterson. High-Dielectric Materials for Fabrication by Two-Photon Polymerization. Presented at *59th Electronic Materials Conference*, South Bend, Indiana, United States, 2017-06-28 - 2017-06-30. (LA-UR-17-25202)

Posters

Andrews, H. L. Current Experimental Work with Diamond Field-Emitter Arrays. Presented at *FEL17*, Santa Fe, New Mexico, United States, 2017-08-20 - 2017-08-25. (LA-UR-17-27452)

Andrews, H. L., D. Kim, K. Nichols, D. Shchegolkov, R. L. Fleming, J. W. I. Lewellen, E. I. Simakov 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-18-23724)

Baker, R. C. Calculating the Electron Emission of Diamond Field Emitters with Nanotips. . (LA-UR-18-26951)

Fleming, R. L. Continuing Experimental Work with Diamond Field-Emitter Array Cathodes. . (LA-UR-17-27013)

Fleming, R. L. Continuing Experimental Work with Diamond Field-Emitter Array Cathodes. Presented at *Vice President of Research (VPR) Visit and Poster Session*, Los Alamos, New Mexico, United States, 2018-03-27 - 2018-03-27. (LA-UR-18-22881)

Fleming, R. L. Focusing Studies of an Electron Beam in Diamond Field Emitter Array Cathodes. Presented at *NAPAC 2019*, Lansing, Michigan, United States, 2019-09-01 - 2019-09-06. (LA-UR-19-28556)

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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-18-23518)

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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.

Technical Outcomes

Through a combination of Los Alamos experimental, theoretical, and engineering expertise, we successfully carried out a joint R&D and established capability for a new heavy quark physics program for sPHENIX. We built a prototype telescope to demonstrate the tracking capability of the Los Alamos led state-of-the-art Monolithic-Active-Pixel-Sensor based Vertex Detector upgrade. We developed new theoretical framework to better understand the physics of quark energy loss in Quark-Gluon-Plasma and published a comprehensive set of predictions.

Publications

Journal Articles

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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.

Technical Outcomes

Our work was based on the hypothesis that chemically reactive ejecta transporting in a reactive gas, such as deuterium (D2), will rapidly break up into smaller fragments in situations where they are otherwise hydrodynamically stable in a nonreactive gas, such as helium (He). The three years of research were characterized by discovery. For example, we see rapid chemically reactive-heating and -breakup processes that are lacking in hydrodynamic models.

Publications

Journal Articles

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Schwarzkopf, J. D., D. G. Sheppard, J. E. Hammerberg, M. M. Schauer, W. T. Buttler and R. K. Schulze. MODELING OF CERIUM EJECTA IN HELIUM AND DEUTERIUM GASES. Presented at *21 st Biennial Conference on Shock Compression of Condensed Matter*. (Portland, Oregon, United States, 2019-06-16 - 2019-06-21). (LA-UR-19-27422)

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Books/Chapters

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Reports

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. Understanding ejecta transport, breakup and conversion: The partition of mass below the Mie scattering resolution limits. Unpublished report. (LA-UR-19-28118)

Buttler, W. T., J. C. Cooley, J. E. Hammerberg, R. K. Schulze, J. D. Schwarzkopf, D. G. Sheppard, J. E. Barefield, J. J. Charonko, J. J. I. Goett, M. Grover, B. M. La Lone, J. G. Mance, R. Manzanares, J. I. Martinez, J. D. Regele, T. A. Saleh, M. M. Schauer, D. W. Schmidt, A. P. Shivprasad, G. D. Stevens, W. D. Turley, R. J. Valencia and S. K. Lamoreaux. Final Report on “Understanding ejecta transport, breakup and conversion processes” [20170082DR]. Unpublished report. (LA-UR-19-31575)

Presentation Slides

Bjorgaard, J. A. Density Functional Theory Study of Cerium Deuterides with Application to Ejecta Break-up in Reactive Gases. Presented at *Science in '3'*, Los Alamos, New Mexico, United States, 2017-06-07 - 2017-06-07. (LA-UR-17-25255)

Bjorgaard, J. A. Density functional theory study of cerium deuterides with application to ejecta break-up in reactive gases. Presented at *American Physical Society Topical Group on Shock Compression of Condensed Matter*, St. Louis, Missouri, United States, 2017-07-09 - 2017-07-15. (LA-UR-17-25329)

Bjorgaard, J. A. Simulations of Material Properties. Presented at *Interview Presentation*, Portland, Oregon, United States, 2018-02-14 - 2018-02-14. (LA-UR-18-21233)

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Buttler, W. T. Ejecta transport breakup and conversion: Update. . (LA-UR-18-30218)

Buttler, W. T. (U) Ejecta transport breakup and conversion: DR Progress report. . (LA-UR-19-21158)

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Buttler, W. T. Ejecta transport, breakup and conversion 3.0. Presented at *NEDPC 2019*, Los Alamos, New Mexico, United States, 2019-10-14 - 2019-10-18. (LA-CP-19-20644)

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Charonko, J. J., J. J. I. Goett, R. Manzanares, J. I. Martinez, D. W. Schmidt, W. T. Buttler, M. Grover, B. La Lone, J. G. Mance, G. Stevens and W. Turley. Measuring the Spatial Evolution of Ejecta Transport Using Particle Image Velocimetry. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK19)*, Portland, Oregon, United States, 2019-06-17 - 2019-06-21. (LA-UR-19-25445)

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Schulze, R. K. Thermochemical and Thermophysical properties for the system of Ce metal and Ce hydride (deuteride). . (LA-UR-19-32722)

Schwarzkopf, J. D., D. G. Sheppard, J. E. Hammerberg, M. M. Schauer, W. T. Buttler and R. K. Schulze. Modeling of Ce ejecta in He (nonreactive) and D2 (reactive) gases. Presented at *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SHOCK19)*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25442)

Shivprasad, A. P., T. A. Saleh, J. R. Wermer, R. K. Schulze and W. T. Buttler. Elastic properties of cerium hydrides and deuterides measured using RUS. Presented at *Topical Group on Shock Compression of Condensed Matter*, Portland, Oregon, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25451)

Understanding New Discoveries by High Altitude Water Cherenkov Observatory of Greater than 10 Tera Electron Volts Galactic Sources

Hui Li
20190049DR

Project Description

This project will utilize the most sensitive all-sky gamma-ray detectors and the state-of-the-art numerical simulation tools in kinetic plasma studies. We expect that this project will enable further development of the sensitive detector technology and new numerical schemes for large-scale simulations, both of which will enhance the LANL's technological and scientific bases. Such development could be integrated into techniques and tools to be used to address LANL's long-term mission needs such as gamma-ray detectors and multi-physics simulations.

Technical Outcomes

We have completed three studies using HAWC observations, including the discovery of > 100 TeV from Crab nebular, a catalog of > 100 TeV sources, and a pulsar wind nebula DA 495 in multi-wavelengths with HAWC, NuSTAR (hard X-ray), XMM-Newton (X-ray) and radio observations. We have also completed several theoretical and numerical studies of particle acceleration in highly magnetized environments to accelerate both electrons and protons.

Publications

Journal Articles

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Polko, P. and H. Li. Self-similar jet models: two new issues. Submitted to *Astrophysical Journal*. (LA-UR-19-30944)

Conference Papers

Malone, K. A. First HAWC Spectra of Galactic Gamma-ray Sources Above 100 TeV and the Implications for Cosmic-ray Acceleration. Presented at *International Cosmic Ray Conference*. (Madison, Wisconsin, United States, 2019-07-24 - 2019-08-01). (LA-UR-19-26623)

Presentation Slides

Li, H. Evolution of Eccentric Planet Orbits and Implications for Global Dust Evolution. Presented at *International Conference on Astrophysical Dynamcis*, Shanghai, China, 2019-07-07 - 2019-07-09. (LA-UR-19-30717)

Malone, K. A. First HAWC Spectra of Galactic Gamma-ray Sources Above 100 TeV and the Implications for Cosmic-ray Acceleration. Presented at *International Cosmic Ray Conference*, Madison, Wisconsin, United States, 2019-07-24 - 2019-08-01. (LA-UR-19-26622)

Malone, K. A. Recent Results from the HAWC Observatory. Presented at *International Symposium on Multiparticle*

Dynamics, Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-13. (LA-UR-19-29009)

Posters

Lu, Y., F. Guo, H. Li and E. P. Liang. Fermi-type particle acceleration from magnetic reconnection at the termination shock of relativistic striped wind. Presented at *Connecting Micro and Macro Scales: Acceleration, Reconnection, and Dissipation in Astrophysical Plasmas*, Santa Barbara, California, United States, 2019-09-09 - 2019-09-12. (LA-UR-19-29037)

Malone, K. A. Observation of the highest-energy gamma-ray sources with the HAWC Observatory. Presented at *LANL Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28439)

Long-pulse, Ultra-high-gradient Radio-frequency Accelerator Structures – Better Performance through Smart Design, Manufacturing and Breakdown Suppression

Frank Krawczyk
20190079DR

Project Description

Particle accelerators are established tools for solving national security challenges, as well as discovery science. Current mission needs with national security implications include the need to study and develop materials under extreme conditions that never have been accessible before, and improve tools for remote sensing in defense from national security threats. These two needs represent the two extremes of system sizes, where accelerators are used. The enabling tools and technologies developed in this project will feed into a follow-on technology development effort with significant impact on the performance and cost of both types of systems. The studies on material extremes require large X-ray free-electron lasers (XFEL), for which new radio-frequency (RF)-structure technology will reduce size (length typically ~ 1000 yards) and complexity, and increase the efficiency of accelerator systems. For remote sensing applications the use of such RF-structures provides a path to trailer-bed mountable mobile systems for detection of special nuclear materials (SNM). With completion of this one year effort novel design and engineering tools will be available for the first ever integrated RF-structure design using designed materials that specifically suppress limiting RF-break-down in high performance operation.

Technical Outcomes

This project extended science simulation tools in Molecular Dynamics to include effects relevant to engineered systems, completing the integration of Lorentz forces and scoping the consideration of thermal fatigue and defect propagation for a complete model of break-down precursors and the actual break-down phenomenon. We also quantitatively confirmed C-band as the most suitable frequency for application to Los Alamos National Laboratory's mission needs, considering both electron (DMMSC) and proton accelerator applications (pRAD).

Publications

Journal Articles

Wang, G., P. Yang and E. R. Batista. Computational screening of 2D coatings for semiconducting photocathodes. Submitted to *Journal of Physical Chemistry Letters*. (LA-UR-19-29869)

Conference Papers

Simakov, E. I., A. W. Garmon, T. C. Germann, M. F. Kirshner, F. L. Krawczyk, J. W. I. Lewellen, D. Perez, G. Wang, A. Fukasawa and J. B. Rosenzweig. High Gradient High Efficiency C-Band Accelerator Structures Research at LANL. Presented at *North American Particle Accelerator Conference*. (Lansing, Michigan, United States, 2019-09-02 - 2019-09-02). (LA-UR-19-28740)

Reports

Krawczyk, F. L. Meeting minutes SLAC/UCLA/LANL Meeting on December 5, 2018. Unpublished report. (LA-UR-18-31874)

Presentation Slides

Kirshner, M. F. RF Sources for High Gradient Accelerators. Presented at *C-Band High Gradient Accelerator Structure Meeting at LANSCE*, Los Alamos, New Mexico, United States, 2018-12-05 - 2018-12-14. (LA-UR-18-31588)

Krawczyk, F. L. LANL Plans on High-Performance RF-structures. Presented at *Towards An Ultra-Compact X-Ray Free Electron Laser Registration*, Los Angeles, California, United States, 2019-01-22 - 2019-01-25. (LA-UR-19-20299)

Krawczyk, F. L. LANL Accelerator Activities for C-band. . (LA-UR-19-21086)

Krawczyk, F. L. LANL Accelerator and Material Science Activities for C-band. Presented at *International Workshop on Breakdown Science and High Gradient Technology" (HG2019)*, Chamonix, France, 2019-06-10 - 2019-06-14. (LA-UR-19-25200)

Krawczyk, F. L., E. I. Simakov, D. Perez, M. F. Kirshner, N. A. Moody, J. W. I. Lewellen, G. Pilania, V. Pavlenko, T. C. Germann and G. Wang. Meeting for the evaluation of potential collaboration among SLAC, UCLA and LANL. . (LA-UR-18-31755)

Krawczyk, F. L., E. I. Simakov, J. W. I. Lewellen, M. F. Kirshner, A. Y. Le, T. C. Germann, D. Perez, G. Wang, G. Pilania, T. A. Jankowski, S. K. Lawrence, A. N. Black and P. J. Gibbs. Long-pulse, Ultra-high-gradient Radio-Frequency Accelerator Structures - Better Performance Through Smart Design, Manufacturing and Breakdown Suppression. Presented at *International Workshop on Future Linear Colliders LCWS 2018*, Arlington, Texas, United States, 2018-10-22 - 2018-10-22. (LA-UR-18-30015)

I. Lewellen, J. W. Thoughts on Materials and Sources. Presented at *DOE Basic Research Needs Workshop*, Tysons Corner, Virginia, United States, 2019-05-06 - 2019-05-08. (LA-UR-19-24074)

Perez, D., A. W. Garmon, T. C. Germann, G. Wang and F. L. Krawczyk. High-Field Materials Modeling Effort at LANL. Presented at *Workshop on compact FEL*, Los Angeles, California, United States, 2019-01-21 - 2019-01-21. (LA-UR-19-20760)

Song, H., A. Le and M. Kirshner. 50 MW C-Band Multiple Beam Klystron (MBK) for High Gradient Accelerators. . (LA-UR-19-27721)

Posters

Simakov, E. I., A. W. Garmon, T. C. Germann, M. F. Kirshner, F. L. Krawczyk, J. W. I. Lewellen, D. Perez, G. Wang, A. Fukasawa and J. B. Rosenzweig. High Gradient High Efficiency C-Band Accelerator Structures Research at LANL. Presented at *North American Particle Accelerator Conference*, Lansing, Michigan, United States, 2019-09-02 - 2019-09-02. (LA-UR-19-28741)

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

Journal Articles

Chen, G., L. Chacon, L. Yin, B. J. Albright, D. J. Stark and R. F. Bird. A semi-implicit, energy- and charge-conserving particle-in-cell algorithm for the relativistic Vlasov-Maxwell equations. Submitted to *Computer Physics Communications*. (LA-UR-19-21811)

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)

*Yin, L., B. J. Albright, D. J. Stark, W. D. Nystrom, R. F. Bird and K. J. Bowers. Saturation of cross-beam energy transfer for multispeckled laser beams involving both ion and electron dynamics. 2019. *Physics of Plasmas*. **26** (8): 082708. (LA-UR-19-24839 DOI: 10.1063/1.5111334)

Presentation Slides

Chen, G., L. Chacon, L. Yin, B. J. Albright, D. J. Stark and R. F. Bird. Modern Algorithms for PIC Simulation of Laser-plasma Interactions (LPI). Presented at *SIME Conference ON NONLINEAR WAVES and COHERENT STRUCTURES*, Anaheim, California, United States, 2018-06-11 - 2018-06-14. (LA-UR-18-25421)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom and R. F. Bird. Isolating the Role of Ion Trapping in the Saturation of Cross-beam Energy Transfer. Presented at *60th Annual APS DPP meeting*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30538)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom and R. F. Bird. Density dependence of stimulated Raman scattering in CBET-amplified multi-speckle beams. Presented at *Anomalous Absorption*, Telluride, Colorado, United States, 2019-06-10 - 2019-06-10. (LA-UR-19-25205)

Stark, D. J., L. Yin, B. J. Albright, W. D. Nystrom and R. F. Bird. Density dependence of the saturation of stimulated Raman scattering in CBET-amplified multi-speckled beams. Presented at *61st Annual APS DPP conference*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30512)

Stark, D. J., L. Yin, G. Chen, R. F. Bird, W. D. Nystrom, L. Chacon and B. J. Albright. Nonlinear Dynamics of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams. . (LA-UR-19-21814)

Stark, D. J., L. Yin, K. L. Nguyen, G. Chen, R. F. Bird, W. D. Nystrom, B. J. Albright and L. Chacon. Nonlinear Dynamics of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams. . (LA-UR-20-21983)

Yin, L. Nonlinear electron and ion dynamics in the saturation of cross-beam energy transfer (CBET). Presented at *61st Annual Meeting of the APS-DPP*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30162)

Yin, L., B. J. Albright, D. J. Stark, R. F. Bird and W. D. Nystrom. Nonlinear electron and ion dynamics in the saturation of cross-beam energy transfer. Presented at *49th Annual Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-09. (LA-UR-19-25133)

Yin, L., B. J. Albright, D. J. Stark, W. D. Nystrom and R. F. Bird. Saturation of Cross-Beam Energy Transfer for Multi-Speckled Laser Beams. Presented at *60th Annual Meeting of the APS Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30314)

Posters

Chen, G., L. Chacon, L. Yin, B. J. Albright, D. J. Stark, R. F. Bird and W. D. Nystrom. Optimizations for a semi-implicit, energy- and charge-conserving particle-in-cell algorithm with iVPIC. Presented at *APS DPP annual meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30950)

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

Journal Articles

Andrews, H. L., K. Nichols, D. Kim, E. I. Simakov, S. Antipov, M. Conde, D. Doran, G. Ha, W. Liu, J. Power, J. Shao, C. Whiteford, E. E. Wisniewski and G. Chen. Shaped Beams from Diamond Field-Emitter Array Cathodes. Submitted to *IEEE Transactions on Plasma Science*. (LA-UR-19-31870)

Kim, D., H. L. Andrews, B. K. Choi, R. L. Fleming, C. Huang, T. J. T. Kwan, J. W. I. Lewellen, K. Nichols, V. Pavlenko and E. I. Simakov. Divergence study and emittance measurements for the electron beam emitted from a diamond pyramid. 2019. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. (LA-UR-19-30904 DOI: 10.1016/j.nima.2019.163055)

Nichols, K., H. L. Andrews, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. Power, J. Shao, C. Whiteford, E. E. Wisniewski, S. Antipov and G. Chen. Demonstration of Transport of a Patterned Electron Beam Produced by Diamond Pyramid Cathode in an RF Gun. Submitted to *AIP: Journal of Physics*. (LA-UR-19-23845)

Conference Papers

Andrews, H. L., K. Nichols, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. Wisniewski, S. Antipov and G. Chen. Diamond Field Emitter Array Cathode Experimental Tests in RF Gun. Presented at *NAPAC 2019*. (Lansing, Michigan, United States, 2019-09-01 - 2019-09-06). (LA-UR-19-29010)

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)

Nichols, K., H. L. Andrews, D. Kim, E. I. Simakov, M. Conde, D. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. E. Wisniewski, S. Antipov and G. Chen. Experimental Results of Dense Array Diamond Field Emitters in RF Gun. Presented at *IPAC*. (Melbourne, Australia, 2019-05-19 - 2019-05-24). (LA-UR-19-24470)

Presentation Slides

Andrews, H. L., D. Kim, K. Nichols, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. E. Wisneiwski, S. P. Antipov and G. Chen. Shaped beams from Diamond Field-Emitter Array Cathodes. Presented at *PPPS2019*, orlando, Florida, United States, 2019-06-23 - 2019-06-28. (LA-UR-19-25996)

Andrews, H. L., K. Nichols, D. Kim, E. I. Simakov, M. Conde, D. S. Doran, G. Ha, W. Liu, J. F. Power, J. Shao, C. Whiteford, E. Wisniewski, S. Anitipov and G. Chen. Shaped Beams from Diamond Field-Emitter Array Cathodes. Presented at *NAPAC 2019*, Lansing, Michigan, United States, 2019-09-01 - 2019-09-06. (LA-UR-19-28834)

Posters

Nichols, K., D. Shchegolkov, E. I. Simakov and H. L. Andrews. MODELING OF DIAMOND FIELD EMITTER ARRAYS FOR SHAPED ELECTRON BEAM PRODUCTION. Presented at *IPAC*, Vancouver, Canada, 2018-04-29 - 2018-05-04. (LA-UR-18-23589)

Stiftel, J. G. Beam shaping for 'shoebox' accelerators. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-26792)

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

Journal Articles

*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*. **97** (7): 072011. (LA-UR-18-20811 DOI: 10.1103/PhysRevD.97.072011)

*Chu, P. -., Y. J. Kim and I. Savukov. Search for an axion-induced oscillating electric dipole moment for electrons using atomic magnetometers. 2019. *Physical Review D*. **99** (7): 075031. (LA-UR-18-28540 DOI: 10.1103/PhysRevD.99.075031)

Chu, P., Y. J. Kim and I. M. Savukov. Comment on ”Search for an axion-induced oscillating electric dipole moment forelectrons using atomic magnetometers”. Submitted to *Physical Review D*. (LA-UR-19-23854)

Chu, P., Y. J. Kim and I. M. Savukov. Search for exotic spin-dependent interactions using polarized helium. Submitted to *Physical Review D*. (LA-UR-20-21170)

*Kim, Y. J., P. Chu, I. Savukov and S. Newman. Experimental limit on an exotic parity-odd spin- and velocity-dependent interaction using an optically polarized vapor. 2019. *Nature Communications*. **10** (1): 2245. (LA-UR-19-20817 DOI: 10.1038/s41467-019-10169-1)

*Young, J. K., C. Ping-Han and I. 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*. **121** (9): 091802. (LA-UR-18-22161 DOI: 10.1103/PhysRevLett.121.091802)

Reports

Kim, Y. J. Development of New Directions in Axion Dark Matter Searches. Unpublished report. (LA-UR-19-22470)

Presentation Slides

Chu, P. Dark matter and fundamental physics using atomic magnetometers. Presented at *Telecon for axion dark matter detection*, Los Alamos, New Mexico, United States, 2019-11-26 - 2019-11-26. (LA-UR-19-31565)

Chu, P., Y. J. Kim and I. M. Savukov. Search for an Electron oscillating electric dipole moment using atomic magnetometers. Presented at *APS April 2019*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23004)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. Experimental constraint on an exotic spin- and velocity-dependent interaction with a spin-exchange relaxation-free magnetometer. Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, Waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30183)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. New constraints on exotic spin- and velocity-dependent interactions of polarized electrons with an atomic magnetometer. Presented at *APS April Meeting 2019*, Denver, Colorado, United States, 2019-04-12 - 2019-04-16. (LA-UR-19-23005)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. New experimental limits on exotic spin- and velocity-dependent interactions with a spin-exchange relaxation-free atomic magnetometer. Presented at *27th International Nuclear Physics Conference*, Glasgow, United Kingdom, 2019-07-29 - 2019-07-29. (LA-UR-19-27147)

Kim, Y. J., P. Chu, I. M. Savukov and S. G. Newman. New constraints on exotic spin- and velocity-dependent interactions of polarized electrons with an atomic magnetometer. Presented at *2019 Fall Meeting of the APS Division of Nuclear Physics*, Crystal City, Virginia, United States, 2019-10-13 - 2019-10-17. (LA-UR-19-30187)

Kim, Y. J., P. Chu and I. M. Savukov. An experimental search for exotic spin-dependent interactions with a spin-exchange relaxation-free magnetometer. Presented at *APS April Meeting*, Columbus, Ohio, United States, 2018-04-14 - 2018-04-14. (LA-UR-18-23132)

Missing Physics behind X-ray Emission from High-Energy-Density Plasmas

Thomas Weber
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 burining plasma. Our project will develop a crucial model which will allow such a temperature diagnostics.

Publications

Journal Articles

*Kagan, G., O. L. Landen, D. Svyatskiy, H. Sio, N. V. Kabadi, R. A. Simpson, M. G. Johnson, J. A. Frenje, R. D. Petrasso, R. C. Shah, T. R. Joshi, P. Hakel, T. E. Weber, H. G. 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. 2019. *Contributions to Plasma Physics*. **59** (2): 181-188. (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)

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

Journal Articles

Gandolfi, S., D. Lonardoni, A. Lovato and M. Piarulli. Quantum Monte Carlo methods and chiral EFT interactions: an overview. Submitted to *Frontiers*. (LA-UR-20-20035)

Lonardoni, D., I. Tews, S. Gandolfi and J. A. Carlson. Nuclear matter and the symmetry energy from local chiral interactions. Submitted to *Physical Review Letters*. (LA-UR-19-32538)

Lynn, J. E., D. Lonardoni, J. A. Carlson, J. W. Chen, W. Detmold, S. Gandolfi and A. Schwenk. Ab initio short-range-correlation scaling factors from light to medium-mass nuclei. Submitted to *Physical Review C*. (LA-UR-19-20911)

Lynn, J., I. Tews, S. Gandolfi and A. Lovato. Quantum Monte Carlo Methods in Nuclear Physics: Recent Advances. Submitted to *Annual Review of Nuclear and Particle Science*. (LA-UR-19-20209)

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. 2019. *The European Physical Journal A*. **55** (6): 97. (LA-UR-19-20198 DOI: 10.1140/epja/i2019-12774-6)

Reports

Gandolfi, S. LDRD Data Sheet. Unpublished report. (LA-UR-19-25844)

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

Journal Articles

Kim, H. I., H. Y. Lee, A. Georgiadou, S. A. Kuvin, L. Zavorka, T. Kawano and M. W. Herman. New evaluation on angular distributions and energy spectra for neutron-induced charged-particle measurements. 2020. *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. 163699. (LA-UR-19-28775 DOI: 10.1016/j.nima.2020.163699)

Lee, H. Y., S. M. Mosby, C. J. Prokop, A. M. Long, J. Goerres, E. Stech and M. Wiescher. Low Energy Neutron-induced Charged-particle (Z) (LENZ) instrument development with a focus on the Pulse Shape Discrimination for double-sided silicon strip detectors at LANSCE. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-19-29340)

Reports

Lee, H. Y. Pinning Down the nu-p Process Importance in Heavy Element Production via Reaction Studies on Radioactive 56Ni at LANSCE. Unpublished report. (LA-UR-17-30772)

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)

Presentation Slides

Birnbaum, E. R. and C. Vermeulen. Isotope Production Facility Capabilities and Nuclear Physics Targetry. Presented at *LANSCE User Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-05. (LA-UR-18-30446)

Grinder, M. M. and H. Y. Lee. Diamond Detectors in High Radiation Background. Presented at *NSSC-LANL Keepin Program presentation*, Los Alamos, New Mexico, United States, 2018-08-08 - 2018-08-08. (LA-UR-18-27519)

Kelly, K. J., H. Y. Lee, B. J. DiGiovine, S. A. Kuvin, L. Zavorka and A. Georgiadou. LANL experimental updates in FY19 on ChiNu and LENZ. Presented at *US Nuclear Data Week*, Brookhaven, New York, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31268)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, S. M. Mosby, F. M. Nortier, C. Vermeulen, P. Tsintari, G. Perdikakis and M. M. Grinder. Constraining the \xce\xbdp-process through the study of neutron-induced charged-particle reactions on short-lived 56Ni. Presented at *APS April Meeting*, Denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23602)

Lee, H. Y., B. J. DiGiovine, L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman, C. Vermeulen, C. Eiroa Lledo, E. R. Birnbaum, M. Brugh, S. A. Kozimor, V. Mocko, F. M. Nortier, H. I. Kim, G. Perdikakis, P. Tsintari, C. Frohlich and M. Grinder. LENZ at LANSCE: neutron-induced charged-particle reaction studies on radioactive nuclei. Presented at *CENTAUR Scientific Advisory Committee Meeting*, Los Alamos, New Mexico, United States, 2019-08-21 - 2019-08-23. (LA-UR-19-28495)

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Lee, H. Y., L. Zavorka, S. A. Kuvin, A. Georgiadou, T. Kawano, M. W. Herman and H. I. Kim. New Evaluation on Angular Distributions and Energy Spectra for Neutron-induced Charged particle Measurements. Presented at *US Nuclear*

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Lee, H. Y., S. A. Kuvin, L. Zavorka, T. Kawano, C. Vermeulen, K. Bennett, E. R. Birnbaum, M. Brugh, F. M. Nortier, G. Perdikakis, P. Tsintari, M. Grinder and C. Frohlich. First Direct Measurement on 56Ni(n,p) Reaction for Astrophysical Implication. Presented at *The Fall Meeting of Division of Nuclear Physics of the American Physical Society*, Waikoloa village, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30291)

Tsintari, P., G. Perdikakis, P. Gastis, J. Dissanayake, J. Davison, Z. Purcell, H. Y. Lee, S. A. Kuvin, L. Zavorka, A. Georgiadou and H. Kim. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *Frontiers Junior Researchers Workshop*, East Lancing, Michigan, United States, 2019-05-20 - 2019-05-21. (LA-UR-19-24752)

Tsintari, P., G. Perdikaks, J. Dissanayake, J. Davison, Z. Purcell, H. Y. Lee, S. A. Kuvin, L. Zavorka, A. Georgiadou and H. I. Kim. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *WE-Heraeus summer school on Nuclear Physics in Astrophysics*, Heidelberg, Germany, 2019-09-10 - 2019-09-14. (LA-UR-19-29020)

Vermeulen, C., H. Y. Lee, E. R. Birnbaum, F. M. Nortier, S. A. Kuvin, K. Bennett and G. Pederkakis. Radioactive Targets at Los Alamos National Laboratory: A quasi-philosophical approach. Presented at *25th Conference on Application of Accelerators in Research and Industry*, Grapevine, Texas, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27361)

Kuvin, S. A., H. Y. Lee, B. J. DiGiovine, C. Vermeulen and C. Eiroa Lledo. Measurement of the\xc2\xa059Ni(n,p) reaction at LANSCE and progress towards the first direct measurement of the 56Ni(n,p) reaction. Presented at *agnew showcase*, los alamos, New Mexico, United States, 2019-12-10 - 2019-12-10. (LA-UR-19-32221)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, M. Grinder, S. M. Mosby, F. M. Nortier, G. Perdikakis, P. Tsintari and C. Vermeulen. Constraining the nu p-process through the study of neutron-induced charged-particle reactions on short-lived 56Ni. Presented at *Conference on Compound Nuclear Reactions*, Berkeley, California, United States, 2018-09-24 - 2018-09-28. (LA-UR-18-29018)

Kuvin, S. A., H. Y. Lee, K. Bennett, E. R. Birnbaum, M. Grinder, S. M. Mosby, F. M. Nortier, G. Perdikakis, P. Tsintari and C. Vermeulen. First Direct Measurement of the 56Ni(n,p) Reaction. Presented at *LANSCE User Group Meeting*, Santa Fe, New Mexico, United States, 2018-11-05 - 2018-11-07. (LA-UR-18-30461)

Kuvin, S. A. and L. Collaboration. Progress towards the first direct measurement of the 56Ni(n,p) reaction. Presented at *Gordon Research Conference*, New London, New Hampshire, United States, 2019-06-16 - 2019-06-16. (LA-UR-19-25358)

Tsintari, P., G. Perdikakis, J. Davison, Z. Purcell, H. Y. Lee, L. Zavorka and C. Frohlich. Optimization of the LENZ detector system at LANL using GEANT4 simulations. Presented at *WE-Heraeus summer school on Nuclear Physics in Astrophysics*, Heidelberg, Germany, 2019-09-10 - 2019-09-14. (LA-UR-19-29021)

Tsintari, P., G. Perdikakis, J. Davison, Z. Purcell and H. Y. Lee. Optimization of the LENZ detector system at LANL for the study of (n,p) reactions with radioactive targets using GEANT4 simulations. . (LA-UR-18-29098)

Posters

Grinder, M., H. Iwasaki, T. Mijatovic, R. Elder, J. Ash, A. Revel, H. Y. Lee and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Implementation of a Radiation-hard Diamond Active Target. Presented at *NSSC University Program Review 2019*, Releigh, North Carolina, United States, 2019-06-04 - 2019-06-06. (LA-UR-19-24418)

Grinder, M., H. Iwasaki, T. Mijatovic, R. Elder, J. Ash, H. Y. Lee and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Diamond Detectors in High Radiation Background. Presented at *The Nuclear Science and Security Consortium Fall Workshop*, Livermore, California, United States, 2018-10-01 - 2018-10-02. (LA-UR-18-29099)

Grinder, M., H. Y. Lee, H. Iwasaki, T. Mijatovic, R. Elder, J. Ash and N. Kobayashi. Precision Lifetime Measurements of Rare Isotopes and Implementation of a Radiation-Hard Active Target. Presented at *NSSC University Program Review 2018*, Ann Arbor, Michigan, United States, 2018-06-05 - 2018-06-07. (LA-UR-18-23629)

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 has 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.

Publications

Journal Articles

*Bellm, E. C., S. R. Kulkarni, M. J. Graham, R. Dekany, R. M. Smith, R. Riddle, F. J. Masci, G. Helou, T. A. Prince, S. M. Adams, C. Barbarino, T. Barlow, J. Bauer, R. Beck, J. Belicki, R. Biswas, N. Blagorodnova, D. Bodewits, B. Bolin, V. Brinnel, T. Brooke, B. Bue, M. Bulla, R. Burruss, S. B. Cenko, C. Chang, A. Connolly, M. Coughlin, J. Cromer, V. Cunningham, K. De, A. Delacroix, V. Desai, D. A. Duev, G. Eadie, T. L. Farnham, M. Feeney, U. Feindt, D. Flynn, A. Franckowiak, S. Frederick, C. Fremling, A. Gal-Yam, S. Gezari, M. Giomi, D. A. Goldstein, V. Z. Golkhou, A. Goobar, S. Groom, E. Hacopians, D. Hale, J. Henning, A. Y. Q. Ho, D. Hover, J. Howell, T. Hung, D. Huppenkothen, D. Imel, W. Ip, Z. Ivezic, E. Jackson, L. Jones, M. Juric, M. M. Kasliwal, S. Kaspi, S. Kaye, M. S. P. Kelley, M. Kowalski, E. Kramer, T. Kupfer, W. Landry, R. R. Laher, C. Lee, H. W. Lin, Z. Lin, R. Lunnan, M. Giomi, A. Mahabal, P. Mao, A. A. Miller, S. Monkewitz, P. Murphy, C. Ngeow, J. Nordin, P. Nugent, E. Ofek, M. T. Patterson, B. Penprase, M. Porter, L. Rauch, U. Rebbapragada, D. Reiley, M. Rigault, H. Rodriguez, J. van Roestel, B. Rusholme, J. van Santen, S. Schulze, D. L. Shupe, L. P. Singer, M. T. Soumagnac, R. Stein, J. Surace, J. Sollerman, P. Szkody, F. Taddia, S. Terek, A. Van Sistine, S. van Velzen, W. T. Vestrand, R. Walters, C. Ward, Q. Ye, P. Yu, L. Yan and J. Zolkower. The Zwicky Transient Facility: System Overview, Performance, and First Results. 2019. *Publications of the Astronomical Society of the Pacific*. **131** (995): 018002. (LA-UR-19-22558 DOI: 10.1088/1538-3873/aaecbe)

*Graham, M. J., S. R. Kulkarni, E. C. Bellm, S. M. Adams, C. Barbarino, N. Blagorodnova, D. Bodewits, B. Bolin, P. R. Brady, S. B. Cenko, C. Chang, M. W. Coughlin, K. De, G. Eadie, T. L. Farnham, U. Feindt, A. Franckowiak, C. Fremling, S. Gezari, S. Ghosh, D. A. Goldstein, V. Z. Golkhou, A. Goobar, A. Y. Q. Ho, D. Huppenkothen, Z. Ivezic, R. L. Jones, M. Juric, D. L. Kaplan, M. M. Kasliwal, M. S. P. Kelley, T. Kupfer, C. Lee, H. W. Lin, R. Lunnan, A. A. Mahabal, A. A. Miller, C. Ngeow, P. Nugent, E. O. Ofek, T. A. Prince, L. Rauch, J. van Roestel, S. Schulze, L. P. Singer, J. Sollerman, F. Taddia, L. Yan, Q. Ye, P. Yu, T. Barlow, J. Bauer, R. Beck, J. Belicki, R. Biswas, V. Brinnel, T. Brooke, B. Bue, M. Bulla, R. Burruss, A. Connolly, J. Cromer, V. Cunningham, R. Dekany, A. Delacroix, V. Desai, D. A. Duev, M. Feeney, D. Flynn, S. Frederick, A. Gal-Yam, M. Giomi, S. Groom, E. Hacopians, D. Hale, G. Helou, J. Henning, D. Hover, L. A. Hillenbrand, J. Howell, T. Hung, D. Imel, W. Ip, E. Jackson, S. Kaspi, S. Kaye, M. Kowalski, E. Kramer, M. Kuhn, W. Landry, R. R. Laher, P. Mao, F. J. Masci, S. Monkewitz, P. Murphy, J. Nordin, M. T. Patterson, B. Penprase, M. Porter, U. Rebbapragada, D. Reiley, R. Riddle, M. Rigault, H. Rodriguez, B. Rusholme, J. van Santen, D. L. Shupe, R. M. Smith, M. T. Soumagnac, R. Stein, J. Surace, P. Szkody, S. Terek, A. Van Sistine, S. van Velzen, W. T. Vestrand, R. Walters, C. Ward, C. Zhang and J. Zolkower. The Zwicky Transient Facility: Science Objectives. 2019. *Publications of the Astronomical Society of the Pacific*. **131** (1001): 078001. (LA-UR-19-30653 DOI: 10.1088/1538-3873/ab006c)

Vestrand, W. T., P. F. Bloser, A. S. Hoover, L. P. Parker and J. Wren. The Mini Astrophysical MeV Background Observatory (MAMBO): A CubeSat for measuring the MeV Extragalactic Gamma-Ray Background. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-26775)

Vestrand, W. T. and L. P. Parker. Optical Emission from Fossil Cosmic Ray Reservoirs. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-27021)

Using Quarkonia to Probe Matter from the Early Universe

Ivan Vitev
20190033ER

Project Description

A millionth of a second after the Big Bang, while still at a temperature of several trillion degrees, the entire universe transitioned through a phase of matter we are only beginning to understand--- the quark-gluon plasma (QGP), a hot and dense soup of the most fundamental microscopic constituents that make up the visible world. As this strongly interacting plasma expanded and cooled down, quarks and gluons clumped together into bound states to form a gas of particles called hadrons. This phase transition is of great interest to particle and nuclear physics, cosmology and astrophysics. It was predicted to affect the density of dark matter, and result in gravitational waves that probe the QGP properties. Heavy ion physics is a forefront area of research at the interface of high-energy and nuclear science that seeks to recreate these primordial states of matter of the early universe in controlled laboratory conditions and pin down their properties by colliding nuclei at ultrarelativistic energies. We will develop a new theory that describes some of the heaviest elementary particles produced in nature, called quarkonia, and use them to determine the properties of a primordial state of matter created in heavy ion collisions and the early universe.

Publications

Journal Articles

Fleming, S., Y. Makris and T. Mehen. An effective field theory approach to quarkonium at small transverse momentum. Submitted to *Journal of High Energy Physics*. (LA-UR-19-31110)

*Gao, A., H. T. Li, I. Moult and H. X. Zhu. Precision QCD Event Shapes at Hadron Colliders: The Transverse Energy-Energy Correlator in the Back-to-Back Limit. 2019. *Physical Review Letters*. **123** (6): 062001. (LA-UR-19-20914 DOI: 10.1103/PhysRevLett.123.062001)

Gutierrez-Reyes, D., Y. Makris, V. P. Vaidya, I. Scimemi and L. Zoppi. Probing Transverse-Momentum Distributions With Groomed Jets. Submitted to *Journal of High Energy Physics*. (LA-UR-19-31102)

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*Li, C. S., H. T. Li, D. Y. Shao and J. Wang. Momentum-space threshold resummation in tW production at the LHC. 2019. *Journal of High Energy Physics*. **2019** (6): 125. (LA-UR-19-21475 DOI: 10.1007/JHEP06(2019)125)

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Makris, Y. and I. M. Vitev. An Effective Theory of Quarkonia in QCD Matter. Submitted to *Journal of High Energy Physics*. (LA-UR-19-25833)

*Sievert, M. D., I. Vitev and B. Yoon. A complete set of in-medium splitting functions to any order in opacity. 2019. *Physics Letters B*. **795**: 502-510. (LA-UR-19-22343 DOI: 10.1016/j.physletb.2019.06.019)

Vitev, I. M. Aspects of heavy flavor jet physics in heavy ion collisions. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30718)

Vitev, I. M. Toward an effective theory of quarkonium production in nuclear matter. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-30716)

Vitev, I. M., B. Yoon, Z. Kang and J. Reiten. Light and heavy flavor dijet production and dijet mass modification in heavy ion collisions}. Submitted to *Physical Review D*. (LA-UR-19-22344)

Reports

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)

Ultra-Cold Neutron Experiment for Proton Branching Ratio in Neutron Beta Decay (UCNProBe)

Zhaowen Tang
20190048ER

Project Description

The free neutron decay lifetime is vital across many fields of physics. The Department of Energy Office of Science, Nuclear Physics has identified resolving the beam and bottle neutron lifetime discrepancy as a prerequisite to the next generation neutron lifetime experiments. The successful execution of this project will position the Laboratory to solve this lifetime discrepancy. The confirmation of the bottle lifetime results will be a vital piece of information for the nuclear physics community and help pave the way for a next generation ultracold neutron (UCN) based lifetime experiment; the confirmation of the beam lifetime results would demonstrate beyond the Standard Model (SM) of physics, and be truly extraordinary.

Publications

Presentation Slides

Hassan, M. T. An experiment to measure the Proton Branching Ratio in Neutron Beta Decay (UCNProBe). Presented at *APS DNP 2019*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30666)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *Particle Physics with Neutrons at the ESS*, stockholm, Sweden, 2018-12-10 - 2018-12-14. (LA-UR-18-31486)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *APS April Meeting 2019*, denver, Colorado, United States, 2019-04-13 - 2019-04-16. (LA-UR-19-23299)

Tang, Z. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *Fundamental physics with neutron beta decay*, Seattle, Washington, United States, 2019-11-04 - 2019-11-08. (LA-UR-19-31233)

Tang, Z., C. Morris, J. H. Choi and D. E. Fellers. Search for the Neutron Decay n\xe2\x9f\xb6\xf0\x9d\x9b\xbe+X, where X is a dark matter particle. Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30026)

Tang, Z., J. C. Lambert, C. Morris and S. Clayton. Ultra-Cold Neutron measurement of Proton branching ratio in neutron Beta decay (UCNProBe). Presented at *5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan*, waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30027)

Wideband Sub-Millimeter Source for Deployed Applications

Kip Bishofberger
20190066ER

Project Description

We are developing a wideband amplifier system that can yield significant power over a wide range of frequencies. The system is compact and power-efficient for low size, weight, and power applications. Project results could potentially impact several Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) mission areas. Several potential future applications are described below. Project results could impact Mono/bistatic Radar Time-domain Spectroscopy. Results from this project could ultimately support a capability to probe a cloud, smoke column, or atmospheric region. A large bandwidth would allow one system to be used to detect a wide variety of chemical signatures. Project results could impact Space-based Spectroscopy; future applications could allow most of the atmospheric column to be analyzed via a system deployed from orbit. Project results could impact Secure Communications; a small wavelength would enable small antennas to communicate (at very high bandwidths), without unintended listeners (e.g., satellites, aircraft, binoculars). Project results could impact Materials Inspection; although dielectrics are transparent, the high resolution anticipated through this project would ultimately allow the detection of millimeter-scale features (e.g., high-Z, circuitry) for improvised explosive device (IED) and special nuclear material (SNM detection).

Publications

Conference Papers

Neben, D. E., K. A. Bishofberger, V. Pavlenko and N. Yampolsky. Design of a Source for Millimeter-wave Ultra-wide Bandwidth Applications Using the Two-stream Instability. Presented at *International Vacuum Electronics Conference*. (Monterey, California, United States, 2020-04-20 - 2020-04-23). (LA-UR-20-21994)

Ultralight Bosonic Dark Matter Search with an Optically Pumped Magnetometer

Leanne Duffy
20190113ER

Project Description

Modern cosmological observations lead to the conclusion that most of the matter in the Universe is of an undiscovered form. Matter that interacts with light contributes only 20% of the Universe’s matter, with the remaining 80% given by dark matter, inferred via its gravitational effects on visible matter and radiation. Discovering the nature of dark matter is one priority of Cosmic Frontier research funded by the Department of Energy Office of Science, High Energy Physics program. Los Alamos National Laboratory has a unique intersection of leadership in axion physics with world-leading magnetic field detection capabilities through the development and application of optically pumped magnetometers, and an existing magnet that can be applied to develop the next level of sensitivity in axion searches. We estimate that our proposed experiment can probe axion specific axion masses with a sensitivity that is up to 4 orders of magnitude beyond the existing best limit. Our ultimate goal is to reveal the nature of the Universe's dark matter. At the very least, we will provide significant new limits on the properties of the dark matter.

Publications

Presentation Slides

Kim, Y. J., P. Chu, I. M. Savukov, S. G. Newman, L. D. Duffy and A. V. Urbaitis. Dark Matter and Fundamental Physics Searches using Atomic Magnetometers. Presented at *CPAD Instrumentation Frontier Workshop 2019*, Madison, Wisconsin, United States, 2019-12-08 - 2019-12-10. (LA-UR-19-31996)

Hot Electron Beam Generation and Transport for Fast Ignition

Sasikumar Palaniyappan
20190124ER

Project Description

Inertial confinement fusion (ICF) is one of the grand challenges of this century due to its potential to provide an unlimited amount of clean energy. In laser-driven ICF, a high-energy nanosecond laser compresses a mixture of deuterium (D) and tritium (T) fuel inside a capsule to very high-density and temperature and initiates nuclear fusion reactions. Despite decades of research, laboratory fusion is still elusive. Electron fast ignition is a variant of ICF where the fuel is first compressed to high density using a long-pulse (nanosecond) laser and then ignited by a hot-electron beam generated from a short-pulse (picosecond) laser interaction with a gold cone tip, where the short pulse laser is usually brought into the assembled dense fuel via a re-entrant cone. The current cone-in-shell design suffers due to large electron beam divergence. This proposal will address the crippling deficiencies in electron fast ignition by generating a near-collimated hot-electron beam using near-critical plasmas and transport it effectively from the source to the dense fuel with the aid of resistive magnetic collimation.

Publications

Journal Articles

Li, F., P. K. Singh, S. Palaniyappan and C. Huang. Parameterization of nonlinear particle resonances in direct laser acceleration. Submitted to *Physical Review Letters*. (LA-UR-20-22447)

Presentation Slides

Huang, C., F. Li, P. K. Singh and S. Palaniyappan. Transport of low-divergence high-current electron beams in a high density plasma. Presented at *49th Annual Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-10 - 2019-06-14. (LA-UR-19-25186)

Li, F., C. Huang, P. K. Singh and S. Palaniyappan. Electron beam properties from combined direct laser acceleration and plasma acceleration in regimes relevant to fast ignition. Presented at *49th Anomalous Absorption Conference*, Telluride, Colorado, United States, 2019-06-09 - 2019-06-14. (LA-UR-19-25253)

Li, F., C. Huang, P. K. Singh and S. Palaniyappan. Towards controlled laser acceleration of electrons in laser-plasma coupling regimes relevant to fast ignition. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30695)

A New Computation Framework for the Nonlinear Beam Dynamics with Radiation Self-fields

Chengkun Huang
20190131ER

Project Description

The development of X-ray Free Electron Lasers (FELs) and compact advanced accelerators provides the foundation to address the control of performance and production of materials at the mesoscale, a major challenge in national security missions. The continuing quest to enhance the performance/functionality of X-ray FELs and advance accelerators demands techniques to manipulate electron beams with the highest brightness. However, nonlinear beam dynamic problems often arise in the generation and control of such beams. State-of-the-art theoretical and simulation models lack the accuracy and physics consistency to fully address these outstanding beam dynamic problems. We will design and implement a new simulation framework to treat the self-consistent dynamics of a relativistic particle beam interacting with its complete radiation self-fields. With the unprecedented accuracy and physics consistency, this tool will be applied to the evaluation of high risk component design in free electron lasers.

Publications

Conference Papers

Li, F., C. Huang, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Validation of a novel method for the calculation of near-field synchrotron radiation. Presented at *10th International Particle Accelerator Conference*. (Melbourne, Australia, 2019-05-19 - 2019-05-24). (LA-UR-19-24377)

Reports

Yeung, O. B. Validation of Two-Dimensional Near-Field Synchrotron Radiation Solver. Unpublished report. (LA-UR-19-27333)

Presentation Slides

Huang, C. Particle accelerators: present, future and the enabling computational modeling. . (LA-UR-19-31915)

Huang, C., F. Li, O. B. Yeung, P. P. Pombrio, B. Shen, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Comparison of Numerical Methods for the Calculation of Synchrotron Radiation from Electrons. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30731)

Li, F., C. Huang, O. B. Yeung, B. Shen, P. P. Pombrio, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Comparison of Numerical Methods for the Calculation of Synchrotron Radiation from Electrons. Presented at *North American Particle Accelerator Conference*, Lansing, Michigan, United States, 2019-09-01 - 2019-09-06. (LA-UR-19-28858)

Shen, B. Numerical Method and Parallelization for the Computation of Synchrotron Radiation. Presented at *Super Computing 2019*, Denver, Colorado, United States, 2019-11-17 - 2019-11-17. (LA-UR-19-27982)

Yeung, O. B. Design and Validation of a Solver for Synchrotron Radiation. Presented at *LANL SULI Presentations, on-site*, Los Alamos, New Mexico, United States, 2019-07-17 - 2019-07-17. (LA-UR-19-27178)

Posters

Li, F., C. Huang, R. V. Garimella, T. J. T. Kwan and B. E. Carlsten. Validation of a novel method for the calculation of near-field synchrotron radiation. Presented at *10th International Particle Accelerator Conference*, Melbourne, Australia, 2019-05-19 - 2019-05-24. (LA-UR-19-24589)

Shen, B. Numerical Method and Parallelization for the Computation of Synchrotron Radiation. Presented at *Super Computing 19*, Denver, Colorado, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-27461)

Shen, B. Numerical Method for the Computation of Synchrotron Radiation in the Near-Field. Presented at *PCSRI Outbrief Presentations*, Los alamos, New Mexico, United States, 2019-07-30 - 2019-07-30. (LA-UR-19-27494)

The Influence of Multiple Scattering on the Opacities of Warm and Hot Dense Matter

Charles Starrett
20190206ER

Project Description

Opacity is a key quantity in weapons physics as well as inertial fusion and astrophysics. Our project will develop an new computational capability for opacity in dense plasmas -- a significant improvement over existing methods. The key advantage of our approach is that plasma effects will be fully accounted for in a non-perturbative way, in contrast to existing methods. We will apply this to open and enigmatic experiments that point to weaknesses in current approaches.

Publications

Reports

Gill, N. M. Modeling of Warm Dense Plasmas for the Determination of Transport Properties and Equation of State. Unpublished report. (LA-UR-20-22190)

Presentation Slides

Starrett, C. E. Electronic structure of Dense Plasma's with the Green's Function Method. . (LA-UR-19-29084)

Posters

Hanson, C. J., M. W. Laraia, C. E. Starrett, N. R. Shaffer and D. P. Kilcrease. Microfield distributions from pseudoatom molecular dynamics & Real-space structures for multiple scattering green's functions. . (LA-UR-19-27904)

Starrett, C. E. Using the Green's Function Multiple Scattering Method to Model Warm and Hot Dense Matter. Presented at *2019 Workshop on Recent Developments in Electronic Structure*, Urbana, Illinois, United States, 2019-05-19 - 2019-05-19. (LA-UR-19-24197)

A Non-Invasive Current Profile Diagnostic for Electron Bunches

Quinn Marksteiner
20190294ER

Project Description

This project will develop an electron beam diagnostic that will help resolve many important physics issues for high energy electron accelerators. This diagnostic will be of particular importance for accelerator capabilities, where a non-invasive diagnostic with short (femtosecond) resolution is needed to address important issues such as the microbunching instability and long-range wakes. In addition, the Department of Energy Office of Science Advanced Accelerator Development Strategy Report specifically calls out the need for diagnostics with femtosecond resolution, for laser-driven plasma wakefield accelerators and for particle-beam-driven plasma wakefield accelerators.

Publications

Presentation Slides

Marksteiner, Q. R., H. L. Andrews, S. Barber, J. E. Coleman, C. Emma, B. W. Ostler, W. P. Romero, R. Ryne and N. Yampolsky. Using off axis undulator radiation as a longitudinal current diagnostic. Presented at *Advanced Control Methods for Particle Accelerators*, Santa Fe, New Mexico, United States, 2019-08-20 - 2019-08-22. (LA-UR-19-28705)

Origin of High-Energy Astrophysical Neutrinos: Multi-messenger Signals from Flares of Extragalactic Jets

Hui Li
20190383ER

Project Description

This project aims at understanding the origin of high-energy astrophysical neutrinos, especially those made by relativistic jets powered by supermassive black holes. This is a fundamental question in our understanding of the cosmos. This project brings together theory, numerical modeling, observations in optical and gamma-rays. It builds capabilities in particle and gamma-ray detectors, as well as large-scale supercomputing techniques that are suitable for next-generation exascale computers and numerical modeling.

Publications

Journal Articles

*Abeysekara, A. U., A. Albert, R. Alfaro, C. Alvarez, J. D. Alvarez, J. R. Angeles Camacho, R. Arceo, J. C. Arteaga-Velazquez, K. P. Arunbabu, D. Avila Rojas, H. A. A. Solares, V. Baghmanyan, E. Belmont-Moreno, S. Y. BenZvi, C. Brisbois, K. S. Caballero-Mora, T. Capistran, A. Carraminana, S. Casanova, U. Cotti, J. Cotzomi, S. Coutino de Leon, E. De la Fuente, C. de Leon, S. Dichiara, B. L. Dingus, M. A. DuVernois, J. C. Diaz-Velez, R. W. Ellsworth, K. Engel, C. Espinoza, B. Fick, H. Fleischhack, N. Fraija, A. Galvan-Gamez, J. A. Garcia-Gonzalez, F. Garfias, M. M. Gonzalez, J. A. Goodman, J. P. Harding, S. Hernandez, J. Hinton, B. Hona, F. Hueyotl-Zahuantitla, C. M. Hui, P. Huntemeyer, A. Iriarte, A. Jardin-Blicq, V. Joshi, S. Kaufmann, D. Kieda, A. Lara, W. H. Lee, H. Leon Vargas, J. T. Linnemann, A. L. Longinotti, G. Luis-Raya, J. Lundeen, K. Malone, S. S. Marinelli, O. Martinez, I. Martinez-Castellanos, J. Martinez-Castro, H. Martinez-Huerta, J. A. Matthews, P. Miranda-Romagnoli, J. A. Morales-Soto, E. Moreno, M. Mostafa, A. Nayerhoda, L. Nellen, M. Newbold, M. U. Nisa, R. Noriega-Papaqui, A. Peisker, E. G. Perez-Perez, J. Pretz, Z. Ren, C. D. Rho, C. Riviere, D. Rosa-Gonzalez, M. Rosenberg, E. Ruiz-Velasco, H. Salazar, F. S. Greus, A. Sandoval, M. Schneider, H. Schoorlemmer, M. S. Arroyo, G. Sinnis, A. J. Smith, R. W. Springer, P. Surajbali, E. Tabachnick, M. Tanner, O. Tibolla, K. Tollefson, I. Torres, T. Weisgarber, S. Westerhoff, J. Wood, T. Yapici, A. Zepeda and H. Zhou. Measurement of the Crab Nebula Spectrum Past 100 TeV with HAWC. 2019. *The Astrophysical Journal*. **881** (2): 134. (LA-UR-19-24703 DOI: 10.3847/1538-4357/ab2f7d)

Guo, F., X. Li, W. S. Daughton, H. Li, Y. Liu, W. Yan and D. D. Ma. Determining the Dominant Acceleration Mechanism during Relativistic Magnetic Reconnection in Large-scale Systems. Submitted to *Physical Review Letters*. (LA-UR-18-31752)

H. Kilian, P. F., X. Li, F. Guo and H. Li. Exploring the acceleration mechanisms for particle injection and power-law formation during trans-relativistic magnetic reconnection. Submitted to *Astrophysical Journal*. (LA-UR-20-20135)

Kong, X., F. Guo, Y. Chen and J. Giacalone. THE ACCELERATION OF ENERGETIC PARTICLES AT CORONAL SHOCKS AND EMERGENCE OF A DOUBLE POWER LAW FEATURE IN PARTICLE ENERGY SPECTRA. Submitted to *Astrophysical Journal*. (LA-UR-19-20913)

Polko, P. and H. Li. Self-similar jet models: two new issues. Submitted to *Astrophysical Journal*. (LA-UR-19-30944)

Zhang, H., X. Li, D. Giannios, F. Guo, Y. Liu and L. Dong. Radiation and Polarization Signatures from Magnetic Reconnection in Relativistic Jets–I. A Systematic Study. Submitted to *Astrophysical Journal*. (LA-UR-20-20194)

Conference Papers

Dong, B., P. F. H. Kilian, X. Li, F. Guo, S. Byna and K. Wu. Terabyte-scale Particle Data Analysis: An ArrayUDF Case Study. Presented at *SSDBM 2019 : 31st International Conference on Scientific & Statistical Database Management*. (Santa Cruz, California, United States, 2019-07-23 - 2019-07-25). (LA-UR-19-24098)

Malone, K. A. Recent Results from the High Altitude Water Cherenkov Observatory. Presented at *International Symposium on Multiparticle Dynamics*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-13). (LA-UR-20-21318)

Reports

Rani, B., H. Zhang, S. Hunter, F. Kislat, M. Boettcher, J. E. McEnery, D. Giannios, F. Guo, H. Li, M. G. Baring, I. Agudo, S. Buson, M. Petropoulou, V. Pavlidou, E. Angelakis, I. Myserlis, Z. Wadiasingh, R. Curado da Silva, P. F. H. Kilian,

S. Guiriec, V. Bozhilov, S. Anton, M. Kazana, P. Coppi, T. M. Venters, F. Longo and E. Bottachini. High-Energy Polarimetry - a new window to probe extreme physics in AGN jets. Unpublished report. (LA-UR-19-22708)

Presentation Slides

Guo, F. IC Project: Magnetic Reconnection versus Shocks: First-principles Kinetic Simulations of Major Particle Acceleration Mechanisms in the Universe. . (LA-UR-19-21782)

H. Kilian, P. F., X. Li, F. Guo and H. Li. How magnetic reconnection injects particles and accelerates them to high energies. Presented at *19th Annual International Astrophysics Conference*, Santa Fe, New Mexico, United States, 2020-03-09 - 2020-03-13. (LA-UR-20-22043)

H. Kilian, P. F. and F. Guo. Particle Acceleration due to Relativistic Reconnection. Presented at *235th AAS meeting*, Honolulu, Hawaii, United States, 2020-01-05 - 2020-01-08. (LA-UR-20-20084)

Li, H. All Hands On Deck: Understanding Astrophysical Jets. . (LA-UR-19-32437)

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 Department of Energy endeavor.

Technical Outcomes

We set up a theoretical framework to connect the new physics generating lepton number non-conservation at very high energy scales to energy scales relevant to nuclear decay. Our work is a key element in the interpretation of upcoming experimental searches. Our analysis has culminated in a master formula for the nuclear half-life. In the process, we discovered several new leading contributions previously missed in the literature, which significantly impacts the measurement of the neutrino mass.

Publications

Journal Articles

*Alioli, S., V. Cirigliano, W. Dekens, J. Vries and E. Mereghetti. Right-handed charged currents in the era of the Large Hadron Collider. 2017. *Journal of High Energy Physics*. **2017** (5): 86. (LA-UR-17-21898 DOI: 10.1007/JHEP05(2017)086)

Brantley, D., E. Mereghetti, J. Balint, E. Mastropas, H. Monge Camacho, K. Orginos, B. Tiburzi and A. Walker-Loud. Strong isospin violation and chiral logarithms in the baryon spectrum. Submitted to *Physical Review C*. (LA-UR-16-29618)

*Cirigliano, V., W. Dekens, E. Mereghetti and A. Walker-Loud. Neutrinoless double beta decay in effective field theory: The light-Majorana neutrino-exchange mechanism. 2018. *Physical Review C*. **97** (6): 065501. (LA-UR-17-28401 DOI: 10.1103/PhysRevC.97.065501)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser, E. Mereghetti, S. Pastore and U. van Kolck. New Leading Contribution to Neutrinoless Double-\xce\xb2 Decay. 2018. *Physical Review Letters*. **120** (20): 202001. (LA-UR-18-21404 DOI: 10.1103/PhysRevLett.120.202001)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser and E. Mereghetti. Neutrinoless double beta decay in chiral effective field theory: lepton number violation at dimension seven. 2017. *Journal of High Energy Physics*. **2017** (12): 82. (LA-UR-17-27799 DOI: 10.1007/JHEP12(2017)082)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser and E. Mereghetti. A neutrinoless double beta decay master formula from effective field theory. 2018. *Journal of High Energy Physics*. **2018** (12): 97. (LA-UR-18-24895 DOI: 10.1007/JHEP12(2018)097)

*Cirigliano, V., W. Dekens, J. de Vries and E. Mereghetti. An \xcf \xb5 # improvement from right-handed currents. 2017. *Physics Letters B*. **767**: 1-9. (LA-UR-16-28961 DOI: 10.1016/j.physletb.2017.01.037)

Cirigliano, V., W. Dekens, M. Graesser and E. Mereghetti. Neutrinoless double beta decay and chiral SU (3). 2017. *Physics Letters B*. **769**: 460-464. (LA-UR-17-20043 DOI: 10.1016/j.physletb.2017.04.020)

Mereghetti, E., V. Cirigliano, W. G. Dekens, J. de Vries, M. L. Graesser, S. Pastore, M. Piarulli, U. Van Kolck and R. B. Wiringa. A renormalized approach to neutrinoless double beta decay. Submitted to *Physical Review C*. (LA-UR-19-26002)

*Pastore, S., J. Carlson, V. Cirigliano, W. Dekens, E. Mereghetti and R. B. Wiringa. Neutrinoless double- decay matrix elements in light nuclei. 2018. *Physical Review C*. **97** (1): 014606. (LA-UR-17-29297 DOI: 10.1103/PhysRevC.97.014606) *de Vries, J., E. Mereghetti, C. Seng and A. Walker-Loud. Lattice QCD spectroscopy for hadronic CP violation. 2017. *Physics Letters B*. **766**: 254-262. (LA-UR-16-29007 DOI: 10.1016/j.physletb.2017.01.017)

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 length 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 and build underlying science of interest to the DOE. The observational signatures published by this work will be directly used by National Aeronautics and Space Administration (NASA) surveys such as James Webb Space Telescope (JWST) to classify supermassive black holes, as well as surveys that collaborate with NASA efforts such as Atcama Large Millimeter Array (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.

Technical Outcomes

This project advanced understanding of how black holes form, how they affect local star formation, how turbulence drives their accretion disks, how they can be distinguished from Pop III star bursts, and their observational signatures. The observational signatures published by this work will be directly used by NASA surveys to classify supermassive black holes. Other notable accomplishments of the project include compelling supercomputer visualizations of black hole physics.

Publications

Journal Articles

Aykutalp, 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. Aykutalp and J. H. Wise. Observational signatures of massive black hole formation in the early Universe. 2018. *Nature Astronomy*. **2** (12): 987-994. (LA-UR-17-30611 DOI: 10.1038/s41550-018-0569-y)

*S. Barrow, K. S., J. H. Wise, A. Aykutalp, B. W. O'Shea, M. L. Norman and H. Xu. First light – II. Emission line extinction, population III stars, and X-ray binaries. 2018. *Monthly Notices of the Royal Astronomical Society*. **474** (2): 2617-2634. (LA-UR-17-28139 DOI: 10.1093/mnras/stx2973)

Clark, S. J. and J. M. Smidt. Answers to Student Interview Questions. Submitted to *Southern Utah University News*. (LA-UR-19-25223)

*Johnson, J. L. and A. Aykutalp. Extreme Primordial Star Formation Enabled by High-redshift Quasars. 2019. *The Astrophysical Journal*. **879** (1). (LA-UR-18-31390 DOI: 10.3847/1538-4357/ab223e)

Lloyd-Ronning, N. M., A. Aykutalp and J. L. Johnson. On the Cosmological Evolution of Long Gamma-Ray Burst Properties. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-19-25015)

*Smidt, J., D. J. Whalen, J. L. Johnson, M. Surace and H. Li. Radiation Hydrodynamical Simulations of the First Quasars. 2018. *The Astrophysical Journal*. **865** (2): 126. (LA-UR-16-28026 DOI: 10.3847/1538-4357/aad7b8)

*Waters, T. and D. Proga. Non-isobaric Thermal Instability. 2019. *The Astrophysical Journal*. **875** (2): 158. (LA-UR-18-30430 DOI: 10.3847/1538-4357/ab10e1)

*Waters, T. and D. Proga. Magnetothermal disc winds in X-ray binaries: poloidal magnetic fields suppress thermal winds. 2018. *Monthly Notices of the Royal Astronomical Society*. (LA-UR-18-25178 DOI: 10.1093/mnras/sty2398)

*Waters, T. and D. Proga. Cloud Coalescence: A Dynamical Instability Affecting Multiphase Environments. *Astrophysical Journal Letters*. **876** (1). (LA-UR-19-26958 DOI: 10.3847/2041-8213/ab12e8)

Reports

Black, W. K. Primordial Origins of Supermassive Black Holes. Unpublished report. (LA-UR-18-26505)

Presentation Slides

Aykutalp, A. Finding infant massive black holes in the early universe with James Webb Space Telescope. . (LA-UR-18-30431)

Johnson, J. L. Formation Mechanisms of Black Hole Seeds in the Early Universe. Presented at *Accretion signatures of the earliest black holes in the universe*, Princeton, New Jersey, United States, 2019-04-03 - 2019-04-05. (LA-UR-19-23095)

Waters, T. R. Thermal Instability in the presence of turbulence. Presented at *Multiphase AGN feeding and feedback*, Sesto, Italy, 2018-07-09 - 2018-07-13. (LA-UR-18-26583)

Posters

Aykutalp, A. Co-evolution of Black Holes and Stellar Populations in the Early Universe. Presented at *2017 LANL Postdoctoral Research Symposium*, Los Alamos, New Mexico, United States, 2017-08-29 - 2017-08-31. (LA-UR-17-27288)

Waters, T. R. and I. D. Ruh. Exploring a new astrophysical gas dynamical instability on GPUs. . (LA-UR-19-26959)

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.

Technical Outcomes

This project successfully created a laboratory turbulent magnetic dynamo, and measured the large fields produced, and a growth rate of those fields twice as fast as models predict. This rate of growth has large implications for the dynamics in an ICF capsule if similar conditions exist, which is likely given that we know the fill-tube makes a jet (similar to the one we made), and which may explain the reduced yields.

Publications

Journal Articles

*Liao, A. S., L. Shengtai, L. Hui, K. Flippo, D. Barnak, K. Van Kelso, C. Fiedler Kawaguchi, A. Rasmus, S. Klein, J. Levesque, C. Kuranz and L. Chikang. Design of a new turbulent dynamo experiment on the OMEGA-EP. 2019. *Physics of Plasmas*. **26** (3): 32306. (LA-UR-18-30966 DOI: 10.1063/1.5081062)

Reports

Rasmus, A. M. Shock driven discrete vortex growth on oblique interfaces. Unpublished report. (LA-UR-18-26572)

Presentation Slides

Flippo, K. A. Platforms for advanced studies of self-generated fields in ICF and Astrophysics and other future designs. . (LA-UR-17-30572)

Flippo, K. A. High Energy Density Hydrodynamics and ICF Experiments at Los Alamos National Lab. . (LA-UR-19-26212)

Flippo, K. A., H. Li, B. J. Albright, A. S. Liao, S. Li, Y. Lu, D. H. Barnak, A. M. Rasmus, C. Y. Fiedler Kawaguchi, K. V. Kelso, T. Weber, E. N. Loomis, Y. H. Kim, T. J. Murphy, A. Zylstra, C. C. Kuranz, S. R. Klein, A. Angulo, J. Levesque, C. Li and P. Tzeferacos. Self-Generated Magnetic Fields in High Energy Density Laboratory Experiments. Presented at *American Physical Society Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30589)

Li, H. Dynamics of Dust-Gas Interactions in Protoplanetary Disks and Implications for Planetesimal Formation. . (LA-UR-17-29301)

Li, H. Exploring Astrophysical Jet Physics Using Laboratory Plasma Experiments. . (LA-UR-17-29300)

Li, H. Laboratory Plasma Astrophysics: Progress and Future Prospects. Presented at *First Asia-Facific Conference on Plasma Physics*, Chengdu, China, 2017-09-18 - 2017-09-22. (LA-UR-17-29302)

Li, H. Modeling of Polarization Signatures of AGN Blazars. . (LA-UR-17-29299)

Liao, A. S. Astrophysical Turbulent Dynamos in High Energy Density Laboratory Plasmas. Presented at *61st Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30707)

Rasmus, A. M., K. A. Flippo, A. V. Stier, T. Weber, G. Williams, D. Marsical, H. Levefre, J. Levesque and C. Kuranz. Fiber Optic Pulsed Polarimetry on the Jupiter Laser Facility. Presented at *NIF/JLF user group meeting*, Livermore, California, United States, 2018-02-05 - 2018-02-07. (LA-UR-18-20853)

Posters

Chien, A., L. Gao, H. Ji, K. Hill, J. Fuchs, S. Chen, A. Fazzini, B. Bleotu, R. Takizawa, A. M. Rasmus, X. Yuan and H. Chen. Magnetically-Driven Reconnection using Laser-Powered Capacitor Coils on the Titan Laser. Presented at *NIF and JLF User Group Meeting 2020*, Livermore, California, United States, 2020-02-03 - 2020-02-05. (LA-UR-20-21800)

Flippo, K. A., A. M. Rasmus, H. Li, S. Li, C. C. Kuranz, J. Levesque, S. Kline and P. Tzeferacos. Toward a turbulent magnetic dynamo platform. Presented at *American Physical Society 59th meeting of the Division of Plasma Physics*, Milwaukee, Wisconsin, United States, 2017-10-23 - 2017-10-23. (LA-UR-17-29699)

Liao, A. S., D. H. Barnak, K. A. Flippo, Y. Lu, S. Li, H. Li, A. M. Rasmus, S. R. Klein, J. Levesque, C. C. Kuranz and C. Li. Turbulent Dynamo in Laboratory Plasma. Presented at *2019 International Conference on Numerical Simulation of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28862)

Liao, A. S., S. Li, H. Li, K. A. Flippo and C. Li. Numerical Simulation of an Experimental Turbulent Dynamo on the OMEGA-EP Laser. Presented at *60th Annual Meeting of the APS Division of Plasma Physics Co-Located with the 71st Annual Gaseous Electronics Conference*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30473)

Liao, A. S., S. Li, K. A. Flippo, H. Li and C. Li. A Turbulent Dynamo Experiment on the OMEGA-EP. Presented at *12th International Conference on High Energy Density Laboratory Astrophysics*, Kurashiki, Japan, 2018-05-28 - 2018-06-01. (LA-UR-18-24529)

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.

Technical Outcomes

We have developed a complete quantum-kinetic description of the early universe from the high temperature epoch of weak decoupling, through Big Bang nucleosynthesis (BBN), to electron-positron violation. Focusing on the neutrino component of the weak plasma in the early universe, which is needed for a precise description of the production of light nuclei in BBN, we have established that the neutrinos exhibit the ubiquitous phenomenon of quantum coherence, which potentially persists to the present day.

Publications

Journal Articles

*Anderson, P. R., E. Mottola and D. H. Sanders. Decay of the de Sitter vacuum. 2018. *Physical Review D*. **97** (6): 065016. (LA-UR-17-28548 DOI: 10.1103/PhysRevD.97.065016)

*Cirigliano, V., M. Paris and S. Shalgar. Collective neutrino oscillations with the halo effect in single-angle approximation. 2018. *Journal of Cosmology and Astroparticle Physics*. **2018** (11): 19-19. (LA-UR-18-25562 DOI: 10.1088/1475-7516/2018/11/019)

*Cirigliano, V., M. W. Paris and S. Shalgar. 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)

*Corian\xc3\xb2, C., M. M. Maglio and E. Mottola. TTT in CFT: Trace identities and the conformal anomaly effective action. 2019. *Nuclear Physics B*. **942**: 303-328. (LA-UR-17-22382 DOI: 10.1016/j.nuclphysb.2019.03.019)

Grohs, E. B., D. Blaschke, V. Cirigliano, G. M. Fuller, L. A. Johns, C. Kishimoto, M. W. Paris and S. Shalgar. Development and persistence of quantum coherence in relic cosmological neutrinos. Submitted to *Physical Review Letters*. (LA-UR-19-32546)

*Grohs, E., G. M. Fuller, C. T. Kishimoto and M. W. Paris. Lepton asymmetry, neutrino spectral distortions, and big bang nucleosynthesis. 2017. *Physical Review D*. **95** (6): 063503. (LA-UR-16-29176 DOI: 10.1103/PhysRevD.95.063503)

*Ma, L., S. Shalgar and H. Duan. Matter parametric neutrino flavor transformation through Rabi resonances. 2018. *Physical Review D*. **98** (10): 103011. (LA-UR-18-25879 DOI: 10.1103/PhysRevD.98.103011)

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. Multi-angle calculation of the matter-neutrino resonance near an accretion disk. 2018. *Journal of Cosmology and Astroparticle Physics*. **2018** (02): 10-10. (LA-UR-17-26195 DOI: 10.1088/1475-7516/2018/02/010)

Reports

Giorgi, E. E. An alternative theory looks at black holes \xe2\x80\xa6 as surfaces, not holes. Unpublished report. (LA-UR-17-21316)

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)

Presentation Slides

Paris, M. W. Quantum Effects on Cosmology: Probing Physics Beyond the Standard Model with Big Bang. . (LA-UR-18-21136)

Paris, M. W. Kinetic theory of neutrinos and nuclei in the 'early' universe. Presented at *2018 Annual Meeting of the APS Four Corners Section*, Salt Lake City, Utah, United States, 2018-10-12 - 2018-10-13. (LA-UR-18-29729)

Paris, M. W., E. B. Grohs, V. Cirigliano, S. M. Shalgar, L. A. Johns and G. Fuller. Precision Constraints on Nuclear and Neutrino Reactions via Big Bang Nucleosynthesis. Presented at *CIPANP 2018 - Thirteenth Conference on the Intersections of Particle and Nuclear Physics*, Palm Springs, California, United States, 2018-05-29 - 2018-06-03. (LA-UR-18-24541)

Paris, M. W. and G. M. Hale. LANL-EDA5 analysis of the 7Be System. Presented at *3rd Consultants' Meeting on R-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region*, Vienna, Austria, 2017-06-28 - 2017-06-30. (LA-UR-17-25143)

Paris, M. W. and G. M. Hale. Nuclear reactions and neutrino kinetics in the early universe. Presented at *Nuclear Processes in Dense Plasmas*, Livermore, California, United States, 2018-07-30 - 2018-08-01. (LA-UR-18-26937)

Beat-Wave Magnetization of a Dense Plasma

Samuel Langendorf
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.

Technical Outcomes

This project investigated two approaches of forming a standoff magnetized target plasma, namely laser beat-wave magnetization and dynamic merging of pre-magnetized plasmas, approaches which could be compatible with innovative fusion approaches such as those pursued in the recent Advanced Research Projects Agency-Energy (ARPA-E) Accelerating Low-Cost Plasma Heating and Assembly (ALPHA) program. The latter approach shows significant promise and will be incorporated as a core concept in an upcoming proposed research effort towards fusion energy development.

Publications

Journal Articles

*Hsu, S. C. and S. J. Langendorf. Magnetized Plasma Target for Plasma-Jet-Driven Magneto-Inertial Fusion. 2018. *Journal of Fusion Energy*. **38** (1): 182-198. (LA-UR-18-21935 DOI: 10.1007/s10894-018-0168-z)

Yates, K. C., T. Awe, B. Bauer, T. Hutchinson, E. Yu and S. Fuelling. Azimuthally correlated surface roughness affecting the formation of plasma on metal conductors driven by a mega-ampere current pulse. Submitted to *Physics of Plasmas*. (LA-UR-19-29358)

Presentation Slides

Byvank, T., S. Langendorf, S. C. Hsu, D. Endrizzi, K. Mccollam, C. Forest, E. Hansen and P. Tzeferacos. Formation of Transient Plasmas with Beta and Hall Parameters Simultaneously Greater than Unity. Presented at *American Physical Society Division of Plasma Physics 2019*, Ft. Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30450)

Byvank, T., S. Langendorf, S. C. Hsu and D. A. Endrizzi. Plasma Jet Collisions for Studying 1) a Novel Fusion Concept and 2) Fundamental Shock Physics. Presented at *Seminar at Wisconsin Plasma Physics Laboratory*, Madison, Wisconsin, United States, 2019-09-26 - 2019-09-26. (LA-UR-19-29435)

Hsu, S. C. Fusion Concept Exploration and Basic Plasma-Shock Research on the Plasma Liner Experiment (PLX) at Los Alamos. . (LA-UR-19-21066)

Hsu, S. C., S. Langendorf, T. Byvank and P. H. Stoltz. w18_plxa Viewgraphs. . (LA-UR-19-21733)

Langendorf, S. and T. Byvank. w18_plxa Final Report Viewgraphs. . (LA-UR-20-21969)

Yates, K. C., S. C. Hsu, D. Montgomery, S. Langendorf, J. P. Dunn, B. Pollock and C. Thoma. Magnetization of a dense plasma via laser beat waves. Presented at *American Physical Society Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30459)

Posters

Yates, K. C., S. C. Hsu, D. Montgomery, J. P. Dunn, S. Langendorf, B. Pollock, T. Johnson, D. Welch and C. Thoma. Laser Beat-Wave Magnetization of a Dense Plasma. Presented at *59th Annual Meeting of the APS Division of Plasma Physics*, Milwaukee, Wisconsin, United States, 2017-10-23 - 2017-10-27. (LA-UR-17-29681)

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.

Technical Outcomes

We developed a novel approach for carrying out non-adiabatic molecular dynamics simulations of warm dense matter. Unlike previous approaches, the theory describes the evolution to thermal equilibrium from an arbitrary initial state. We developed a simulation capability to implement the new theoretical framework in existing quantum molecular dynamics codes. We applied the capability to perform the first evaluation of the electron-ion temperature relaxation rates in representative warm dense matter materials of various electronic complexity.

Publications

Journal Articles

*Baalrud, S. D. and J. Daligault. Transport regimes spanning magnetization-coupling phase space. 2017. *Physical Review E*. **96** (4): 043202. (LA-UR-17-25086 DOI: 10.1103/PhysRevE.96.043202)

*Baalrud, S. D. and J. Daligault. Mean force kinetic theory: A convergent kinetic theory for weakly and strongly coupled plasmas. 2019. *Physics of Plasmas*. **26** (8): 082106. (LA-UR-19-22330 DOI: 10.1063/1.5095655)

*Daligault, J. Crossover from Classical to Fermi Liquid Behavior in Dense Plasmas. 2017. *Physical Review Letters*. **119** (4): 045002. (LA-UR-17-22894 DOI: 10.1103/PhysRevLett.119.045002)

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. and D. Mozyrsky. Nonadiabatic quantum molecular dynamics with detailed balance. 2018. *Physical Review B*. **98** (20): 205120. (LA-UR-17-26600 DOI: 10.1103/PhysRevB.98.205120)

Daligault, J. and J. Simoni. Theory of the electron-ion temperature relaxation rate spanning the hot solid metals and plasma phases. 2019. *Physical Review E*. **100** (4): 043201. (LA-UR-19-24626 DOI: 10.1103/PhysRevE.100.043201)

*Simoni, J. and J. Daligault. First-Principles Determination of Electron-Ion Couplings in the Warm Dense Matter Regime. 2019. *Physical Review Letters*. **122** (20): 205001. (LA-UR-19-22811 DOI: 10.1103/PhysRevLett.122.205001)

Simoni, J. and J. O. Daligault. Calculation of electron-ion temperature equilibration rates and friction coefficients in plasma and liquid metals using quantum molecular dynamics. Submitted to *Physical Review E*. (LA-UR-19-31346)

Presentation Slides

Simoni, J. First Principles Determination of Electron-Ion Energy Relaxation Rates in the Warm Dense Matter Regime. Presented at *61st Annual Meeting of the APS Division of Plasma Physics*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30616)

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.

Technical Outcomes

Project was completed and major objectives were achieved. A patent was obtained on the high-tensile-strength, High-Gradient-Insulators which demonstrated a vacuum, DC standoff of >100kV/cm. Several novel concepts, including UV LED photocathodes, and pulsed thermionic cathodes were advanced for the first time.

Publications

Conference Papers

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)

Presentation Slides

Watson, S. A. MEXRAY - A Low Power Source With Space Potential. . (LA-UR-19-21089)

Winch, N. M., S. A. Watson, E. B. Sorensen and D. Platts. Mechanical X-ray (MEXRAY) Generator for MeV Radiography. Presented at *2018 Symposium on Radiation Measurements and Applications (SORMA XVII)*, Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-11. (LA-UR-18-21628)

Posters

Watson, S. A., N. M. Winch, E. B. Sorensen, D. Platts, J. M. Thompson and L. E. Bronisz. Portable Megavolt X-ray Generator (MEXRAY). Presented at *IEEE Nuclear Science Symposium and Medical Imaging Conference*, Sydney, Australia, 2018-11-11 - 2018-11-11. (LA-UR-18-30451)

Winch, N. M., S. A. Watson, E. B. Sorensen and D. Platts. MEchanical X-RAY (MEXRAY) Generator for MeV Radiography. Presented at *2018 Symposium on Radiation Measurements and Applications (SORMA XVII)*, Ann Arbor, Michigan, United States, 2018-06-11 - 2018-06-11. (LA-UR-18-25007)

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.

Technical Outcomes

This project has moved the development of advance photocathodes forward by demonstrating how the design and careful control of materials properties can impact the optimization and control of their spectral response and emission properties. We are now positioned to compete on a broader-scale for funding in targeted applications where we can build on these innovative techniques to address internal and external missions and establish LANL as a leader in the development of next-generation, high-performance photocathodes.

Publications

Presentation Slides

Pavlenko, V., A. Scheinker, M. A. Hoffbauer, F. Liu and N. A. Moody. Towards adaptive, automated growth of photocathodes. Presented at *Photocathode Physics for Photoinjectors (P3) Workshop*, Santa Fe, New Mexico, United States, 2018-10-15 - 2018-10-17. (LA-UR-18-29735)

Posters

Alexander, A., S. Kandil, G. Esparza, V. Pavlenko, F. Liu, J. Smedley, N. A. Moody, D. Sievenpiper and P. Bandaru. The utility of nanoscale science and structural mechanisms in\xc2\xa0optimizing emittance and quantum efficiency. Presented at *Photocathode Physics for Photoinjectors (P3) Workshop*, Santa Fe, New Mexico, United States, 2018-10-15 - 2018-10-17. (LA-UR-18-29514)

Laboratory Demonstration of the High-electron Mobility Transistors (HEMT)-Driven Accelerator

Dinh Nguyen
20190601ER

Project Description

We are demonstrating electron beam acceleration in a compact accelerator powered with microwave power from solid-state transistors and deliver key technical results that will support the deployment of compact accelerators for space and other applications. This new compact and efficient accelerator configuration will also have potential impact on the future designs of high-energy electron accelerators that will be used for a number of Department of Energy(DOE)/National Nuclear Security Administration(NNSA) and National Aeronautics Space Administration (NASA) missions ranging from the Accelerators-in-space program supporting beam based space sciences to X-ray free-electron lasers (FEL) such as the Linac Coherent Light Source at SLAC and the proposed MaRIE (Matter Radiation Interaction in Extremes) X-ray FEL at Los Alamos National Laboratory.

Technical Outcomes

We have demonstrated energy and density modulations, and acceleration of electron beams in three C-band cavities driven by high-electron mobility transistors (HEMTs). Starting with continuous electron beams, we observed energy modulation up to 11 keV in one cavity, and energy gain of 34 keV in three HEMT-powered cavities. This demonstration is a key milestone in our effort to design, build and test a compact electron accelerator powered by low-voltage DC power supplies for space missions.

Publications

Journal Articles

*I. Lewellen, J. W., C. E. Buechler, B. E. Carlsten, G. E. Dale, M. A. Holloway, D. E. Patrick and D. C. Nguyen. Space-Borne Electron Accelerator Design. 2019. *Frontiers in Astronomy and Space Sciences*. **6**. (LA-UR-19-20168 DOI: 10.3389/fspas.2019.00035)

Presentation Slides

Carlsten, B. E. Radiation Belt Remediation Using Space-Based Antennas and Electron Beams. Presented at *Jefferson Laboratory Colloquium*, Newport News, Virginia, United States, 2018-10-31 - 2018-10-31. (LA-UR-18-25900)

Application-specific Critical and Subcritical Benchmarks for Nuclear Data and Analytical Methods Validation

Jesson Hutchinson
20190606ER

Project Description

Radiation transport simulations are used for all aspects of the nuclear industry including defense programs, nonproliferation, counterproliferation, nuclear energy, space applications (National Aeronautics and Space Administration), criticality safety, medical physics, and others. These simulations require nuclear data; therefore, accurate nuclear data is essential to produce accurate results. This research will develop advanced tools that could result in the design of new critical and subcritical experiments that will ultimately lead to nuclear data improvements. As nuclear data improves, the understanding of device performance and criticality will also be improved. This work will require recent and new simulation tools and will result in better understanding of cross-section sensitivities for systems which are very relevant to the weapons and nonproliferation programs. The experiments will be designed for the National Criticality Experiments Research Center (but experiment execution is outside the scope of this project and is part of the future work).

Technical Outcomes

Validated nuclear cross-section data are required to maximize confidence in predictive radiation transport simulations. Benchmark experiments that are similar to an application are used to validate nuclear data for that application. The ARCHIMEDES project developed and refined tools (for sensitivity analysis, gap analysis, and experiment optimization) that will be employed to design new benchmark experiments. The goal of such experiments will be to maximum nuclear data improvements for specific nuclear weapons and global security applications.

Publications

Conference Papers

Hutchinson, J. D., J. L. Alwin, R. M. Bahran, T. J. Grove, R. C. Little, I. J. Michaud, W. L. Myers, A. T. McSpaden, M. E. Rising, T. A. Smith, N. W. Thompson and D. K. Hayes. CRITICALITY TESTING OF RECENT MEASUREMENTS AT THE NATIONAL CRITICALITY EXPERIMENTS RESEARCH CENTER. Presented at *International Conference on Nuclear Criticality*. (Paris, France, 2019-09-15 - 2019-09-15). (LA-UR-19-25271)

Hutchinson, J. D., J. L. Alwin, T. J. Grove, N. A. Kleedtke, J. A. Kulesza, A. T. McSpaden, I. J. Michaud, M. E. Rising, T. A. Smith, N. W. Thompson and R. C. Little. Sensitivity Studies, Gap Analysis, and Benchmark Experiment Optimization for Reactor Applications. Presented at *PHYSOR*. (Cambridge, United Kingdom, 2020-03-30 - 2020-03-30). (LA-UR-19-31133)

Kulesza, J. A., J. L. Alwin, J. D. Hutchinson, E. F. Shores and R. C. Little. l3d2vtk: An MCNPTools Utility to Enable LNK3DNT File Visualization & Post-processing. Presented at *2019 ANS Winter Meeting and Nuclear Technology Expo*. (Washington, District Of Columbia, United States, 2019-11-17 - 2019-11-21). (LA-UR-19-24947)

Michaud, I. J., N. A. Kleedtke, J. D. Hutchinson, T. A. Smith, R. C. Little, T. J. Grove and M. E. Rising. Designing Critical Experiments using Gaussian Process Optimization. Presented at *ANS Winter Meeting and Nuclear Technology Expo 2019*. (Washington, District Of Columbia, United States, 2019-11-17 - 2019-11-21). (LA-UR-19-25783)

Thompson, N. W., J. D. Hutchinson, T. E. Cutler, W. L. Myers and D. K. Hayes. Preliminary Designs for Criticality Safety Benchmarks – Iron/Steel/Chromium Series. Presented at *2019 American Nuclear Society Winter Meeting and Nuclear Technology Expo*. (Washington, District Of Columbia, United States, 2019-11-17 - 2019-11-21). (LA-UR-19-26433)

Presentation Slides

Hutchinson, J. D., J. L. Alwin, J. A. Arthur, R. M. Bahran, T. J. Grove, J. A. Kulesza, I. J. Michaud, A. T. McSpaden, M. E. Rising, T. A. Smith, N. W. Thompson and R. C. Little. ARCHIMEDES: Application-specific experiments for nuclear data and analytical methods validation. . (LA-UR-19-24291)

Hutchinson, J. D., J. L. Alwin, J. A. Arthur, R. M. Bahran, T. J. Grove, J. A. Kulesza, I. J. Michaud, A. T. McSpaden, M.

E. Rising, T. A. Smith, N. W. Thompson and R. C. Little. ARCHIMEDES: Application-specific experiments for nuclear data and analytical methods validation. . (LA-UR-19-26387)

Hutchinson, J. D., J. L. Alwin, R. M. Bahran, T. J. Grove, R. C. Little, I. J. Michaud, A. T. McSpaden, W. L. Myers, M. E. Rising, T. A. Smith, N. W. Thompson and D. K. Hayes. Criticality Testing of Recent Measurements at the National Criticality Experiments Research Center. Presented at *International Conference on Nuclear Criticality*, Paris, France, 2019-09-16 - 2019-09-16. (LA-UR-19-28889)

Kulesza, J. A., J. L. Alwin, J. D. Hutchinson, E. F. Shores and R. C. Little. l3d2vtk: An MCNPTools Utility to Enable LNK3DNT File Visualization & Post-processing. Presented at *2019 ANS Winter Meeting and Nuclear Technology Expo*, Washington, District Of Columbia, United States, 2019-11-17 - 2019-11-21. (LA-UR-19-31429)

Little, R. C., J. D. Hutchinson, J. L. Alwin, R. M. Bahran, T. J. Grove, I. J. Michaud, A. T. McSpaden, M. E. Rising, T. A. Smith and N. W. Thompson. The Los Alamos ARCHIMEDES Project: Application-specific experiments for nuclear data and analytical methods validation. Presented at *Cross Section Evaluation Working Group (CSEWG) Meeting*, Upton, New York, United States, 2019-11-04 - 2019-11-06. (LA-UR-19-31175)

Michaud, I. J., N. A. Kleedtke, J. D. Hutchinson, T. A. Smith, R. C. Little, T. J. Grove and M. E. Rising. Designing Critical Experiments using Gaussian Process Optimization. Presented at *American Nuclear Society Winter Meeting and Expo*, Washington, District Of Columbia, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-31529)

Smith, T. A. ARCHIMEDES Application: ADS & Krusty. . (LA-UR-19-24500)

Thompson, N. W., J. D. Hutchinson, T. E. Cutler, W. L. Myers and D. K. Hayes. Preliminary Designs for Criticality Safety Benchmarks – Iron/Steel/Chromium Series. Presented at *American Nuclear Society Winter Meeting and Expo, 2019*, Washington, District Of Columbia, United States, 2019-11-17 - 2019-11-21. (LA-UR-19-31543)

Non-invasive Pipe Pressure Monitoring for Safeguards

Alessandro Cattaneo
20190638ER

Project Description

Today, the on-line enrichment monitor (OLEM) is the preeminent tool for safeguards monitoring at gas centrifuge enrichment plants (GCEP). OLEM often relies upon operator owned or shared instruments for pressure measurement. However, if the reported pressure at OLEM were surreptitiously dropped in half by a non-cooperative operator, the enrichment could be doubled, and because the total mass of U-235 detected by OLEM is unaltered, the system would not detect a change in enrichment. A new solution to independently and noninvasively determine the pressure inside GCEPs' pipes would greatly increase the confidence in uranium enrichment measurements collected with OLEM when there is reduced confidence in operator data. We propose to monitor the fluid pressure inside gas-carrying pipes by measuring temperature compensated hoop and axial strain using an optical interferometry approach that takes advantage of state-of-the-art Fiber Bragg Grating (FBG) sensors externally applied to the pipe surface, and high sensitivity interrogation based on swept-wavelength infrared laser technology. The project is relevant to the International Atomic Energy Agency (IAEA) priorities and a broad set of DOE/NNSA/Nuclear Nonproliferation programs. For this reason, the project will likely strengthen the LANL privileged relationship with key political and industrial figures active on the international nuclear safeguards stage.

Technical Outcomes

We successfully demonstrated the ability and convenience to use optical fiber Bragg gratings (FBG) interrogation to measure the axial and hoop strain on commercial four-inch tubes and pipes. Vacuum induced strains were measured at room temperature on a table top, and resolution was demonstrated in the tens of nano-strains; that is to say, ten parts in a billion or, equivalently the length of approximately ten atoms of Fe on our pipes circumference.

Publications

Reports

Jaime, M. RR2016 Summary Report Dilatometry Under Pressure: Unveiling Universal Static Properties of Quantum Critical Points. Unpublished report. (LA-UR-19-30096)

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 (kiloelectron volts) 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.

Publications

Journal Articles

Carlsten, B. E., P. M. Anisimov, C. W. Barnes, Q. R. Marksteiner, R. R. Robles and N. Yampolsky. High-Brightness Beam Technology Development for a Future Dynamic Mesoscale Materials Science Capability. 2019. *Instruments*. **3** (4): 52. (LA-UR-19-28549 DOI: 10.3390/instruments3040052)

Presentation Slides

Anisimov, P. M. High-Efficiency Free Electron Lasers with Pinched Electron Beams. Presented at *Physics & Applications of High Efficiency Free-Electron Lasers Workshop*, Los Angeles, California, United States, 2018-04-11 - 2018-04-13. (LA-UR-18-23463)

Anisimov, P. M., Q. R. Marksteiner, R. R. Robles, J. W. I. Lewellen, N. Yampolsky and B. E. Carlsten. Laser Assisted Bunch Compression for High Energy X-ray Free Electron Lasers. Presented at *FEL 2019*, Hamburg, Germany, 2019-08-26 - 2019-08-30. (LA-UR-19-28673)

Carlsten, B. E. Accelerator Challenges for XFELs with Very High X-Ray Energies. Presented at *39th International Free-Electron Laser Conference*, Hamburg, Germany, 2019-08-26 - 2019-08-30. (LA-UR-19-28626)

Posters

Robles, R. R., J. E. Williams and P. M. Anisimov. Increasing High-Energy XFEL Efficiency with a Transverse Gradient Undulator. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-26791)

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.

Publications

Journal Articles

*Alioli, S., W. Dekens, M. Girard and E. Mereghetti. NLO QCD corrections to SM-EFT dilepton and electroweak Higgs boson production, matched to parton shower in POWHEG. 2018. *Journal of High Energy Physics*. **2018** (8): 205. (LA-UR-18-23399 DOI: 10.1007/JHEP08(2018)205)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser, E. Mereghetti, S. Pastore and U. van Kolck. New Leading Contribution to Neutrinoless Double-\xce\xb2 Decay. 2018. *Physical Review Letters*. **120** (20): 202001. (LA-UR-18-21404 DOI: 10.1103/PhysRevLett.120.202001)

*Cirigliano, V., W. Dekens, J. de Vries, M. L. Graesser and E. Mereghetti. A neutrinoless double beta decay master formula from effective field theory. 2018. *Journal of High Energy Physics*. **2018** (12): 97. (LA-UR-18-24895 DOI: 10.1007/JHEP12(2018)097)

Mereghetti, E., A. Walker-Loud, C. Drischler, A. N. Nicholson, W. Haxton, K. McElvain and P. Vranas. Towards grounding nuclear physics in QCD. Submitted to *European Physical Journal A. Hadrons and Nuclei*. (LA-UR-19-30583)

Mereghetti, E., K. Fuyuto, W. G. Dekens, J. de Vries and G. Zhou. Sterile neutrinos and neutrinoless double beta decay in effective field theory. Submitted to *Journal of High Energy Physics*. (LA-UR-20-21376)

Mereghetti, E., V. Cirigliano, W. G. Dekens, J. de Vries, M. L. Graesser, S. Pastore, M. Piarulli, U. Van Kolck and R. B. Wiringa. A renormalized approach to neutrinoless double beta decay. Submitted to *Physical Review C*. (LA-UR-19-26002)

Wang, X. B., A. C. Hayes, J. Carlson, G. X. Dong, E. Mereghetti, S. Pastore and R. B. Wiringa. Comparison between variational Monte Carlo and shell model calculations of neutrinoless double beta decay matrix elements in light nuclei. 2019. *Physics Letters B*. **798**: 134974. (LA-UR-19-25587 DOI: 10.1016/j.physletb.2019.134974)

Conference Papers

Mereghetti, E. Lattice QCD and nuclear physics for searches of physics beyond the Standard Model. Presented at *36th Annual International Symposium on Lattice Field Theory*. (Lansing, Michigan, United States, 2018-07-22 - 2018-07-28). (LA-UR-18-30382)

Presentation Slides

Mereghetti, E. Electric dipole moments of light nuclei. Presented at *Atomic Nuclei as Laboratories for BSM physics*, Trento, Italy, 2019-04-15 - 2019-04-19. (LA-UR-19-30719)

Mereghetti, E. An Effective Field Theory Approach to neutrinoless double beta decay. . (LA-UR-19-30720)

Mereghetti, E. Constraining BSM physics with hadronic and nuclear physics. Presented at *Hadron 2019*, Guilin, China, 2019-08-16 - 2019-08-21. (LA-UR-19-28353)

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 the Department of Energy Office of Science. 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.

A Multidimensional Multiscale Vlasov-Fokker-Planck Algorithm for Modeling High Energy Density and Inertial Confinement Fusion Applications

William Taitano
20190529ECR

Project Description

After the failed attempt of ignition at the National Ignition Facility (NIF), the predictive capabilities of our radiation hydrodynamic (rad-hydro) codes have been put into question. At the moment, it is not clear if the mismatch between calculations and experiments is caused by missing physics (e.g., kinetic plasma effects) in our rad-hydro codes, or inferior algorithms used therein. The project will build foundational algorithmic capabilities which will allow us to investigate the role of these 'missing physics' in our rad-hydro simulations and ultimately, increase our predictive capabilities for related laboratory experiments.

Publications

Reports

Taitano, W., L. Chacon and A. N. Simakov. The Annual IC Progress Report. Unpublished report. (LA-UR-20-22359)

Adaptive Process Control for Beyond-State-of-the-Art Alkali Antimonide Photocathodes

Vitaly Pavlenko
20190536ECR

Project Description

Hard X-ray free electron lasers such as Linac Coherent Light Source-II (LCLS-II) and Matter-Radiation Interactions in Extremes (MaRIE) are considered essential to enable sustainable stockpile stewardship. Reliable operation and performance of such billion-dollar facilities depends on a tiny but critical piece, a photocathode (laser-triggered source of electrons). Fabrication of one of the most important photocathode types, alkali antimonides, to this day remains an art, as opposed to a technological process that applies to every other part of the system. We believe that we possess the knowledge required to eliminate the vulnerability and poor reproducibility associated with a human-controlled process and deliver the first-ever fully automated photocathode growth system.

Publications

Posters

Alexander, A. M., F. Liu, V. Pavlenko, N. A. Moody, J. M. Smedley and P. Bandaru. Interference Enhanced Photocathodes. Presented at *Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28528)

A Dual n-gamma Detector Array to Correct Neutron Transport Simulations

Keegan Kelly
20190588ECR

Project Description

Monte Carlo simulations of nuclear systems are essential for the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) national nuclear security missions. These simulations contain ambiguities because they include commonly-encountered neutron scattering cross sections that are poorly known, poorly measured, and estimated from nuclear models. This project aims to resolve these ambiguities by taking advantage of recent developments in detector technologies to create a detector system capable of yielding accurate and complete measurements of these cross sections and the corresponding angular distributions.

Publications

Conference Papers

Kelly, K. J., M. J. Devlin and J. M. O'Donnell. Development of a Highly-Segmented Dual n-gamma Detector Array for Neutron Scattering Measurements at LANL. Presented at *SORMAWest 2020*. (Berkeley, California, United States, 2020-06-01 - 2020-06-04). (LA-UR-20-21042)

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.

Technical Outcomes

This project explored a new technique for relativistic radiation magnetohydrodynamics, specifically for astrophysical applications, but with an eye toward a broader set of applications in the future. The work in the project contributed to multiple publications and led to follow on work by a postdoc that has produced the only fully relativistic radiation magnetohydrodynamics code capable of modeling all regimes of radiation MHD with full, time-dependent transport.

Publications

Journal Articles

Mabanta, Q. A., J. W. Murphy and J. C. Dolence. Convection-Aided Explosions in One-Dimensional Core-Collapse Supernova Simulations I: Technique and Validation. Submitted to *Astrophysical Journal*. (LA-UR-19-20695)

*Radice, D., A. Burrows, D. Vartanyan, M. A. Skinner and J. C. Dolence. Electron-capture and Low-mass Iron-core-collapse Supernovae: New Neutrino-radiation-hydrodynamics Simulations. 2017. *The Astrophysical Journal*. **850** (1): 43. (LA-UR-17-20973 DOI: 10.3847/1538-4357/aa92c5)

*Richers, S., H. Nagakura, C. D. Ott, J. Dolence, K. Sumiyoshi and S. Yamada. A Detailed Comparison of Multidimensional Boltzmann Neutrino Transport Methods in Core-collapse Supernovae. 2017. *The Astrophysical Journal*. **847** (2): 133. (LA-UR-17-24929 DOI: 10.3847/1538-4357/aa8bb2)

*Ryan, B. R., S. M. Ressler, J. C. Dolence, A. Tchekhovskoy, C. Gammie and E. Quataert. The Radiative Efficiency and Spectra of Slowly Accreting Black Holes from Two-temperature GRRMHD Simulations. 2017. *The Astrophysical Journal*. **844** (2): L24. (LA-UR-17-25079 DOI: 10.3847/2041-8213/aa8034)

*Ryan, B. R., S. M. Ressler, J. C. Dolence, C. Gammie and E. Quataert. Two-temperature GRRMHD Simulations of M87. 2018. *The Astrophysical Journal*. **864** (2): 126. (LA-UR-18-23675 DOI: 10.3847/1538-4357/aad73a)

*Skinner, M. A., J. C. Dolence, A. Burrows, D. Radice and D. Vartanyan. Fornax: A Flexible Code for Multiphysics Astrophysical Simulations. 2019. *The Astrophysical Journal Supplement Series*. **241** (1): 7. (LA-UR-18-25082 DOI: 10.3847/1538-4365/ab007f)

*Vartanyan, D., A. Burrows, D. Radice, M. A. Skinner and J. Dolence. Revival of the fittest: exploding core-collapse supernovae from 12 to 25\xc2\xa0M\xe2\x8a\x99. 2018. *Monthly Notices of the Royal Astronomical Society*. **477** (3): 3091-3108. (LA-UR-18-20409 DOI: 10.1093/mnras/sty809)

*Vartanyan, D., A. Burrows, D. Radice, M. Aaron Skinner and J. Dolence. A successful 3D core-collapse supernova explosion model. 2019. *Monthly Notices of the Royal Astronomical Society*. **482** (1): 351-369. (LA-UR-18-28730 DOI: 10.1093/mnras/sty2585)

Presentation Slides

Dolence, J. C. Simulations of Core-Collapse Supernova Explosions. Presented at *XXX IUPAP Conference on Computational Physics*, Davis, California, United States, 2018-07-29 - 2018-07-29. (LA-UR-18-27079)

Dolence, J. C. Full Transport GR Neutrino Radiation MHD and Nucleosynthesis in Neutron Star Merger Disks. Presented at *Explosive Nucleosynthesis in the Supernova and Merging-Neutron-Star Contexts*, Princeton, New Jersey, United States, 2019-05-22 - 2019-05-24. (LA-UR-19-24793)

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 implications 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.

Technical Outcomes

This work was fundamental to establish the steps for the search for gluon condensates in high energy collisions. We developed the initial steps for the fabrication of a particle tracker based on triangular extruded scintillators to be installed in LHCb. This Physics program was awarded one of the three DOE/OS early career awards in Nuclear Physics in 2018.

Publications

Presentation Slides

Durham, J. M. Production measurements in heavy ion and fixed target collisions at LHCb. Presented at *2018 Santa Fe Jets and Heavy Flavor Workshop*, Santa Fe, New Mexico, United States, 2018-01-29 - 2018-01-29. (LA-UR-18-20816)

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.

Technical Outcomes

We have demonstrated that intense laser-driven plasma could convert up to 5% of the laser energy into mega electron volt (MeV) x-rays. We have also demonstrated that the laser-driven MeV x-ray source size is 80 microns, which is an order of magnitude smaller than the conventional sources. We have also radiographed a wide variety of dense objects demonstrating the viability of laser-based MeV x-ray sources for radiography applications.

Publications

Journal Articles

*Fernandez, J. C., D. Cort Gautier, C. Huang, S. Palaniyappan, B. J. Albright, W. Bang, G. Dyer, A. Favalli, J. F. Hunter, J. Mendez, M. Roth, M. Swinhoe, P. A. Bradley, O. Deppert, M. Espy, K. Falk, N. Guler, C. Hamilton, B. M. Hegelich, D. Henzlova, K. D. Ianakiev, M. Iliev, R. P. Johnson, A. Kleinschmidt, A. S. Losko, E. McCary, M. Mocko, R. O. Nelson, R. Roycroft, M. A. Santiago Cordoba, V. A. Schanz, G. Schaumann, D. W. Schmidt, A. Sefkow, T. Shimada, T. N. Taddeucci, A. Tebartz, S. C. Vogel, E. Vold, G. A. Wurden and Y. Lin. Laser-plasmas in the relativistic-transparency regime: Science and applications. 2017. *Physics of Plasmas*. **24** (5): 056702. (LA-UR-17-22372 DOI: 10.1063/1.4983991)

Palaniyappan, S., C. Huang, D. C. Gautier, F. Fiuza, W. Ma, J. Schreiber, J. C. Fernandez, A. J. Raymer, R. N. Mortensen, R. P. Gonzales, S. L. Reid, T. Shimada and R. P. Johnson. Collisionless shock acceleration of carbon ions from 1um-laser-driven near-critical plasma. Submitted to *Nature Physics*. (LA-UR-18-27131)

*Palaniyappan, S., D. C. Gautier, B. J. Tobias, J. C. Fernandez, J. Mendez, T. Burris-Mog, C. K. Huang, A. Favalli, J. F. Hunter, M. E. Espy, D. W. Schmidt, R. O. Nelson, A. Sefkow, T. Shimada and R. P. Johnson. MeV bremsstrahlung X rays from intense laser interaction with solid foils. 2018. *Laser and Particle Beams*. **36** (4): 502-506. (LA-UR-18-25214 DOI: 10.1017/S0263034618000551)

Reports

Tobias, B. J., S. Palaniyappan, D. C. Gautier, J. Mendez, T. J. Burris-Mog, C. Huang, A. Favalli, J. F. Hunter, M. A. Espy, D. W. Schmidt, R. O. Nelson, A. Sefkow, T. Shimada, R. P. Johnson and J. C. Fernandez. Quantification of uncertainty in photon source spot size inference during laser-driven radiography experiments at TRIDENT. Unpublished report. (LA-UR-17-28604)

Presentation Slides

Huang, C. Particle accelerators: present, future and the enabling computational modeling. . (LA-UR-19-31915)

Huang, C., S. Palaniyappan, F. Fiuza, D. C. Gautier, W. Ma, J. Schreiber, J. C. Fernandez, A. J. Raymer, R. N. Mortensen, R. P. Gonzales, S. L. Reid, T. Shimada and R. P. Johnson. Collisionless shock acceleration of carbon ions from 1\xf0\x9d\x9d\x81m laser-driven near-critical plasma. Presented at *60th Annual Meeting of the APS Division of Plasma Physics*, Portland, Oregon, United States, 2018-11-05 - 2018-11-09. (LA-UR-18-30522)

Tobias, B. J., S. Palaniyappan, D. C. Gautier, J. Mendez, T. J. Burris-Mog, C. Huang, A. Favalli, J. F. Hunter, M. A. Espy, D. W. Schmidt, R. O. Nelson, A. Sefkow, T. Shimada, R. P. Johnson and J. C. Fernandez. Laser-Driven Radiography Experiments at TRIDENT. Presented at *Radiography Workshop*, Los Alamos, New Mexico, United States, 2017-09-28 - 2017-09-29. (LA-UR-17-28559)

Posters

Huang, C., S. Palaniyappan, D. C. Gautier, R. P. Johnson, T. Shimada, J. C. Fernandez, F. S. Tsung and W. B. Mori. Proton Deflectometry Of Laser-Driven Relativistic Electron Jet From Thin Foil. Presented at *59th Annual Meeting of the APS Division of Plasma Physics*, Milwaukee, Wisconsin, United States, 2017-10-23 - 2017-10-27. (LA-UR-17-29822)

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.

Publications

Journal Articles

*Bertolini, D., D. Kolodrubetz, D. Neill, P. Pietrulewicz, I. W. Stewart, F. J. Tackmann and W. J. Waalewijn. Soft functions for generic jet algorithms and observables at hadron colliders. 2017. *Journal of High Energy Physics*. **2017** (7): 99. (LA-UR-17-23006 DOI: 10.1007/JHEP07(2017)099)

*Larkoski, A. J., I. Moult and D. Neill. Factorization and resummation for groomed multi-prong jet shapes. 2018. *Journal of High Energy Physics*. **2018** (2): 144. (LA-UR-17-29531 DOI: 10.1007/JHEP02(2018)144)

Neill, D. A. and F. Ringer. Soft Fragmentation on the Celestial Sphere. Submitted to *Journal of High Energy Physics*. (LA-UR-20-21841)

*Neill, D., A. Papaefstathiou, W. J. Waalewijn and L. Zoppi. Phenomenology with a recoil-free jet axis: TMD fragmentation and the jet shape. 2019. *Journal of High Energy Physics*. **2019** (1): 67. (LA-UR-18-30361 DOI: 10.1007/JHEP01(2019)067)

*Neill, D. and W. J. Waalewijn. Entropy of a Jet. 2019. *Physical Review Letters*. **123** (14): 142001. (LA-UR-18-30360 DOI: 10.1103/PhysRevLett.123.142001)

Jets in Strongly Interacting Plasmas

Andrey Sadofyev
20170666PRD1

Project Description

The 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 the European Organization for Nuclear Research (CERN). An extremely dense and hot "fireball" is created in collisions of heavy ions and consists of the elementary constituents of matter, quark, 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.

Publications

Journal Articles

*Avdoshkin, A., A. V. Sadofyev and V. I. Zakharov. IR properties of chiral effects in pionic matter. 2018. *Physical Review D*. **97** (8): 085020. (LA-UR-17-31504 DOI: 10.1103/PhysRevD.97.085020)

*Brewer, J., K. Rajagopal, A. Sadofyev and W. van der Schee. Evolution of the mean jet shape and dijet asymmetry distribution of an ensemble of holographic jets in strongly coupled plasma. 2018. *Journal of High Energy Physics*. **2018** (2): 15. (LA-UR-17-29843 DOI: 10.1007/JHEP02(2018)015)

*Hirono, Y., D. E. Kharzeev and A. V. Sadofyev. Dynamics of Vortices in Chiral Media: The Chiral Propulsion Effect. 2018. *Physical Review Letters*. **121** (14): 142301. (LA-UR-18-22126 DOI: 10.1103/PhysRevLett.121.142301)

*Huang, X. and A. V. Sadofyev. Chiral vortical effect for an arbitrary spin. 2019. *Journal of High Energy Physics*. **2019** (3): 84. (LA-UR-18-24524 DOI: 10.1007/JHEP03(2019)084)

Sadofyev, A., W. van der Schee and J. Brewer. Jet shape modifications in holographic dijet systems. Submitted to *Physical Review Letters*. (LA-UR-18-30400)

Sadofyev, A. and E. Mottola. Chiral Waves on the Fermi-Dirac Sea: Quantum Superfluidity and the Axial Anomaly. Submitted to *Physical Review D*. (LA-UR-19-27117)

Sadofyev, A. and J. Reiten. Drag force to all orders in gradients. Submitted to *Journal of High Energy Physics*. (LA-UR-20-20237)

*Sadofyev, A. and S. Sen. Chiral anomalous dispersion. 2018. *Journal of High Energy Physics*. **2018** (2): 99. (LA-UR-17-31502 DOI: 10.1007/JHEP02(2018)099)

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.

Technical Outcomes

This project resulted in new methods for performing real-time Compton imaging on low space weight and power devices. We have developed a FPGA-based Compton imaging pipeline that performs both event reconstruction and mapping. Our reconstruction step pioneered FPGA-based Compton event reconstruction. The pipeline's mapping step produces naive backprojected maps for Compton events over four-pi steradians, and includes a noise suppressing filtering step. This pipeline has been validated with simulations and with data acquired in lab.

Publications

Journal Articles

*Appel, J. W., Z. Xu, I. L. Padilla, K. Harrington, B. Pradenas Marquez, A. Ali, C. L. Bennett, M. K. Brewer, R. Bustos, M. Chan, D. T. Chuss, J. Cleary, J. Couto, S. Dahal, K. Denis, R. Dunner, J. R. Eimer, T. Essinger-Hileman, P. Fluxa, D. Gothe, G. C. Hilton, J. Hubmayr, J. Iuliano, J. Karakla, T. A. Marriage, N. J. Miller, C. Nunez, L. Parker, M. Petroff, C. D. Reintsema, K. Rostem, R. W. Stevens, D. A. N. Valle, B. Wang, D. J. Watts, E. J. Wollack and L. Zeng. On-sky Performance of the CLASS Q-band Telescope. 2019. *The Astrophysical Journal*. **876** (2): 126. (LA-UR-18-30124 DOI: 10.3847/1538-4357/ab1652)

*Kusaka, A., J. Appel, T. Essinger-Hileman, J. A. Beall, L. E. Campusano, H. Cho, S. K. Choi, K. Crowley, J. W. Fowler, P. Gallardo, M. Hasselfield, G. Hilton, S. P. Ho, K. Irwin, N. Jarosik, M. D. Niemack, G. W. Nixon, M. Nolta, L. A. J. Page, G. A. Palma, L. Parker, S. Raghunathan, C. D. Reintsema, J. Sievers, S. M. Simon, S. T. Staggs, K. Visnjic and K. Yoon. Results from the Atacama B-mode Search (ABS) experiment. 2018. *Journal of Cosmology and Astroparticle Physics*. **2018** (09): 5-5. (LA-UR-18-23879 DOI: 10.1088/1475-7516/2018/09/005)

Parker, L. P., Z. Li, S. Naess, S. Aiola, J. W. Appel, R. J. Bond, E. Calabrese, S. K. Choi, T. Essinger-Hileman, J. Dunkley, J. Fowler, P. Gallardo, J. Hubmayr, M. D. Niemack, L. Page, B. Partridge, M. Salatino, C. Sifon, S. M. Simon, S. T. Staggs, E. Storer and E. Wollack. The Cross Correlation of the ABS and ACT Maps. Submitted to *Astrophysical Journal*. (LA-UR-20-21154)

*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. 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. 2018. *The Astrophysical Journal*. **863** (2): 121. (LA-UR-18-20165 DOI: 10.3847/1538-4357/aad283)

Conference Papers

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)

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)

Posters

Parker, L. P., S. Grifffin, C. Kierans, A. Shoenwald, P. Shawhan, R. Caputo, J. McEnery and J. Perkins. Progress towards the Silicon Tracker for the All-sky Medium Energy Gamma-ray Observatory Prototype. Presented at *IEEE Nuclear Science Symposium (NSS) and Medical Imaging Conference (MIC)*, Manchester, United Kingdom, 2019-10-26 - 2019-11-02. (LA-UR-19-30803)

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. The Department of Energy(DOE)/National Nuclear Security Administration(NNSA) 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.

Publications

Journal Articles

Mansoor, M. M., S. M. Dalton, A. A. Martinez, T. Desjardins, J. J. Charonko and K. P. Prestridge. The effect of initial conditions on mixing transition of the Richtmyer-Meshkov instability. Submitted to *Journal of Fluid Mechanics*. (LA-UR-19-31658)

Conference Papers

Mansoor, M. M., S. M. Dalton, T. Desjardins, A. A. Martinez, J. J. Charonko and K. P. Prestridge. THE EFFECT OF INITIAL CONDITIONS ON THE LATE-TIME DEVELOPMENT OF RICHTMYER-MESHKOV INSTABILITY. Presented at *Eleventh International Symposium on Turbulence and Shear Flow Phenomena (TSFP11)*. (Southampton, United Kingdom, 2019-07-30 - 2019-08-02). (LA-UR-19-23718)

Presentation Slides

Prestridge, K. P., M. M. Mansoor, A. A. Martinez, S. M. Dalton and T. Desjardins. Effects of initial conditions on shock-driven instabilities and turbulent mixing. Presented at *Eleventh International Symposium on Turbulence and Shear Flow Phenomena (TSFP11)*, Southampton, United Kingdom, 2019-07-30 - 2019-08-02. (LA-UR-19-27196)

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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 Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions in the long term.

Publications

Journal Articles

*Akiyama, K., A. Alberdi, W. Alef, K. Asada, R. Azulay, A. Baczko, D. Ball, M. Balokovic, J. Barrett, D. Bintley, L. Blackburn, W. Boland, K. L. Bouman, G. C. Bower, M. Bremer, C. D. Brinkerink, R. Brissenden, S. Britzen, A. E. Broderick, D. Broguiere, T. Bronzwaer, D. Byun, J. E. Carlstrom, A. Chael, C. Chan, S. Chatterjee, K. Chatterjee, M. Chen, Y. Chen, I. Cho, P. Christian, J. E. Conway, J. M. Cordes, G. B. Crew, Y. Cui, J. Davelaar, M. De Laurentis, R. Deane, J. Dempsey, G. Desvignes, J. Dexter, S. S. Doeleman, R. P. Eatough, H. Falcke, V. L. Fish, E. Fomalont, R. Fraga-Encinas, P. Friberg, C. M. Fromm, J. L. Gomez, P. Galison, C. F. Gammie, R. Garcia, O. Gentaz, B. Georgiev, C. Goddi, R. Gold, M. Gu, M. Gurwell, K. Hada, M. H. Hecht, R. Hesper, L. C. Ho, P. Ho, M. Honma, C. L. Huang, L. Huang, D. H. Hughes, S. Ikeda, M. Inoue, S. Issaoun, D. J. James, B. T. Jannuzi, M. Janssen, B. Jeter, W. Jiang, M. D. Johnson, S. Jorstad, T. Jung, M. Karami, R. Karuppusamy, T. Kawashima, G. K. Keating, M. Kettenis, J. Kim, J. Kim, J. Kim, M. Kino, J. Y. Koay, P. M. Koch, S. Koyama, M. Kramer, C. Kramer, T. P. Krichbaum, C. Kuo, T. R. Lauer, S. Lee, Y. Li, Z. Li, M. Lindqvist, K. Liu, E. Liuzzo, W. Lo, A. P. Lobanov, L. Loinard, C. Lonsdale, R. Lu, N. R. MacDonald, J. Mao, S. Markoff, D. P. Marrone, A. P. Marscher, I. Marti-Vidal, S. Matsushita, L. D. Matthews, L. Medeiros, K. M. Menten, Y. Mizuno, I. Mizuno, J. M. Moran, K. Moriyama, M. Moscibrodzka, C. Mueller, H. Nagai, N. M. Nagar, M. Nakamura, R. Narayan, G. Narayanan, I. Natarajan, R. Neri, C. Ni, A. Noutsos, H. Okino, H. Olivares, G. N. Ortiz-Leon, T. Oyama, F. Ozel, D. C. M. Palumbo, N. Patel, U. Pen, D. W. Pesce, V. Pietu, R. Plambeck, A. PopStefanija, O. Porth, P. Ben, J. A. Preciado-Lopez, D. Psaltis, H. Pu, V. Ramakrishnan, R. Rao, M. G. Rawlings, A. W. Raymond, L. Rezzolla, B. Ripperda, F. Roelofs, A. Rogers, E. Ros, M. Rose, A. Roshanineshat, H. Rottmann, A. L. Roy, C. Ruszczyk, B. R. Ryan, K. L. J. Rygl, S. Sanchez, D. Sanchez-Arguelles, M. Sasada, T. Savolainen, F. P. Schloerb, K. Schuster, L. Shao, Z. Shen, D. Small, B. W. Sohn, J. SooHoo, F. Tazaki, P. Tiede, R. P. J. Tilanus, M. Titus, K. Toma, P. Torne, T. Trent, S. Trippe, S. Tsuda, I. van Bemmel, H. J. van Langevelde, D. R. van Rossum, J. Wagner, J. Wardle, J. Weintroub, N. Wex, R. Wharton, M. Wielgus, G. N. Wong, Q. Wu, A. Young, K. Young, Z. Younsi, F. Yuan, Y. Yuan, J. A. Zensus, G. Zhao, S. Zhao, Z. Zhu, J. Algaba, A. Allardi, R. Amestica, U. Bach, C. Beaudoin, B. A. Benson, R. Berthold, J. M. Blanchard, R. Blundell, S. Bustamente, R. Cappallo, E. Castillo-Dominguez, C. Chang, S. Chang, S. Chang, C. Chen, R. Chilson, T. C. Chuter, R. C. Rosado, I. M. Coulson, T. M. Crawford, J. Crowley, J. David, M. Derome, M. Dexter, S. Dornbusch, K. A. Dudevoir, S. A. Dzib, C. Eckert, N. R. Erickson, W. B. Everett, A. Faber, J. R. Farah, V. Fath, T. W. Folkers, D. C. Forbes, R. Freund, A. I. Gomez-Ruiz, D. M. Gale, F. Gao, G. Geertsema, D. A. Graham, C. H. Greer, R. Grosslein, F. Gueth, N. W. Halverson, C. Han, K. Han, J. Hao, Y. Hasegawa, J. W. Henning, A. Hernandez-Gomez, R. Herrero-Illana, S. Heyminck, A. Hirota, J. Hoge, Y. Huang, C. M. V. Impellizzeri, H. Jiang, A. Kamble, R. Keisler, K. Kimura, Y. Kono, D. Kubo, J. Kuroda, R. Lacasse, R. A. Laing, E. M. Leitch, C. Li, L. C. -. Lin, C. Liu, K. Liu, L. Lu, R. G. Marson, P. L. Martin-Cocher, K. D. Massingill, C. Matulonis, M. P. McColl, S. R. McWhirter, H. Messias, Z. Meyer-Zhao, D. Michalik, A. Montana, W. Montgomerie, M. Mora-Klein, D. Muders, A. Nadolski, S. Navarro, C. H. Nguyen, H. Nishioka, T. Norton, G. Nystrom, H. Ogawa, P. Oshiro, T. Oyama, S. Padin, H. Parsons, S. N. Paine, J. Penalver, N. M. Phillips, M. Poirier, N. Pradel, R. A. Primiani, P. A. Raffin, A. S. Rahlin, G. Reiland, C. Risacher, I. Ruiz, A. F. Saez-Madain, R. Sassella, P. Schellart, P. Shaw, K. M. Silva, H. Shiokawa, D. R. Smith, W. Snow, K. Souccar, D. Sousa, T. K. Sridharan, R. Srinivasan, W. Stahm, A. A. Stark, K. Story, S. T. Timmer, L. Vertatschitsch, C. Walther, T. Wei, N. Whitehorn, A. R. Whitney, D. P. Woody, J. G. A. Wouterloot, M. Wright, P. Yamaguchi, C. Yu, M. Zeballos and L. Ziurys. First M87 Event Horizon Telescope Results. II. Array and Instrumentation. 2019. *The Astrophysical Journal Letters*. **875** (1). (LA-UR-19-26510 DOI: 10.3847/2041-8213/ab0c96)

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Akiyama, K., B. R. Ryan and E. H. T. Collaboration. First M87 Event Horizon Telescope Results VI: The Shadow and Mass of the Central Black Hole. Submitted to *Astrophysical Journal Letters*. (LA-UR-19-31648)

Ryan, B. R. and J. C. Dolence. MOCMC: Method of Characteristics Moment Closure, a Numerical Method for Covariant Radiation Magnetohydrodynamics. Submitted to *Astrophysical Journal. Supplement Series*. (LA-UR-19-24802)

Presentation Slides

Dolence, J. C. Full Transport GR Neutrino Radiation MHD and Nucleosynthesis in Neutron Star Merger Disks. Presented at

Explosive Nucleosynthesis in the Supernova and Merging-Neutron-Star Contexts, Princeton, New Jersey, United States, 2019-05-22 - 2019-05-24. (LA-UR-19-24793)

Ryan, B. R. MOCMC Status Report & Rad Hydro Issues. Presented at *TCAN 2020*, New York, New York, United States, 2020-01-09 - 2020-01-11. (LA-UR-20-20323)

Ryan, B. R. and J. C. Dolence. Method of Characteristics Moment Closure, a Numerical Method for Covariant Radiation Magnetohydrodynamic. Presented at *The 26th International Conference on Transport Theory (ICTT-26)*, Paris, France, 2019-09-23 - 2019-09-27. (LA-UR-19-29627)

Ryan, B. R. and J. C. Dolence. METHOD OF CHARACTERISTICS MONTE CARLO. Presented at *Horizon Collaboration Meeting 2019*, Princeton, New Jersey, United States, 2019-04-14 - 2019-04-16. (LA-UR-19-23499)

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

Journal Articles

Chen, L., H. Li, H. Shao and J. Wang. Higgs boson pair production via gluon fusion at N^{3}LO in QCD. Submitted to *Physical Review Letters*. (LA-UR-19-30443)

Chen, L., H. Li, H. Shao and J. Wang. The gluon-fusion production of Higgs boson pair: N^{3}LO QCD corrections and top-quark mass effects. Submitted to *JHEP*. (LA-UR-20-20034)

*Gao, A., H. T. Li, I. Moult and H. X. Zhu. Precision QCD Event Shapes at Hadron Colliders: The Transverse Energy-Energy Correlator in the Back-to-Back Limit. 2019. *Physical Review Letters*. **123** (6): 062001. (LA-UR-19-20914 DOI: 10.1103/PhysRevLett.123.062001)

*Li, C. S., H. T. Li, D. Y. Shao and J. Wang. Momentum-space threshold resummation in tW production at the LHC. 2019. *Journal of High Energy Physics*. **2019** (6): 125. (LA-UR-19-21475 DOI: 10.1007/JHEP06(2019)125)

Li, H. T. and I. Vitev. Jet splitting function in the vacuum and QCD medium. *PoS - Proceedings of Science*. (LA-UR-19-20679 DOI: 10.22323/1.345.0077)

*Li, H. T. and I. Vitev. Inclusive heavy flavor jet production with semi-inclusive jet functions: from proton to heavy-ion collisions. 2019. *Journal of High Energy Physics*. **2019** (7): 148. (LA-UR-19-20952 DOI: 10.1007/JHEP07(2019)148)

Li, H. and I. M. Vitev. Jet charge modification in dense QCD matter. Submitted to *Physical Review D*. (LA-UR-19-30442)

Conference Papers

Li, H. Jet charge in heavy-ion collisions. Presented at *https://indico.cern.ch/event/761800/*. (Santa Fe, New Mexico, United States, 2019-09-09 - 2019-09-09). (LA-UR-20-21864)

Conservative Slow-Manifold Integrators

Joshua Burby
20180756PRD4

Project Description

Physical systems and their computational modeling in national security applications often encounter extreme scale separation. The inherent stiffness in the physical models presents a grand challenge in multiscale simulations and predictive science. The current project seeks to develop a new paradigm in multiscale simulations via the so-called conservative slow manifold integrators. The key innovation is based on two fundamental properties of stiff systems that have been largely overlooked by previous investigators: (1) in the presence of irrelevant timescales, dynamics occur on invariant sets known as slow manifolds; (2) systems with conservation laws aways possess multi-linear skew-symmetric brackets that generalize Poisson brackets. Through the identification of slow manifolds, we can systematically identify dependent variables for various systems that nonlinearly separate the relevant and irrelevant timescales. In terms of those variables, we will then discretize the relevant skew-symmetric bracket in order to derive nonlinearly-implicit time integrators that preserve any number of first integrals exactly. This new advance will lead to groundbreaking simulations for topical problems in magnetic and inertial confinement fusion physics where the numerical and physical implications of stiffness are poorly understood.

Publications

Journal Articles

Burby, J. W. Guiding center dynamics as motion on a slow manifold in loop space. Submitted to *Journal of Mathematical Physics*. (LA-UR-19-24299)

Burby, J. W., E. Hirvijoki, D. Pfefferle and A. J. Brizard. Energy and momentum conservation in the Euler-Poincar\xc3\xa9 formulation of local Vlasov-Maxwell-type systems. Submitted to *Physics of Plasmas*. (LA-UR-19-32412)

Burby, J. W., N. Kallinikos and R. S. MacKay. Some mathematics for quasi-symmetry. Submitted to *Journal of Mathematical Physics*. (LA-UR-19-32407)

Burby, J. W. and D. E. Ruiz. Variational nonlinear WKB in the Eulerian frame. Submitted to *Journal of Mathematical Physics*. (LA-UR-19-21078)

Burby, J. W. and T. T. Klotz. Slow manifold reduction for plasma science. Submitted to *Communications in Nonlinear Science and Numerical Simulation*. (LA-UR-19-32243)

Reports

Klotz, T. and J. W. Burby. Slow Manifolds of fast-slow systems, the Vlasov-Maxwell System, and Control of Confined Plasma. Unpublished report. (LA-UR-19-27827)

Presentation Slides

Burby, J. W. Integrating guiding center motion in loop space. . (LA-UR-19-22767)

Burby, J. W. Compatibility Conditions for Quasisymmetry. . (LA-UR-19-27161)

Burby, J. W. Slow manifold integrators and the errors the commit. . (LA-UR-19-28965)

Burby, J. W. Slow manifold integrators: basic theory. Presented at *Nambe Meeting*, Los Alamos, New Mexico, United States, 2020-01-22 - 2020-01-22. (LA-UR-20-20600)

Burby, J. W. Slow manifold integrators: by way of computational Hamiltonian mechanics. Presented at *Structure-Preserving Geometric Discretization of Physical Systems*, Princeton, New Jersey, United States, 2020-02-17 - 2020-02-18. (LA-UR-20-21533)

Posters

Burby, J. W. Slow manifold integrator for electromagnetic PIC. Presented at *2019 APS DPP meeting*, Fort Lauderdale, Florida, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30654)

Matter and Nuclei at Neutron-Rich Extremes

Ingo Tews
20190617PRD1

Project Description

The work will involve large-scale calculations of atomic nuclei and of dense nucleonic matter present in neutron stars. Advancing our ability to calculate the properties and reactions of atomic nuclei will allow us to advance the state of the art in predicting nuclear reactions in regimes where experiments are difficult or impossible, like reactions on unstable nuclei.

Publications

Journal Articles

Brown, S. M., C. D. Capano, I. Tews, S. De, B. Margalit, D. A. Brown, B. Krishnan, S. Reddy and S. Kumar. Stringent constraints on neutron-star radii frommultimessenger observations and nuclear theory. Submitted to *Nature Astronomy*. (LA-UR-19-28442)

Dietrich, T., M. W. Coughlin, P. T. H. Pang, M. Bulla, J. Heinzel, L. Issa, I. Tews and S. Antier. New Constraints on the Supranuclear Equation of State and the Hubble Constant from Nuclear Physics--Multi-Messenger Astronomy. Submitted to *Science*. (LA-UR-20-21470)

Lonardoni, D., I. Tews, S. Gandolfi and J. A. Carlson. Nuclear matter and the symmetry energy from local chiral interactions. Submitted to *Physical Review Letters*. (LA-UR-19-32538)

Lonardoni, D. and I. Tews. Local chiral EFT potentials in nuclei and neutron matter: results and issues. Submitted to *PoS - Proceedings of Science*. (LA-UR-19-22185 DOI: 10.22323/1.317.0100)

Piarulli, M. and I. Tews. Local Nucleon-Nucleon and Three-Nucleon Interactions Within Chiral Effective Field Theory. 2020. *Frontiers in Physics*. **7**: 245. (LA-UR-19-30461 DOI: 10.3389/fphy.2019.00245)

Tews, I. Quantum Monte Carlo methods for astrophysical applications. Submitted to *Frontiers in Physics*. (LA-UR-19-32577)

Tews, I., J. Margueron and S. Reddy. To which extend nuclear physics and GW170817 constrain the neutron star equation of state?. Submitted to *Proceedings for the CUSTIPEN XiAMEN Workshop*. (LA-UR-19-24461)

Tews, I., Z. Davoudi, A. Ekstrom, J. Holt and J. Lynn. New Ideas in Constraining Nuclear Forces. Submitted to *Journal of Physics G: Nuclear and Particle Physics*. (LA-UR-19-32540)

Presentation Slides

Tews, I. Chiral effective field theory for the nuclear equation of state and neutron-star mergers. Presented at *2019 Fall Meeting of the APS Division of Nuclear Physics*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-17. (LA-UR-19-30581)

Tews, I. Chiral Effective Field Theory, Dense Nuclear Matter, and Neutron-Star Mergers. Presented at *JINA-INT Workshop Dense Matter & Neutron Star Mergers*, Seattle, Washington, United States, 2019-12-16 - 2019-12-18. (LA-UR-19-32539)

Tews, I. Stringent constraints on neutron-star radii from neutron-star mergers and chiral effective field theory. Presented at *Hirschegg 2020*, Hirschegg, Austria, 2020-01-13 - 2020-01-13. (LA-UR-20-20236)

Tews, I. Constraining the neutron-star equation of state and radius with chiral effective field theory and observations. Presented at *Ringberg conference*, Kreuth, Germany, 2020-01-13 - 2020-01-13. (LA-UR-20-20431)

Tews, I. From nuclei to neutron stars with local chiral interactions. Presented at *Theory Seminar at Washington University in St. Louis*, St. Louis, Missouri, United States, 2020-02-27 - 2020-02-27. (LA-UR-20-21840)

Posters

Tews, I. Matter and Nuclei at Neutron-rich Extremes. . (LA-UR-19-25831)

Tews, I. Neutron-Star Mergers as Probes for Nuclear Physics. Presented at *NUCLEI SciDAC PI meeting*, Rockville, Maryland, United States, 2019-07-15 - 2019-07-18. (LA-UR-19-26620)

State-of-the-Art Predictions for the Matter-Antimatter Asymmetry

Christopher Lee
20190622PRD2

Project Description

This project addresses two of the great open scientific questions of our day, which are also two of the top research priorities of the Department of Energy Office of Science: “What is the origin of the matter-antimatter asymmetry?” and “What lies beyond the Standard Model of Particle Physics?” The first question addresses the origin of all visible matter in our universe today, which cannot be explained by the current Standard Model of Particle physics, thus connecting it to the second question. Answers to these require the development of frontier theoretical and computational tools as well as experimental techniques to probe physical phenomena lying beyond the Standard Model that could provide these answers. In addition, the theoretical tools are applicable to studying other physical systems, such as supernovae and how the propagation of neutrinos through them affects the dynamics of their explosions, while the experiments develop cutting-edge technology and capabilities in accelerator science and in trapping and measuring precisely ultracold neutrons. At the conclusion of our project, besides having such new tools and capabilities, we expect to have made a major step towards understanding how the matter in the universe could have been generated in its first few moments of existence.

Publications

Journal Articles

Fuyuto, K., M. Ramsey-Musolf, C. Chiang, G. Cottin and Y. Du. Collider Probes of Real Triplet Scalar Dark Matter. Submitted to *Journal of High Energy Physics*. (LA-UR-20-22358)

Fuyuto, K., W. S. Hou and E. Senaha. Cancellation mechanism for the electron electric dipole moment connected with bray asymmetry of the Universe. Submitted to *Physical Review Letters*. (LA-UR-19-30968)

Mereghetti, E., K. Fuyuto, W. G. Dekens, J. de Vries and G. Zhou. Sterile neutrinos and neutrinoless double beta decay in effective field theory. Submitted to *Journal of High Energy Physics*. (LA-UR-20-21376)

Phase Diagrams and Conductivity in the Interiors of White Dwarf Stars

Didier Saumon
20190624PRD2

Project Description

The extreme conditions found in stars and the wide range of multi-physics problems that must be solved to understand them overlaps considerably with the science of national security at the Laboratory. Astrophysics is a field where advanced models can be developed and tested and then applied to national security challenges. White dwarf stars in particular present exotic physical conditions not found in any other type of star and pose challenging problems to solve. The proposed work will address the calculation of material properties that are difficult to model, in particular the melting of mixtures and heat transport. These are two essential components for the modeling of white dwarfs. Our accurate plasma models and calculations will lead to better white dwarf models, with consequences for several fields of astrophysics. Moreover, the methods and tools we will develop are more generally applicable to the melting of pure substances and alloys, as well as heat transport in systems such as inertial confinement fusion. We anticipate that they will find fruitful applications in several areas of high energy density physics of relevance to national security, such as stockpile stewardship, where accurate material properties are a critical element to our theoretical understanding.

Publications

Journal Articles

Blouin, S., M. C. Lam, N. C. Hambly, N. Lodieu, E. Harvey, R. J. Smith, H. Zhang and M. C. G\xc3\xa1lvez Ortiz. Discovery of an Ultra-Cool White Dwarf Benchmark in Common Proper Motion with an M Dwarf. Submitted to *Monthly Notices of the Royal Astronomical Society*. (LA-UR-19-31660)

Blouin, S. and P. Dufour. The evolution of carbon-polluted white dwarfs at low effective temperatures. 2019. *Monthly Notices of the Royal Astronomical Society*. **490** (3): 4166-4174. (LA-UR-19-29175 DOI: 10.1093/mnras/stz2915)

Conference Papers

Blouin, S. and P. Dufour. The Spectral Evolution of Cool White Dwarfs. Presented at *IAU Symposium 357: White Dwarfs as probes of fundamental physics and tracers of planetary, stellar & galactic evolution*. (Hilo, Hawaii, United States, 2019-10-21 - 2019-10-25). (LA-UR-19-31433)

Presentation Slides

Blouin, S. The spectral evolution of cool white dwarfs. Presented at *International Astronomical Union Symposium 357: White Dwarfs as probes of fundamental physics and tracers of planetary, stellar & galactic evolution*, Hilo, Hawaii, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-29925)

Blouin, S. When The Fit Is Just Right: Improved Cool White Dwarf Atmosphere Models. Presented at *235th Meeting of the American Astronomical Society*, Honolulu, Hawaii, United States, 2020-01-04 - 2020-01-08. (LA-UR-19-32098)

Searching for Dark Matter with Fixed Target Experiments

Daniele Spier Moreira Alves
20190626PRD2

Project Description

The high level goal is explore the theory and interpretation of experimental data to discover the nature of dark matter in the Universe, an unknown form of matter in galaxies that is six times more abundant than ordinary matter. The expected outcome is a further understanding of the fundamental constituents of the Universe, either by discovering new forms of matter, of by ruling out existing theories that attempt to explain dark matter. This project addresses the challenges defined as high priority scientific goals by the DOE SC Particle Physics Project Prioritization Panel (a subpanel of the High Energy Physics Advisory Panel), the 2015 Department of Energy Office of Science (SC) Nuclear Physics Long-Range Plan, and the Laboratory's Strategic Investment Plan, specifically in its Nuclear and Particle Futures pillar.

Publications

Journal Articles

deNiverville, P., A. Berlin, A. Ritz, N. Toro and P. Schuster. On sub-GeV Dark Matter Production at Fixed-Target Experiments. Submitted to *Physical Review D*. (LA-UR-20-22261)

deNiverville, P., L. Buonocore and C. Frugiuele. The hunt for sub-GeV dark matter at neutrino facilities: a survey of past and present experiments. Submitted to *Journal of High Energy Physics*. (LA-UR-19-32644)

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.

Technical Outcomes

Astrophysical observations suggest 85% of the matter in the Universe is dark matter. We searched for gamma-ray signals from cosmic dark-matter interactions with the Fermi Satellite and the High Altitude Water Cherenkov (HAWC) observatory. Though no signal was found, we were able to exclude models that were previously unexplored. With HAWC's high-energy reach we were able to search for signals from heavy dark matter for the first time.

Publications

Journal Articles

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Albert, A. Multi-messenger Observations of a Binary Neutron Star Merger. Submitted to *Astrophysical Journal*. (LA-UR-18-29823)

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Albert, A. Constraining the p\xc2\xaf/p Ratio in TeV Cosmic Rays with Observations of the Moon Shadow by HAWC. Submitted to *Physical Review D*. (LA-UR-18-29826)

Albert, A. Dark Matter Limits From Dwarf Spheroidal Galaxies with The HAWC Gamma-Ray Observatory. Submitted to *Astrophysical Journal*. (LA-UR-18-29824)

Albert, A. Extended gamma-ray sources around pulsars constrain the origin of the positron flux at Earth. Submitted to *Science*. (LA-UR-18-29827)

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Presentation Slides

Albert, A. Diffuse Gamma-ray Emission Modeling Near the Galactic Center and the 3 GeV Excess. Presented at *APS April Meeting*, Salt Lake City, Utah, United States, 2016-04-16 - 2016-04-16. (LA-UR-16-22730)

Albert, A. Probing Dark Matter with Cosmic Messengers. Presented at *3rd Kobayashi Maskawa International Symposium*, Nagoya, Japan, 2017-01-05 - 2017-01-07. (LA-UR-16-29532)

Albert, A. How to Read a Science Headline. . (LA-UR-17-27280)

Albert, A. Recent Results from the HAWC Gamma-ray Observatory. Presented at *CIPANP 2018*, Palm Springs, California, United States, 2018-05-29 - 2018-05-29. (LA-UR-18-24585)

Albert, A. Recent Results from the HAWC Gamma-ray Observatory. Presented at *2018 Santa Fe Summer Workshop in Particle Physics*, Santa Fe, New Mexico, United States, 2018-07-02 - 2018-07-06. (LA-UR-18-25882)

Albert, A. Searching for Dark Matter Gamma Rays from Dwarf Galaxies. Presented at *14th Rencontres du Vietnam Very High Energy Phenomena in the Universe*, Quy Nhon, Vietnam, 2018-08-12 - 2018-08-18. (LA-UR-18-27499)

Albert, A. High-energy Particle Physics -- In Space!. . (LA-UR-18-28474)

Albert, A. M. Search for Dark Matter Gamma-ray Emission from M31 with HAWC. Presented at *APS April Meeting 2018*, Columbus, Ohio, United States, 2018-04-14 - 2018-04-17. (LA-UR-18-23130)

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 Department of Energy 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.

Technical Outcomes

3D simulations of supernovae (SNe) were performed, explaining a subpopulation of Galactic white dwarfs and isotopes prevalent in the Milky Way (published in three articles). 60Fe detection prospects in SN remnants via EM emission, based on a suite of new simulations and were also published. Work begin on simulations of low-Mach variable density turbulent jets in xRage in collaboration with the Extreme Fluids group at LANL. Jones is now staff in XCP-2.

Publications

Journal Articles

*Davis, A., S. Jones and F. Herwig. Convective boundary mixing in a post-He core burning massive star model. 2019. *Monthly Notices of the Royal Astronomical Society*. **484** (3): 3921-3934. (LA-UR-17-30635 DOI: 10.1093/mnras/sty3415)

*Jones, S. W., H. Moeller, C. L. Fryer, C. J. Fontes, R. Trappitsch, W. P. Even, A. Couture, M. R. Mumpower and S. Safi-Harb. 60Fe in core-collapse supernovae and prospects for X-ray and gamma-ray detection in supernova remnants. 2019. *Monthly Notices of the Royal Astronomical Society*. **485** (3): 4287-4310. (LA-UR-18-24048 DOI: 10.1093/mnras/stz536)

Jones, S., B. C\xc3\xb4t\xc3\xa9 and M. Pignatari. CHROMIUM NUCLEOSYNTHESIS AND CARBON-SILICON SHELL MERGERS IN MASSIVE STARS. Submitted to *Astrophysical Journal Letters*. (LA-UR-19-24678)

*Jones, S., B. Cote, F. K. Ropke and S. Wanajo. A New Model for Electron-capture Supernovae in Galactic Chemical Evolution. 2019. *The Astrophysical Journal*. **882** (2): 170. (LA-UR-19-25987 DOI: 10.3847/1538-4357/ab384e)

Jones, S., C. L. Fryer, F. Roepke, A. Ruiter and R. Reifarth. Remnants and ejecta of high-density oxygen-neon deflagrations; Constraints on the explosion mechanism and frequency of electron-capture supernovae. Submitted to *Astronomy & Astrophysics*. (LA-UR-18-26774)

Kirsebom, O., S. Jones, F. Roepke, S. Ohlmann, H. Fynbo, K. Riisager, G. Mart\xc3\xadnez-Pinedo, H. Moeller, D. Str\xc3\xb3mberg, K. Langanke, A. Kankainen, M. Hukkanen, W. Trzaska, S. Rinta-Antila, T. Eronen, I. Moore, A. Jokinen, H. Penttil\xc3\xa4 and J. Aeystoe. An electron-capture ignited thermonuclear explosion. Submitted to *Science*. (LA-UR-18-26043)

Reports

Fryer, C. L. and S. Jones. Turbulence in Supernova Progenitors. Unpublished report. (LA-UR-18-25735)

Jones, S. Turbulence in Supernova Progenitors. Unpublished report. (LA-UR-17-29474)

Presentation Slides

Jones, S. Modelling stars near the electron-capture supernova limit. Presented at *Stellar Hydro Days IV*, Victoria, Canada, 2017-05-29 - 2017-06-02. (LA-UR-17-24214)

Jones, S. Constraining simulations of stars and supernovae. . (LA-UR-18-28435)

Jones, S. Deflagrations and Convection 1. . (LA-UR-19-21963)

Jones, S. Signatures of thermonuclear electron-capture supernovae. Presented at *Electron-capture initiated stellar collapse*, Leiden, Netherlands, 2019-05-20 - 2019-05-24. (LA-UR-19-24801)

Jones, S., C. L. Fryer, W. P. Even, C. J. Fontes and H. Moeller. STELLAR ORIGIN OF 60Fe AND OBSERVATION PROSPECTS. . (LA-UR-18-25639)

Measurement of Cross Sections Crucial for Constraining Stellar Nucleosynthesis

Christopher Prokop
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.

Technical Outcomes

A successful measurement of the 65Cu(n,g) cross section was performed resulting in a Physical Review C article. Advances in acquisition, analysis, and simulation benefits future DANCE measurements. New collaborations with Texas A&M University through NNSA center of excellence CENTAUR increased our measurement capability. Steps have been taken to develop and characterize detectors for a (d,pg) transfer reaction campaign to inform neutron-capture cross sections away from stability.

Publications

Journal Articles

*Prokop, C. J., A. Couture, S. Jones, S. Mosby, G. Rusev, J. Ullmann and M. Krticka. Measurement of the 65Cu(n,\xce\xb3) cross section using the Detector for Advanced Neutron Capture Experiments at LANL. 2019. *Physical Review C*. **99** (5): 055809. (LA-UR-19-20879 DOI: 10.1103/PhysRevC.99.055809)

Presentation Slides

Prokop, C. J. Measurement of 65Cu(n,gamma) Cross Section using DANCE. Presented at *SSAA Center For Excellence Workshop*, Los Alamos, New Mexico, United States, 2018-03-14 - 2018-03-15. (LA-UR-18-22131)

Prokop, C. J. The Value of Undergraduate Research From the Perspective of an Early-Career Nuclear Scientist. Presented at *25th Conference on Application of Accelerators in Research and Industry*, Grapevine, Texas, United States, 2018-08-12 - 2018-08-17. (LA-UR-18-27712)

Prokop, C. J. Neutron-Capture Measurements with DANCE for Constraining s-process Nucleosynthesis. . (LA-UR-19-23206)

Prokop, C. J. Constraining Nuclear Level Density at the MORDOR Facility. Presented at *Workshop on Opportunities with a Neutron Target Facility*, Santa Fe, New Mexico, United States, 2019-08-19 - 2019-08-20. (LA-UR-19-28336)

Prokop, C. J. Neutron Capture for Applications. Presented at *Nuclear Data Workshop*, Livermore, California, United States, 2019-09-09 - 2019-09-13. (LA-UR-19-28939)

Prokop, C. J. Measurement of neutron-capture cross sections of copper isotopes with DANCE for constraining s-process nucleosynthesis. Presented at *ACS Fall Meeting*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-30158)

Prokop, C. J., A. J. Couture, S. Jones, S. M. Mosby, K. J. Kelly, G. Y. Rusev, J. L. Ullmann and J. Winkelbauer. Measurement of the 65Cu(n,\xf0\x9d\x9b\xbe) Cross Section for Constraining s-process Nucleosynthesis. Presented at *APS DNP*, Waikoloa, Hawaii, United States, 2018-10-23 - 2018-10-27. (LA-UR-18-30247)

Analyticity, Unitarity, and the Behavior of Neutrino Scattering

Vincenzo Cirigliano
20190619PRD1

Project Description

This project will help elucidating the mysteries associated with the most elusive of the known elementary particles, the neutrino, which is also the second most abundant particle in our universe. The Department Of Energy Office of Science is engaged in long-term investments in understanding the nature of neutrino, which include the billion-dollar Deep Underground Neutrino Experiment, which will shoot a beam of neutrinos from Fermilab (Batavia, Illinois) to Sanford Lab (South Dakota). Key to the interpretation of the experimental results is our theoretical understanding of how neutrinos interact with the nuclei that make up the detector at Sanford Lab. This project aims to put on a firm theoretical basis our understanding of the energy-dependence of neutrino interactions with neutrons, protons, and nuclei. The work is theoretical in nature and will have a pure "paper and pencil" component, a computational component, and a data analysis component.

Technical Outcomes

The outcome of this project has been affected by Dr. Kobach's leaving LANL only three months into the project. In this short time, Dr. Kobach has set up a new parameterization for the so-called vector and axial form factors of the nucleon controlling scattering of neutrinos off nuclei. The results are technically sound, but the analysis is still preliminary and has not led to a publication.

Science of Signatures

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 outperfroms 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.

Publications

Presentation Slides

Boshier, M. G. DOE HEP and Quantum Sensing Research at Los Alamos National Laboratory. Presented at *Argonne Workshop on Quantum Sensing*, Chicago, Illinois, United States, 2017-12-12 - 2017-12-12. (LA-UR-17-31155)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31463)

Boshier, M. G. Two Experiments in Atomtronics: Quantum Interference in an Atomtronic SQUID and a Waveguide Sagnac Atom Interferometer. Presented at *2019 Benasque Atomtronics Workshop*, Benasque, Spain, 2019-05-05 - 2019-05-17. (LA-UR-19-24576)

Boshier, M. G. Lessons Learned From Developing Quantum Sensors. Presented at *STEP Workshop on Quantum Sensors*, McLean, Virginia, United States, 2019-09-10 - 2019-09-10. (LA-UR-19-29036)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *Quantum Technologies and Sensing Workshop*, Manchester, United Kingdom, 2019-10-27 - 2019-10-27. (LA-UR-19-30772)

Boshier, M. G. Atomtronics for Quantum Sensing. Presented at *Seminar at Purdue University*, West Lafayette, Indiana, United States, 2019-11-12 - 2019-11-12. (LA-UR-19-31593)

Boshier, M. G. A Moving Waveguide Sagnac Atom Interferometer. Presented at *Workshop on Inertial Sensing*, Brighton, United Kingdom, 2019-11-29 - 2019-11-29. (LA-UR-19-32050)

Boshier, M. G., C. Ryu and C. Samson. Quantum \xc2\xa0Interference\xc2\xa0in\xc2\xa0an \xc2\xa0Atomtronic\xc2\xa0SQUID. Presented at *PQE-2018*, Snowbird, Utah, United States, 2018-01-08 - 2018-01-12. (LA-UR-18-20219)

Boshier, M. G. and C. Ryu. Atomtronics for Quantum Sensing. Presented at *2018 CINT User Meeting*, Santa Fe, New Mexico, United States, 2018-09-24 - 2018-09-25. (LA-UR-18-29086)

Henderson, K. C. Symmetry and How it Breaks. Presented at *New Mexico History Museum*, Santa Fe, New Mexico, United States, 2019-02-22 - 2019-02-22. (LA-UR-19-21059)

Kim, H. Detailed balance of thermalization dynamics in Rydberg quantum simulators. Presented at *LANL Quantum DAY*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31537)

Kurkcuoglu, D. M. Quantum simulation and quantum technologies with cold atoms. . (LA-UR-20-22384)

Martin, M. J., C. Ryu and M. G. Boshier. Quantum technologies with ultracold atoms. Presented at *UC Quantum Information Science Research Workshop*, Berkeley, California, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24127)

Posters

Boshier, M. G. and C. Ryu. Sensing with Atomtronics Circuits and Devices. Presented at *SOS capability review*, Los Alamos, New Mexico, United States, 2018-04-24 - 2018-04-25. (LA-UR-18-23422)

Cassidy, M. C. Presentation2. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27193)

Hurd, S. J. Optimum Transportation of Cold Atoms. Presented at *Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27140)

Hurd, S. J. symposium poster sara hurd 2019. Presented at *Student Symposium*, Las Alamos, New Mexico, United States, 2019-08-07 - 2019-08-07. (LA-UR-19-27933)

Kim, H., J. Ferreras Fuertes, K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu and M. G. Boshier. Progress Toward Atomtronics Sagnac Interferometer. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28645)

Kurkcuoglu, D. M. Unconventional color superfluidity in ultra-cold fermions: Quintuplet pairing, quintuple point and pentacriticality. Presented at *39th CNLS Strongly Correlated Systems Conference*, Santa Fe, New Mexico, United States, 2019-04-29 - 2019-05-03. (LA-UR-19-23837)

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

Journal Articles

Cardin, A. E., S. R. M. Silva, S. R. Vardeny, W. J. Padilla, A. B. Saxena, A. J. Taylor, W. J. de Melo Kort-Kamp, H. Chen, D. A. R. Dalvit and A. K. Azad. Surface-Wave-Assisted Nonreciprocity in Spatio-Temporally Modulated Metasurfaces. Submitted to *Nature Communications*. (LA-UR-19-30765)

*Chang, C., W. J. M. Kort-Kamp, J. Nogan, T. S. Luk, A. K. Azad, A. J. Taylor, D. A. R. Dalvit, M. Sykora and H. Chen. High-Temperature Refractory Metasurfaces for Solar Thermophotovoltaic Energy Harvesting. 2018. *Nano Letters*. **18** (12): 7665-7673. (LA-UR-18-27846 DOI: 10.1021/acs.nanolett.8b03322)

Chen, H., C. Chang, A. J. Taylor, Z. Zhao, S. Fan and D. Li. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. Submitted to *Physical Review Letters*. (LA-UR-18-31108)

Chen, H., J. Zhang, X. Wei, I. D. Rukhlenko and W. Zhu. Electrically Tunable Metasurface with Independent Frequency and Amplitude Modulations. Submitted to *Advanced Materials*. (LA-UR-19-29711)

Chen, H., W. J. de Melo Kort-Kamp, D. A. R. Dalvit, A. K. Azad, C. Chang, J. Nogan, Z. Yang, W. Ross and T. S. Luk. Highly Plasmonic Titanium Nitride by Room-Temperature Sputtering. Submitted to *Scientific Reports*. (LA-UR-19-29707)

Chen, H., Z. Zhao, D. Li, A. J. Taylor, S. Fan and C. Chang. Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. Submitted to *Physical Review Letters*. (LA-UR-19-29771)

*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. 2018. *Applied Physics Letters*. **113** (6): 061111. (LA-UR-18-29890 DOI: 10.1063/1.5040162)

Cheong, S., D. Talbayev, V. Kiryukhin and A. Saxena. Broken symmetries, non-reciprocity, and multiferroicity. 2018. *npj Quantum Materials*. **3** (1): 19. (LA-UR-18-20267 DOI: 10.1038/s41535-018-0092-5)

R. Dalvit, D. A., F. Intravaia, D. Oelschlager, D. Reiche and K. Busch. Rolling Quantum Friction. Submitted to *Physical Review Letters*. (LA-UR-18-29152)

R. Dalvit, D. A., F. Intravaia and K. Busch. Fluctuation-induced phenomena in photonic systems: Introduction. Submitted to *Journal of the Optical Society of America B: Optical Physics*. (LA-UR-19-23024)

Dandoloff, R. and A. Saxena. XY Model on Interacting Parallel Planes with a Soliton. Submitted to *Physics Letters. Section A: General, Atomic and Solid State Physics*. (LA-UR-17-31143)

*Belen Farias, M., W. J. M. Kort-Kamp and D. A. R. Dalvit. Quantum friction in two-dimensional topological materials. 2018. *Physical Review B*. **97** (16): 161407. (LA-UR-17-29840 DOI: 10.1103/PhysRevB.97.161407)

*Gaididei, Y., V. P. Kravchuk, F. G. Mertens, O. V. Pylypovskyi, A. Saxena, D. D. Sheka and O. M. Volkov. Localization of magnon modes in a curved magnetic nanowire. 2018. *Low Temperature Physics*. **44** (7): 634-643. (LA-UR-18-20270 DOI: 10.1063/1.5041428)

*M. Kort-Kamp, W. J., F. J. Culchac, R. B. Capaz and F. A. Pinheiro. Photonic spin Hall effect in bilayer graphene moir\xc3\xa9 superlattices. 2018. *Physical Review B*. **98** (19): 195431. (LA-UR-18-27864 DOI: 10.1103/PhysRevB.98.195431)

*Ledwith, P., W. J. M. Kort-Kamp and D. A. R. Dalvit. Topological phase transitions and quantum Hall effect in the graphene family. 2018. *Physical Review B*. **97** (16): 165426. (LA-UR-17-30904 DOI: 10.1103/PhysRevB.97.165426)

Muniz, Y., A. Manjavacas, C. Farina, D. A. R. Dalvit and W. J. de Melo Kort-Kamp. Unraveling the decay mechanisms of two-quanta spontaneous photonic transitions. Submitted to *Nature Photonics*. (LA-UR-20-20456)

*Muniz, Y., F. S. S. da Rosa, C. Farina, D. Szilard and W. J. M. Kort-Kamp. Quantum two-photon emission in a photonic cavity. 2019. *Physical Review A*. **100** (2): 023818. (LA-UR-19-21860 DOI: 10.1103/PhysRevA.100.023818)

*M. Rao, S. J., G. Kumar, A. K. Azad and D. R. Chowdhury. Ultrafast Relaxation of Charge Carriers Induced Switching in Terahertz Metamaterials. 2018. *Journal of Infrared, Millimeter, and Terahertz Waves*. **39** (12): 1211-1220. (LA-UR-18-30111 DOI: 10.1007/s10762-018-0547-6)

*Rodriguez-Lopez, P., W. J. M. Kort-Kamp, D. A. R. Dalvit and L. M. Woods. Nonlocal optical response in topological phase transitions in the graphene family. 2018. *Physical Review Materials*. **2** (1): 014003. (LA-UR-17-30514 DOI: 10.1103/PhysRevMaterials.2.014003)

Sanders, S., W. J. M. Kort-Kamp, D. A. R. Dalvit and A. Manjavacas. Nanoscale transfer of angular momentum mediated by the Casimir torque. 2019. *Communications Physics*. **2** (1): 71. (LA-UR-18-29153 DOI: 10.1038/s42005-019-0163-3)

M. Silva, S. R., A. K. Azad, D. A. R. Dalvit, H. Chen, J. J. Rushton, W. J. de Melo Kort-Kamp, A. J. Taylor, J. Singleton and A. Rahman. Metasurface-based ultra-lightweight high-gain off-axis flat parabolic reflectarray for microwave beam collimation/focusing. 2019. *Applied Physics Letters*. **9** (1): 18984. (LA-UR-19-22629 DOI: 10.1038/s41598-019-55221-8)

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*Wei, M., X. Hao, A. B. Saxena, W. Qin and S. Xie. Optical Helicity-Manipulated Photocurrents and Photovoltages in Organic Solar Cells. 2018. *The Journal of Physical Chemistry C*. **122** (23): 12566-12571. (LA-UR-18-20268 DOI: 10.1021/acs.jpcc.8b03537)

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Presentation Slides

Azad, A. K. HARNESSING LIGHT-METASURFACE INTERACTIONS FOR ENABLING TECHNOLOGIES. Presented at *IEEE Research and Applications of Photonics In Defense Conference*, Miramar Beach, Florida, United States, 2018-08-20 - 2018-08-20. (LA-UR-18-29352)

Azad, A. K. Dominating the Electromagnetic Spectrum with Spatio-Temporal Modulated Metasurfaces. . (LA-UR-19-20934)

Azad, A. K. LDRD-DR appraisal. . (LA-UR-20-21824)

Azad, A. K., A. E. Cardin, S. R. M. Silva and S. R. Vardeny. Dynamic metasurfaces. . (LA-UR-19-20931)

Azad, A. K. and S. R. Vardeny. LDRD-DR presentation. . (LA-UR-20-21825)

Chen, H. Few-Layer THz Metasurfaces for Effective Control of Amplitude, Phase and Polarization States. Presented at *The 4th International Symposium on Microwave/Terahertz Science and Applications & the 8th International Symposium on Terahertz Nanoscience*, Okayama, Japan, 2017-11-19 - 2017-11-23. (LA-UR-17-30608)

Chen, H. Exotic Properties of Metasurfaces and Their Applications. Presented at *Seminar at University of New Mexico*, Albuquerque, New Mexico, United States, 2018-02-09 - 2018-02-09. (LA-UR-18-21182)

Chen, H. Narrowband Terahertz Bandpass Filters Based on Metasurfaces. Presented at *SPIE Defense + Commercial Sensing*, Orlando, Florida, United States, 2018-04-15 - 2018-04-19. (LA-UR-18-23323)

Chen, H. Hybrid Graphene Metasurfaces for High-Speed Mid-Infrared Modulation. Presented at *The 5th International Conference on Frontiers of Plasmonics (FOP5)*, Nanjing, China, 2018-04-20 - 2018-04-24. (LA-UR-18-23324)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversion. Presented at *The 9th International Symposium on Ultrafast Phenomena and Terahertz Waves (ISUPTW 2018)*, Changsha, China, 2018-04-23 - 2018-04-23. (LA-UR-18-23594)

Chen, H. Hybrid Graphene Metasurface for High-Speed Mid-Infrared Modulation. Presented at *Excited State Process in Electronic and Bio Nanomaterials (ESP-2018)*, Santa Fe,

New Mexico, United States, 2018-06-04 - 2018-06-07. (LA-UR-18-25014)

Chen, H. Broadband THz Linear Polarization Rotation and Linear-to-Circular Polarization Conversion Using Metasurfaces. Presented at *OSA Advanced Photonics Congress*, Zurich, Swaziland, 2018-07-02 - 2018-07-05. (LA-UR-18-25397)

Chen, H. Hybrid Graphene Metasurface for High-Speed Mid-Infrared Light Modulation and Single-Pixel Imaging. Presented at *META 2018*, Marseille, France, 2018-06-24 - 2018-06-24. (LA-UR-18-26353)

Chen, H. Achromatic Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces. . (LA-UR-19-20968)

Chen, H. Metasurfaces for Manipulating Terahertz Radiation. . (LA-UR-19-25954)

Chen, H. Hybrid Graphene Metasurfaces for High-Speed Mid-Infrared Light Modulation and Single-Pixel Imaging. Presented at *ICMAT 2019*, Singapore, Singapore, 2019-06-24 - 2019-06-24. (LA-UR-19-25955)

Chen, H. Metasurfaces – Achromatic Polarization Conversion and Efficient Optical Modulation. Presented at *Seminar at Argonne National Laboratory*, Lemont, Illinois, United States, 2019-09-11 - 2019-09-11. (LA-UR-19-29185)

Chen, H. Metasurfaces for Broadband Terahertz Polarization Conversions. Presented at *MTSA 2019*, Busan, Korea, South, 2019-09-30 - 2019-09-30. (LA-UR-19-29968)

Cooke, B. J., J. H. Goglio, J. J. Rushton and A. K. Azad. Transition to Mission Applications. . (LA-UR-19-20956)

R. Dalvit, D. A. Nonreciprocal Metasurfaces. . (LA-UR-19-20945)

de Melo Kort-Kamp, W. J., D. A. R. Dalvit, S. R. M. Silva and J. J. Rushton. Modeling and Simulation of Static Metasurfaces. . (LA-UR-19-20946)

Saxena, A. B. Nonreciprocity and broken symmetry in photonics: Implications for materials. Presented at *SPIE Optics and Photonics Congress*, San Diego, California, United States, 2018-08-20 - 2018-08-20. (LA-UR-18-27771)

M. Silva, S. R., W. J. de Melo Kort-Kamp, D. A. R. Dalvit, J. J. Rushton, A. K. Azad and H. Chen. Metasurface-based Static Reflectarray Antenna. . (LA-UR-19-20933)

Vardeny, S. R. and A. K. Azad. Testbeds for Active/Dynamic Metamaterial Antennas (ADMA). Presented at *DR Review*, Los Alamos, New Mexico, United States, 2020-02-25 - 2020-02-25. (LA-UR-20-21849)

Posters

Azad, A. K., S. Kramadhati, S. R. M. Silva, N. S. Sirica and H. Chen. Flat Ultrathin Metasurface Parabolic Reflector for THz Applications. . (LA-UR-19-20932)

Cardin, A. E., S. R. M. Silva, S. R. Vardeny, H. Chen and A. K. Azad. Agile Metasurfaces for Beam Manipulation. Presented at *LANL 2019 Student Symposium*, Loa Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27733)

Chen, H., A. D. Tang, S. R. M. Silva, P. L. Cantu, P. Nath and C. Corbella Bagot. Development of an Alvarez metalens in the microwave regime. . (LA-UR-19-20970)

de Melo Kort-Kamp, W. J. Topological Phase Transitions in the Photonic Spin Hall Effect. . (LA-UR-19-20927)

Saxena, A. B. Nonreciprocity and Broken Symmetry. . (LA-UR-19-20944)

Vardeny, S. R. Phase Distribution Surface Controller for Spatio-Temporal Modulated Metasurface Antennas. Presented at *DR Review*, Los Alamos, New Mexico, United States, 2019-02-05 - 2019-02-05. (LA-UR-19-20953)

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

Journal Articles

Carlson, R. K., S. M. Clegg, P. Yang and E. R. Batista. Mechanistic Study of Copper Dissolution in Nitric Acid. Submitted to *Inorganic Chemistry*. (LA-UR-20-20214)

*Currier, R. P., T. B. Peery, M. F. Herman, R. F. Williams, R. Michalczyk, T. E. Larson, D. M. Labotka, J. E. Fessenden and S. M. Clegg. Azeotropic isotopologues. 2019. *Fluid Phase Equilibria*. **493**: 188-195. (LA-UR-18-30223 DOI: 10.1016/j.fluid.2019.04.006)

Dorhout, J. M., K. L. Nowak-Lovato, A. S. Anderson, E. R. Batista, R. K. Carlson, Z. Li, R. K. Martinez, M. P. Wilkerson, S. M. Clegg and R. P. Currier. Characterization of Nitrogen-Containing Species Produced from Nitric Acid/Water Systems. Submitted to *Journal of Physical Chemistry A*. (LA-UR-19-24140)

Dorhout, J. M., K. L. Nowak-Lovato, A. S. Anderson, R. K. Martinez, Z. Li, M. P. Wilkerson and S. M. Clegg. Production of Nitrogen-Containing Species in Nitric Acid/Water Systems. Submitted to *Journal of Physical Chemistry A*. (LA-UR-19-20615)

Dorhout, J. M., K. L. Nowak-Lovato, R. K. Carlson, R. P. Currier, A. S. Anderson, E. R. Batista, Z. Li, R. K. Martinez, M. P. Wilkerson and S. M. Clegg. Characterization of Nitrogen-Containing Species Produced From Nitric Acid/Water Systems. Submitted to *Journal of Molecular Spectroscopy*. (LA-UR-20-20673)

Gayday, I., A. Teplukhin, B. K. Kendrick and D. Babikov. Asymmetric-top rotor terms and Coriolis couplings in hyper-spherical coordinates: On alternative choices of z-axis and the structure of Hamiltonian matrix, with application to ozone. Submitted to *Journal of Chemical Physics*. (LA-UR-19-31077)

Gayday, I., A. Teplukhin, B. K. Kendrick and D. Babikov. On the Role of Rotation-Vibration Coupling in the Spectra of Ozone Isotopomers. Submitted to *The Journal of Chemical Physics*. (LA-UR-19-32237)

Larson, T. E., G. B. Perkins, R. F. Williams, J. E. Fessenden, S. M. Clegg and R. P. Currier. Partitioning of oxygen isotopes during the aqueous solvation of nitric acid. 2020. *Fluid Phase Equilibria*. **506**: 112364. (LA-UR-19-25191 DOI: 10.1016/j.fluid.2019.112364)

Li, Z., K. L. Nowak-Lovato, A. S. Anderson, S. M. Clegg, R. K. Martinez, J. M. Dorhout and R. K. Carlson. Sequential cryogenic separation of NOx species (NO + NO2) for online nitrogen isotopic analysis using EA-IRMS. Submitted to *Rapid Communications in Mass Spectrometry*. (LA-UR-19-20860)

M. Mallory, E. J., T. B. Peery and M. F. Francis. Statistical representations and unbiased metrics for stable isotope fractionation. Submitted to *Chemical Geology*. (LA-UR-20-20132)

Teplukhin, A. and B. K. Kendrick. Three-dimensional potential energy surfaces of ArNO (X 2\xce\xa0). Submitted to *Journal of Chemical Physics*. (LA-UR-20-20133)

Conference Papers

Peery, T. B., R. P. Currier, E. J. M. Mallory and S. M. Clegg. Statistical Reference States in Stable Isotope Fractionation and Chemistry. Presented at *LDRD 20180066DR third-year review*. (Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15). (LA-UR-20-20149)

Books/Chapters

Clegg, S. M., K. L. Nowak-Lovato, R. P. Currier, J. E. Fessenden and R. K. Martinez. Surface Monitoring, Verification and Accounting (MVA) for Geologic Sequestration Storage. (LA-UR-18-26244)

Clegg, S. M., K. L. Nowak-Lovato, R. P. Currier, J. E. Fessenden and R. K. Martinez. Surface Monitoring, Verification and Accounting (MVA) for Geologic Sequestration Storage. (LA-UR-19-27356)

Presentation Slides

Carlson, R. K. Copper Dissolution in Nitric Acid: Unraveling a Century of Hypotheses. Presented at *ACS National Meeting*, San Diego, California, United States, 2019-08-26 - 2019-08-26. (LA-UR-19-28350)

Carlson, R. K. and E. R. Batista. Cu + HNO3 Dissolution: Mechanism and Fractionation. Presented at *DR Review*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20870)

Clegg, S. M. Venus Elemental and Mineralogical Camera (VEMCam). . (LA-UR-18-26082)

Currier, R. P., T. B. Peery, M. F. Herman, R. F. Williams, R. Michalczyk, T. E. Larson, G. B. Perkins, J. E. Fessenden, R. K. Martinez, A. L. Reyes-Newell, D. M. Labotka and S. M. Clegg. Isotopologues at an Azeotrope. Presented at *Invited Chemistry Department seminar (Tulane University)*, New Orleans, Louisiana, United States, 2019-10-21 - 2019-10-21. (LA-UR-19-30264)

Currier, R. P., T. B. Peery, M. Herman, D. M. Labotka, J. E. Fessenden, R. K. Martinez, A. L. Reyes-Newell and S. M. Clegg. Phase Equilibrium Physically or Chemically Driven Fractionation?. Presented at *Presentation for LDRD-DR Mid-Term Review Meeting*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20802)

Dorhout, J. M., K. L. Nowak-Lovato, R. K. Carlson, E. R. Batista, Z. Li, M. P. Wilkerson and S. M. Clegg. Stable-Isotope Fractionation of Nitrogen by Metals in Nitric Acid. Presented at *ACS Southwest Regional Meeting*, El Paso, Texas, United States, 2019-11-12 - 2019-11-16. (LA-UR-19-31174)

Kendrick, B. K. APH3D: A Parallel Code Suite for Computing Quantum Dynamics of A + BC Reactions and Triatomic Spectra. Presented at *2019 MolSSI Workshop on Rovibrational Molecular Spectroscopy*, Blacksburg, Virginia, United States, 2019-11-14 - 2019-11-15. (LA-UR-19-31395)

Kendrick, B. K. and A. Teplukhin. Quantum Mechanical Theory of Stable Isotope Fractionation. Presented at *DR Appraisal meeting for Fundamental Physics and Interpretation of Stable Isotope Fractionation*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20572)

Kendrick, B. K. and A. Teplukhin. Quantum Mechanical Treatment of Stable Isotope Fractionation. . (LA-UR-20-20202)

Nowak-Lovato, K. L., J. M. Dorhout, Z. Li, R. K. Martinez and A. S. Anderson. NOx Fractionation - Experimental. . (LA-UR-19-20749)

Nowak-Lovato, K. L., R. K. Carlson, J. M. Dorhout, Z. Li, R. K. Martinez and A. S. Anderson. NOx summary. . (LA-UR-20-20477)

Posters

Beveridge, A. C., K. L. Nowak-Lovato, S. M. Clegg, R. K. Martinez, A. L. Reyes-Newell, A. S. Anderson, E. R. Batista, R. K. Carlson, B. K. Kendrick and A. Teplukhin. NOx and SOx Photochemistry Experiments. Presented at *LDRD Review Meeting*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20789)

Carlson, R. K., S. M. Clegg, P. Yang and E. R. Batista. Nitrogen Isotope Fractionation During the Dissolution of Copper by Nitric Acid. Presented at *LDRD Project Review*, Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20268)

Dorhout, J. M., A. S. Anderson, K. L. Nowak-Lovato, R. K. Martinez, G. B. Perkins, Z. Li, M. P. Wilkerson and S. M. Clegg. Stable-Isotope Fractionation of Nitrogen Species by Copper in Nitric Acid/Water Systems. . (LA-UR-20-20391)

Dorhout, J. M., A. S. Anderson, K. L. Nowak-Lovato, R. K. Martinez, Z. Li, M. P. Wilkerson and S. M. Clegg. Production of Nitrogen Species in Nitric Acid/Water Systems. . (LA-UR-19-20603)

Dorhout, J. M., A. S. Anderson, K. L. Nowak-Lovato, R. K. Martinez, Z. Li, M. P. Wilkerson and S. M. Clegg. Stable-Isotope Fractionation of Nitrogen Species by Copper or Uranium in Nitric Acid/Water Systems. . (LA-UR-19-20606)

Dorhout, J. M., Z. Li, S. M. Clegg, K. L. Nowak-Lovato, A. S. Anderson, M. P. Wilkerson and R. K. Martinez. Stable-Isotope Fractionation of Nitrogen by Uranium in Nitric Acid. Presented at *Pu Futures*, San Diego, California, United States, 2018-09-09 - 2018-09-14. (LA-UR-18-28511)

Kendrick, B. K. and A. Teplukhin. Quantum Mechanical Description of Isotope Effects in SO2. . (LA-UR-20-20203)

Labotka, D. M., G. B. Perkins, R. P. Currier and S. M. Clegg. Oxygen-17 Fractionation Dynamics. . (LA-UR-19-20619)

Li, Z., K. L. Nowak-Lovato, A. S. Anderson, J. M. Dorhout, R. K. Carlson, R. K. Martinez and S. M. Clegg. Cryogenic separation of NOx species (NO + NO2) for on-line nitrogen isotopic analysis using EA-IRMS. . (LA-UR-19-20835)

Li, Z., K. L. Nowak-Lovato, A. S. Anderson, J. M. Dorhout, R. P. Currier, S. M. Clegg, R. K. Martinez and R. K. Carlson. Sequential cryogenic separation and purification of NOx species (NO + NO2) for on-line nitrogen isotopic analysis using EA-IRMS. . (LA-UR-20-20022)

Peery, T. B., E. J. M. Mallory, R. P. Currier, M. F. Herman and S. M. Clegg. On Statistics & Standard Reference States in the Fractionation of Stable Isotopes. Presented at *LDRD-*

DR 20180066DR mid-term review at LANL, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20703)

Peery, T. B., E. J. M. Mallory, R. P. Currier and S. M. Clegg. Statistical Reference States in Stable Isotope Fractionation and Chemistry. Presented at *LDRD 20180066DR Third-Year Internal Review*, Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20153)

Teplukhin, A. and B. K. Kendrick. Quantum mechanical description of isotope effects in ArNO and NO2. Presented at *LDRD project review*, Los Alamos, New Mexico, United States, 2019-02-04 - 2019-02-04. (LA-UR-19-20518)

Teplukhin, A. and B. K. Kendrick. Quantum mechanical description of isotope effects in ArNO and NO2. Presented at *LDRD project review*, Los Alamos, New Mexico, United States, 2020-01-15 - 2020-01-15. (LA-UR-20-20204)

Teplukhin, A. and B. K. Kendrick. Bound states calculation for ArNO on a three-dimensional potential energy surface. Presented at *The 67th Pacific Conference on Spectroscopy and Dynamics*, San Diego, California, United States, 2020-01-30 - 2020-02-02. (LA-UR-20-20507)

Hyperspectral Xray Imaging (HXI): Nanochemical Analysis of Actinide and Explosive Materials (U)

Mark Croce
20190002DR

Project Description

Small particles containing uranium compounds can come from almost anywhere in the nuclear fuel cycle or on the road to making a nuclear bomb. Characterization of their detailed chemical form is needed to understand potential material origins, history, and environmental fate. The International Atomic Energy Agency (IAEA) and the United States Air Force Technical Applications Center (AFTAC) have stated that chemical speciation, especially uranium oxidation state, is very important for small particles. Outside of the brightest light sources, mammoth synchrotron laboratories, there is no x-ray chemical analysis method that provides a comprehensive determination of actinide (uranium, plutonium) chemical form and the spatial resolution needed to study microscopic samples with nanoscale heterogeneity. We will develop the first comprehensive chemical analysis capability in a regular laboratory for such particles by combining ultra-high-resolution microcalorimeter x-ray detectors with a scanning electron microscope, and interpreting the data with advanced theoretical methods. There are few institutions in a position to fully implement this technology. Only Los Alamos is in a position to develop this technology for laboratory-based materials analysis, and only Los Alamos has a nuclear materials mandate. This project will create a new analytical capability to support national security priorities.

Publications

Journal Articles

Carpenter, M. H., M. P. Croce, Z. K. Baker, E. R. Batista, M. P. Caffrey, C. J. Fontes, K. E. Koehler, S. E. Kossmann, K. G. McIntosh, M. W. Rabin, B. W. Renck, G. L. Wagner, M. P. Wilkerson, P. Yang, M. D. Yoho, J. N. Ullom, D. A. Bennett, G. C. O'Neil, C. D. Reintsema, D. R. Schmidt, G. C. Hilton, D. S. Swetz, D. T. Becker, J. D. Gard, J. Imrek, J. A. B. Mates, K. M. Morgan, D. Yan, A. L. Wessels, R. H. Cantor, J. A. Hall and D. T. Carver. Hyperspectral X-ray Imaging. Submitted to *Journal of Low Temperature Physics*. (LA-UR-19-27148)

Presentation Slides

Croce, M. P. New Analytical Capabilities with Microcalorimeters. . (LA-UR-19-27141)

Croce, M. P. Microcalorimeter Technology for Enhanced Safeguards Capabilities. Presented at *INMM-ESARDA-INMMJ Workshop*, Tokyo, Japan, 2019-10-07 - 2019-10-07. (LA-UR-19-29984)

Croce, M. P. IAEA Sample Results and Microcalorimeter Capabilities. . (LA-UR-19-30668)

Croce, M. P. Non-Destructive Evaluation Capabilities with Calorimetry and Microcalorimetry. Presented at *2019 Pit CEPPC*, Los Alamos, New Mexico, United States, 2019-06-19 - 2019-06-19. (LA-UR-19-30824)

Croce, M. P. LANL LTD Projects. . (LA-UR-19-31710)

Koehler, K. E. Microcalorimeters: A Bright, Bold Future. Presented at *SeeLANL*, Los Alamos, New Mexico, United States, 2020-01-13 - 2020-01-13. (LA-UR-20-20224)

Koehler, K. E. and C. J. Fontes. Spectral Calculations of X-ray Emission for Microcalorimeter Measurements: Theoretical basis for small mystery peaks in experimental x-ray measurements. Presented at *MetroMMC Stakeholder Meeting*, Saclay, France, 2019-10-24 - 2019-10-24. (LA-UR-19-30853)

Posters

Carpenter, M. H., K. G. McIntosh, J. N. Ullom, D. A. Bennett, D. S. Swetz, C. D. Reintsema, J. D. Gard, D. T. Becker, J. A. B. Mates, K. M. Morgan, J. Imrek, A. L. Wessels and M. P. Croce. Development of a Wide-Range X-ray Emission Spectroscopy Measurement System with Transition Edge Sensors and Microwave Multiplexed Readout. Presented at *Low Temperature Detectors 18*, Milan, Italy, 2019-07-22 - 2019-07-26. (LA-UR-19-26750)

Croce, M. P., Z. K. Baker, E. R. Batista, M. P. Caffrey, M. H. Carpenter, C. J. Fontes, K. E. Koehler, S. E. Kossmann, S. A. Kozimor, K. G. McIntosh, M. W. Rabin, B. W. Renck, G. L. Wagner, P. Yang, M. D. Yoho, M. P. Wilkerson, D. T. Becker, D. A. Bennett, J. D. Gard, J. Imrek, J. A. B. Mates, K. M. Morgan, G. C. O'Neil, C. D. Reintsema, D. R. Schmidt, D. S. Swetz, A. L. Wessels, J. N. Ullom, R. H. Cantor, J. A. Hall and D. T. Carver. Hyperspectral X-ray Imaging. Presented at *18th International Workshop on Low Temperature Detectors*, Milan, Italy, 2019-07-22 - 2019-07-22. (LA-UR-19-26600)

Koehler, K. E., C. J. Fontes, E. R. Batista, M. H. Carpenter, S. A. Kozimor, K. G. McIntosh, C. M. Smith, G. L. Wagner, P. Yang and M. P. Croce. Dirac-Fock-Slater Calculations for Low Intensity X-ray Features. Presented at *International Workshop on Theory Frontiers in Actinide Sciences*, Santa Fe, New Mexico, United States, 2020-02-02 - 2020-02-05. (LA-UR-20-20828)

A Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) Future (U)

Scott Twary
20190167DR

Project Description

Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/CRISPR-associated (Cas) genome engineering is rapidly advancing into all aspects of biology. This work will explore the application of novel CRISPR engineering techniques to regulate stem cell differentiation into muscle and neuron cells. Controlled interactions of these cells will then form functional neuromuscular junctions (NMJs). Effective optimized development of functional NMJs has application to traumatic injury repair, disease therapy, chemical agent testing platforms, and advanced cell biology. Varied genome engineering approaches will create multiple clonal cell lines for in depth characterization of cellular responses to targeted genetic engineering. These lines will be sequenced for genomic modifications, gene regulation responses, gene expression changes, and cellular physical response variation. The integrated analysis will provide a foundational basis for identifying aberrant cell responses to targeted genome engineering. Optimized differentiation of stem cells will provide a capability resource that will enhance biomedical applications, develop chem/bio testing platforms, and advance understanding of genetic responses.

Publications

Journal Articles

Jacobs, L. L. Soil Prokaryotic Cell Size Correlates with Ecosystem Productivity. Submitted to *Soil Biology & Biochemistry*. (LA-UR-19-31347)

Pellenz, S., M. Phelps, W. Tang, B. Hovde, R. Sinit, W. Fu, H. Li, E. Chen and R. Monnat. New human chromosomal safe harbor sites for genome engineering with CRISPR/Cas9, TAL effector and homing endonucleases. Submitted to *Human Gene Therapy*. (LA-UR-19-20028)

Reports

Hovde, B. and J. K. Jurss. Computationally locating off-target effects of CRISPR/Cas9 in human embryonic stem cells. Unpublished report. (LA-UR-19-28097)

Presentation Slides

Hraber, P. T. Cyberbiosecurity: \xe2\x80\xa8Emerging Research Field \xe2\x80\xa8or Movie-Plot Threat?. Presented at *UNM Computer Science Department Seminar*, Albuquerque, New Mexico, United States, 2019-09-25 - 2019-09-25. (LA-UR-19-29607)

Hraber, P. T. Cyberbiosecurity: \xe2\x80\xa8Emerging Research Field \xe2\x80\xa8or Movie-Plot Threat?. Presented at *UNM Computer Science Department Seminar*, Albuquerque, New Mexico, United States, 2019-09-25 - 2019-09-25. (LA-UR-19-29643)

Posters

Davis-Anderson, K. L., S. N. Micheva-Viteva, E. A. Solomon, J. C. Sanchez, S. N. Twary and R. S. Iyer. CRISPR-Cas9 Directed Reprogramming of Stem Cells into Motor Neurons for Neuromuscular Junction Organoid. Presented at *2019 CBD S&T Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-18. (LA-UR-19-31218)

Hovde, B. and J. K. Jurss. CRISPR Off-Target Damage Analysis. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-06. (LA-UR-19-27822)

Rodriguez, A. M. Motor Neuron Differentiation from Human Embryonic Stem Cells. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-26136)

Sanchez, J. C., K. L. Davis-Anderson, E. A. Solomon, R. S. Iyer, S. N. Micheva-Viteva and S. N. Twary. The development of a model for the human neuromuscular junction. Presented at *Cell Symposia: Engineering Organoids and Organs*, San Diego, California, United States, 2019-08-25 - 2019-08-27. (LA-UR-19-28075)

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.

Technical Outcomes

This DR has successfully developed and built two working instruments, Jouster and Flowster, which are 20 to 10 million times more sensitive for the transformative measurement of J-coupled Spectroscopy (JCS) at Earth's magnetic field (50 µT). The JCS spectra observed are unique to the structure of small molecules, such as chemical warfare agents, allowing identification and quantification. While Flowster is a portable, fluidics-based instrument, both produce JCS data that is complementary to superconducting NMR instruments.

Publications

Journal Articles

Baumann, D. O., J. C. Gordon and R. F. Williams. Peptoid Siderophore Analogues. Submitted to *Actinide Research Quarterly*. (LA-UR-18-31782)

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)

Evans, A. C. Flow Chemistry Panel Discussion for Chimica Oggi. Submitted to *Chimica Oggi*. (LA-UR-19-23228)

Kaseman, D. C., A. Gamble Jarvi, X. Y. Gan, S. Saxena and J. E. Millstone. Evolution of Surface Copper(II) Environments in Cu2-xSe Nanoparticles. 2018. *Chemistry of Materials*. **30** (20): 7313-7321. (LA-UR-18-28650 DOI: 10.1021/acs.chemmater.8b03967)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, M. A. Alvarez, A. V. Urbaitis, M. T. Janicke, P. Nath, M. A. Espy and R. F. Williams. Design and Implementation of a J-Coupled Spectrometer for Multidimensional Structure and Relaxation Detection at Ultra-Low Magnetic Fields. Submitted to *Review of Scientific Instruments*. (LA-UR-19-29923)

*Zhang, G., J. Wu, H. Zeng, M. C. Neary, M. Devany, S. Zheng and P. A. Dub. Dearomatization and Functionalization of Terpyridine Ligands Leading to Unprecedented Zwitterionic Meisenheimer Aluminum Complexes and Their Use in Catalytic Hydroboration. 2019. *ACS Catalysis*. **9** (2): 874-884. (LA-UR-18-24664 DOI: 10.1021/acscatal.8b04096)

*Zhang, G., J. Wu, S. Zheng, M. C. Neary, J. Mao, M. Flores, R. J. Trovitch and P. A. Dub. Redox-Noninnocent Ligand-Supported Vanadium Catalysts for the Chemoselective

Reduction of C\xe2\x95\x90X (X = O, N) Functionalities. 2019. *Journal of the American Chemical Society*. **141** (38): 15230-15239. (LA-UR-19-22935 DOI: 10.1021/jacs.9b07062)

Reports

Evans, A. C. Summary of Talk at CPAC Rome 2019 Workshop. Unpublished report. (LA-UR-19-23868)

Nelson, T. R. LDRD Data Sheet Template. Unpublished report. (LA-UR-17-31085)

Presentation Slides

Baumann, D. O. Solving Problems with Synthesis. . (LA-UR-19-24796)

Chen, J. C., R. Michalczyk, M. Blum, R. F. Williams and P. S. Anderson. Multidisciplinary approach to understanding structure / function relationships in DFPase, a nerve agent-degrading enzyme. Presented at *CBD S&T*, Long Beach, California, United States, 2017-11-28 - 2017-11-28. (LA-UR-17-30495)

Dub, P. Metal–Ligand Bifunctional Catalysis: The “Accepted” Mechanism, the Issue of Concertedness, and the Function of the Ligand in Catalytic Cycles Involving Hydrogen Atoms. Presented at *ACS Meeting in New Orleans*, New Orleans, Louisiana, United States, 2018-03-18 - 2018-03-18. (LA-UR-18-22171)

Dub, P., J. G. Schmidt, J. C. Gordon and R. F. Williams. Catalytic Hydrogenation of Olefinic and/or Chiral Esters at Room Temperature without Affecting E/Z Ratio and Racemization. Presented at *2018 ACS Meeting in New Orleans*, New Orleans, Louisiana, United States, 2018-03-18 - 2018-03-18. (LA-UR-18-22172)

Espy, M. A. and R. F. Williams. Chemical Threat Signatures and Detection by Ultralow Field Magnetic Resonance. Presented at *Science of Signatures Capability Review*, Los Alamos, New Mexico, United States, 2018-04-25 - 2018-04-25. (LA-CP-18-20265)

Evans, A. C. Tunable Chiroptical Induction Using Synchrotron-Sourced Circularly Polarized Light. Presented at *SelectBio Flow Chemistry Conference 2018*, Miami, Florida, United States, 2018-11-12 - 2018-11-13. (LA-UR-18-30808)

Evans, A. C. “Continuous Biocatalytic Manufacturing Approaches for the Synthesis of Drugs”. Presented at *CPAC Rome Workshop*, Rome, Italy, 2019-03-25 - 2019-03-27. (LA-UR-19-22552)

Janicke, M. T. Big Science at a National Lab, 99Mo Medical Isotope Production at Los Alamos National Laboratory. Presented at *Chemical Engineering Department Seminar, The City College of New York*, New York, New York, United States, 2017-10-02 - 2017-10-02. (LA-UR-17-28777)

Janicke, M. T., D. Kaseman, P. E. Magnelind, R. K. Frankle, A. V. Urbaitis, J. L. Yoder, M. A. Alvarez, M. A. Espy and R. F. Williams. Earth’s Field NMR and small molecule spectroscopy. Presented at *NIST Workshop on Low Field Magnetic Resonance*, Boulder, Colorado, United States, 2019-08-12 - 2019-08-13. (LA-UR-19-28088)

Janicke, M. T., M. A. Espy, M. Malone, T. R. Nelson, R. F. Williams and D. Kaseman. LANL Capabilities for Opioid Screener (DHS proposal preparation with QFS). . (LA-UR-19-22320)

Janicke, M. T., S. Widgeon Paisner, D. Kaseman, P. Nath, A. V. Urbaitis, M. A. Espy, R. F. Williams, J. L. Yoder, M. A. Alvarez and P. E. Magnelind. Low Field Magnetic Resonance Approaches for National Security Challenges. Presented at *Seminar- Lawrence Livermore National Lab*, Livermore, California, United States, 2019-04-09 - 2019-04-09. (LA-UR-19-23213)

Kaseman, D. Pipe-VIZ: THE lifeline for YOUR waterline. Presented at *Disruptech*, Los Alamos, New Mexico, United States, 2019-07-11 - 2019-07-11. (LA-UR-19-26403)

Kaseman, D. Chemical Warfare Agents Detection via Portable Low-Field Nuclear Magnetic Resonance. Presented at *Techwatch*, Washington D.C., Virginia, United States, 2020-03-11 - 2020-03-11. (LA-UR-20-22174)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Ubiquitous Identification of Organophosphorus Compounds with a Fieldable Earth’s Magnetic Field Spectrometer. Presented at *GRC: Chemical and Biological Terrorism Defense (GRS)*, Ventura, California, United States, 2019-03-02 - 2019-03-08. (LA-UR-19-21785)

Michalczyk, R. High and Low Field NMR Research at LANL. . (LA-CP-18-20170)

Minko, Y., R. F. Williams, C. E. Strauss and J. G. Schmidt. Novel Metal-chelating and Stimuli-responsive Peptoid Oligomers. Presented at *ACS National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22698)

Widgeon, S. Investigations of structure and chemistry by nuclear magnetic resonance. . (LA-UR-18-30755)

Williams, R. F., M. A. Espy, M. A. Alvarez, R. J. Batrice, M. T. Janicke, P. E. Magnelind, R. Michalczyk, T. R. Nelson, J. L. Yoder, A. V. Urbaitis, D. Kaseman and S. Widgeon Paisner. Identification of Organophosphorus Chemical Warfare Agents (CWAs), Precursors, and Decomposition Products with a Fieldable NMR Spectrometer Using Earth's Magnetic Field. Presented at *American Chemical Society, Fall 2019 National Meeting and Exposition*, San Diego, California, United States, 2019-08-25 - 2019-08-29. (LA-UR-19-28455)

Williams, R. F., M. A. Espy, T. H. Erkkila, M. T. Janicke, D. Kaseman, P. E. Magnelind, R. Michalczyk, P. Nath, T. R. Nelson, J. G. Schmidt, S. Widgeon Paisner, A. V. Urbaitis, J. L. Yoder and M. A. Alvarez. Nuclear Magnetic Resonance at Low to Ultra-Low Magnetic Fields for Signature Detection of Chemical Warfare Agents and Emerging Threat Materials. Presented at *PANIC - Practical Applications of NMR in*

Industry Conference, Hilton Head Island, South Carolina, United States, 2019-03-03 - 2019-03-07. (LA-UR-19-21909)

Yoder, J. L. Ultra Low Field NMR in B Division. Presented at *Neal Woodbury LANL visit*, Los Alamos, New Mexico, United States, 2018-07-16 - 2018-07-16. (LA-UR-18-26426)

Posters

Baumann, D. O., J. G. Schmidt, J. C. Gordon and R. F. Williams. Progress Towards a Peptoid Siderophore Analogue. Presented at *ACS Spring 2019 National Meeting & Exposition*, Orlando, Florida, United States, 2019-03-31 - 2019-04-04. (LA-UR-19-22699)

Dub, P. Title 1: The Effect of M–L Antiferromagnetic Coupling in Catalysis Title 2: Zwitterionic Meisenheimer Aluminum Complexes: tour de force Molecular Catalysts based on the Most Abundant Metal in the Earth’s Crust. Presented at *2018 Gordon Research Conference on Organometallic Chemistry*, Newport, Rhode Island, United States, 2018-07-08 - 2018-07-08. (LA-UR-18-25394)

Frankle, R. K. Fieldable chemical analysis using J-coupled spectroscopy at earth's magnetic field. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-26829)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Ubiquitous Identification of Organophosphorus Chemical Warfare Agents (CWAs), Precursors, and Decomposition Products with a Fieldable Spectrometer using Earth’s Magnetic Field. Presented at *Gordon Research Conference: Chemical and Biological Terrorism Defense (GRS)*, Ventura, California, United States, 2019-03-02 - 2019-03-08. (LA-UR-19-21813)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. Ubiquitous Identification of Organophosphorus Chemical Warfare Agents (CWAs), Precursors, and Decomposition Products with a Fieldable Spectrometer using Earth’s Magnetic Field. Presented at *Experimental Conference on Nuclear Magnetic Resonance*, Pacific Grove, California, United States, 2019-04-07 - 2019-04-12. (LA-UR-19-22821)

Michalczyk, R. and R. F. Williams. High and Low Field NMR at LANL. Presented at *EMSL Integration 2018: Molecular Structure and Dynamics in Biology and the Environment*, Richland, Washington, United States, 2018-08-06 - 2018-08-08. (LA-UR-18-27391)

Minko, Y., J. G. Schmidt, C. E. Strauss, J. C. Gordon and R. F. Williams. New generation of stimuli-responsive peptoids. Presented at *Los Alamos National Laboratory 2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-27. (LA-UR-19-28548)

Nath, P., E. M. Higgins, Y. J. Kim, I. M. Savukov, C. Hilty, P. L. Volegov, M. A. Espy and R. F. Williams. Backpack NMR: Towards the Miniaturization of Nuclear Magnetic Resonance (NMR) based Metabolic Profiling as a Field Forward Diagnostic Tool. Presented at *CBD S&T Conference 2017*, Long Beach, California, United States, 2017-11-28 - 2017-11-28. (LA-UR-17-30726)

Widgeon Paisner, S., M. T. Janicke, D. Kaseman, J. L. Yoder, M. A. Espy and R. F. Williams. Simultaneous Elemental Analysis and T2 Relaxation Measurements using CPMG. Presented at *Experimental Nuclear Magnetic Resonance Conference*, Pacific Grove, CA, California, United States, 2019-04-08 - 2019-04-12. (LA-UR-19-22879)

Widgeon, S., D. Kaseman, R. K. Frankle, M. T. Janicke, M. A. Espy and R. F. Williams. Simultaneous Elemental Analysis and Physical Characterization of Chemical Threat Agents. Presented at *2018 Postdoc Research Symposium*, Los Alamos, New Mexico, United States, 2018-08-28 - 2018-08-28. (LA-UR-18-27984)

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.

Technical Outcomes

This project built and demonstrated a CubeSat-ready high-resolution hyperspectral imager, the first CubeSat instrument capable of high-sensitivity trace gas imaging. Advanced computationally efficient hyperspectral gas retrieval algorithms were developed to enable rapid on-board processing to address the CubeSat downlink bandwidth bottleneck. Tested on the actual CubeSat processor with real-world data, these algorithms were demonstrated to yield an over 20x reduction in processing time compared to standard methods, with negligible loss of sensitivity or accuracy.

Publications

Journal Articles

Herman, J., N. Abuhassan, J. Kim, J. Kim, M. Dubey, M. Raponi and M. Tzortziou. Underestimation of column NO amounts from the OMI satellite compared to diurnally varying ground-based retrievals from multiple PANDORA spectrometer instruments. 2019. *Atmospheric Measurement Techniques*. **12** (10): 5593-5612. (LA-UR-19-23208 DOI: 10.5194/amt-12-5593-2019)

Conference Papers

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)

Theiler, J. P. and S. P. Love. Algorithm development with on-board and ground-based components for hyperspectral gas detection from small satellites. Presented at *SPIE Defense+Commercial Sensing*. (Baltimore, Maryland, United States, 2019-04-15 - 2019-04-18). (LA-UR-19-23278)

Presentation Slides

Dubey, M. K. Remote Sensing Capabilities and Needs at LANL: Synergy with Montana. Presented at *Montana Lab Day*, Butte, Montana, United States, 2019-10-08 - 2019-10-09. (LA-UR-19-30054)

Hickey, A. M. and J. G. Teague. Modeling the On Orbit Heating Environment of Small Satellites. Presented at *ISR student division presentations*, Los Alamos, New Mexico, United States, 2017-07-27 - 2017-07-27. (LA-UR-17-26445)

Love, S. P., L. A. Ott, J. P. Theiler, B. R. Foy, C. L. Safi, M. E. Dale, C. G. Peterson, A. A. Guthrie, N. Dallmann, K. G. Boyd, P. S. Stein, J. Wren, M. C. (. Proicou and M. K. Dubey. CubeSat-Based High-Resolution Hyperspectral Imagers for Atmospheric Trace Gas Monitoring. Presented at *99th Annual Meeting of the American Meteorological Society*, Phoenix, Arizona, United States, 2019-01-06 - 2019-01-10. (LA-UR-18-31779)

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, 2018-04-16 - 2018-04-19. (LA-UR-18-23215)

Posters

Love, S. P., L. A. Ott, J. P. Theiler, B. R. Foy, C. L. Safi, M. E. Dale, C. G. Peterson, A. A. Guthrie, N. Dallmann, K. G. Boyd, P. S. Stein, J. Wren, M. C. (. Proicou and M. K. Dubey. High-resolution hyperspectral imaging of dilute gases from CubeSat platforms. Presented at *American Geophysical Union 2018 Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31235)

Love, S. P., M. K. Dubey, J. P. Theiler, B. R. Foy, L. A. Ott, M. E. Dale, C. L. Safi, M. C. Proicou, K. G. Boyd, P. S. Stein, J. Wren and C. G. Peterson. Agile Spectral Reconnaissance from CubeSats. . (LA-CP-18-20125)

Hyperspectral X-ray Imaging (HXI) for Scanning Electron Microscopes

Mark Croce
20190493DR

Project Description

Particulate samples containing uranium, plutonium, post-blast residues, and these materials in combination can come from almost anywhere in the nuclear fuel cycle or on the road to making a nuclear weapon. Their detailed chemical form is a crucial link to material origin and history. We will develop the first rapid capability to determine the chemical form of microscopic samples with nanoscale heterogeneity with small-scale instrumentation suitable for almost any lab. The International Atomic Energy Agency (IAEA) and the Air Force Technical Applications Center (AFTAC) have stated chemical speciation is very important for small particles. This work directly addresses the Los Alamos National Laboratory goals of revolutionizing measurement for nuclear, radiological and explosive materials by developing novel analytical methods capable of extracting weak or unintended signatures.

Technical Outcomes

This project has demonstrated scientific viability and developed a detailed research and development plan for the development of Hyperspectral X-ray Imaging. Initial measurements on pure uranium reference materials were performed. Preliminary atomic models were applied to predict x-ray emission features and develop instrument specifications and a plan for theory. The design of a microcalorimeter x-ray fluorescence instrument was completed.

Publications

Presentation Slides

McIntosh, K. G., M. H. Carpenter, A. S. Hoover, E. R. Batista, K. E. Koehler, M. P. Wilkerson, P. Yang, S. A. Kozimor, G. L. Wagner, Z. K. Baker, M. P. Croce, M. W. Rabin and G. J. Havrilla. Actinide Characterization using Selective Optics and High Resolution X-ray Spectroscopy. Presented at *Denver X-Ray Conference*, Lombard, Illinois, United States, 2019-08-05 - 2019-08-09. (LA-UR-19-27813)

Posters

Croce, M. P., E. R. Batista, M. H. Carpenter, G. J. Havrilla, A. S. Hoover, K. E. Koehler, S. A. Kozimor, K. G. McIntosh, V. Mocko, M. W. Rabin, M. P. Wilkerson, P. Yang, D. Becker, D. Bennett, J. Gard, J. Mates, D. Schmidt, J. Ullom and R. Cantor. Progress in Microcalorimeters for Nuclear Material Analysis. Presented at *Applied Superconductivity Conference*, Seattle, Washington, United States, 2018-10-28 - 2018-10-28. (LA-UR-18-30054)

High Energy Lightning: Understanding Relations Between Energetic Particles and Lightning Discharges in Thunderclouds

Xuan-Min Shao
20170179ER

Project Description

This project directly addresses Department of Energy(DOE)/National Nuclear Security Administration(NNSA) 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.

Publications

Journal Articles

*Bowers, G. S., W. Blaine, X. Shao, B. Dingus, D. M. Smith, M. Schneider, F. Martinez-McKinney, M. P. McCarthy, S. BenZvi, L. Nellen and N. Fraija. Combining Cherenkov and scintillation detector observations with simulations to deduce the nature of high-energy radiation excesses during thunderstorms. 2019. *Physical Review D*. **100** (4): 043021. (LA-UR-19-25406 DOI: 10.1103/PhysRevD.100.043021)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine and B. L. Dingus. Improving RF Lightning Mapping Accuracy with “Focused” Interferometry. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-19-24094)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine and B. L. Dingus. “Focused Interferometry” and Fine Structure of Lightning-Initiating Fast Positive Streamers. Submitted to *Journal of Geophysical Research: Atmospheres*. (LA-UR-19-32549)

*Shao, X., C. Ho, M. Caffrey, P. Graham, B. Haynes, G. Bowers, W. Blaine, B. Dingus, D. Smith and H. Rassoul. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations of Lightning Discharges: Revealing New Physics Insights Into Breakdown Processes. 2019. *Journal of Geophysical Research: Atmospheres*. **123** (18): 10-10. (LA-UR-18-24675 DOI: 10.1029/2018JD029096)

Conference Papers

Bowers, G. S., X. 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., 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 Conference on Atmospheric Electricity*. (Nara, Japan, 2018-06-17 - 2018-06-22). (LA-UR-18-23483)

Presentation Slides

Bowers, G. S., D. M. Smith, M. P. McCarthy, J. R. Dwyer, X. Shao and B. L. Dingus. Gamma-ray Signatures of Neutrons from Terrestrial Gamma-ray Flahses. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31117)

Bowers, G. S., W. G. Blaine, X. Shao, B. L. Dingus, M. P. McCarthy, M. Schneider, J. Chaffi and D. Smith. HAWC & GODOT Observation of Thunderstorm Ground Enhancements. Presented at *American Geophysical Union 2018*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31303)

Bowers, G. S. and D. M. Smith. Neutrons From Terrestrial Gamma-ray Flashes. Presented at *American Geophysical Union*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31120)

Bowers, G. S. and X. Shao. Understanding Electromagnetic Pulse & Energetic Particle Signatures from Lightning. Presented at *Interagency Technical Nuclear Forensics Technical Overview (ITNFTR)*, Oak Ridge, Tennessee, United States, 2018-06-30 - 2018-06-30. (LA-UR-18-25311)

Shao, X. Ionosphere disturbances introduced by thunderstorms and lightning discharges. Presented at *International Symposium on Lightning Physics and Lightning Meteorology*, Beijing, China, 2017-09-24 - 2017-09-27. (LA-UR-17-28257)

Shao, X., C. Ho, G. S. Bowers, W. G. Blaine, B. L. Dingus, M. P. Caffrey, P. S. Graham, W. B. Haynes, D. Smith and H. Rassoul. Broadband RF interferometric and polarization observations of lightning discharges correlated with gamma flux detection. Presented at *16th International Conference on Atmospheric Electricity*, Nara, Japan, 2018-06-17 - 2018-06-22. (LA-UR-18-25227)

Shao, X., C. Ho, M. P. Caffrey, P. S. Graham, W. B. Haynes, B. L. Dingus and G. S. Bowers. Broadband RF Interferometric and Polarization Observations of Lightning Discharge Processes. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-30958)

Shao, X., G. S. Bowers, C. Ho, B. L. Dingus, J. S. Bull and C. S. Meierbachtol. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations Reveal new Physics Insights into Lightning Discharge Processes. Presented at *American Geophysical Union Fall meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31981)

Shao, X., G. S. Bowers, W. G. Blaine, C. Ho and B. L. Dingus. Broadband RF Interferometric Mapping and Polarization (BIMAP) Observations of Mini-Discharges in Thunderstorms. Presented at *American Geophysical Union Fall meeting, 2018*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31298)

Shao, X., J. S. Bull and C. S. Meierbachtol. Signatures of RF Polarization Related to Relativistic Discharge Processes. Presented at *American Geophysical Union Fall Meeting*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-31977)

Posters

Blaine, W. G., G. S. Bowers, X. Shao and B. L. Dingus. Simulating Electric Field Effects on Cosmic Ray Particle and Radio Frequency Observations. Presented at *American Geophysical Union (AGU) Fall Meeting 2018*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31431)

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).

Publications

Presentation Slides

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-17-29752)

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-19-31476)

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Ultra-low field MRI and Current Density Imaging. Presented at *SBMT2018*, Los Angeles, California, United States, 2018-04-13 - 2018-04-13. (LA-UR-18-23160)

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Current-density imaging and magnetic resonance-based electrical impedance tomography at ultra-low fields. Presented at *Biomag2018*, Philadelphia, Pennsylvania, United States, 2018-08-26 - 2018-08-30. (LA-UR-18-28117)

Posters

Magnelind, P. E., M. A. Espy, A. N. Matlashov, S. G. Newman, H. J. Sandin, A. V. Urbaitis and P. L. Volegov. Current-density imaging and magnetic resonance-based electrical impedance tomography at ultra-low fields. Presented at *Biomag2018*, Philadelphia, Pennsylvania, United States, 2018-08-26 - 2018-08-30. (LA-UR-18-28116)

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

Journal Articles

Filin, D., I. M. Savukov and J. P. Colgan. CI- MBPT line strengths and atomic probabilities for some transitions of neutral bromine and iodine. Submitted to *Physical Review A*. (LA-UR-20-20076)

*Savukov, I. M. and P. M. Anisimov. Configuration-interaction many-body perturbation theory for La ii electric-dipole transition probabilities. 2019. *Physical Review A*. **99** (3): 032507. (LA-UR-18-30155 DOI: 10.1103/PhysRevA.99.032507)

Presentation Slides

Savukov, I. M. Application of many-body perturbation theory to actinide atoms. Presented at *Atomic Physics 2018*, Boston, Massachusetts, United States, 2018-10-26 - 2018-10-27. (LA-UR-18-29977)

Savukov, I. M. Ab initio precision CI-MBPT calculations for noble-gas atoms. Presented at *Atomic Physics 2018*, Boston, Massachusetts, United States, 2018-10-26 - 2018-10-27. (LA-UR-18-30184)

Savukov, I. M. Accurate calculations of La II transition probabilities with CI-MBPT method. Presented at *ICAMDATA-2018*, Cambridge, Massachusetts, United States, 2018-11-11 - 2018-11-15. (LA-UR-18-30699)

Savukov, I. M. Atomic structure calculations of complex atoms: review. . (LA-UR-19-23852)

Savukov, I. M. CI-MBPT calculations of energies, transitions, and g factors of La II and La I. Presented at *50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics*, Milwaukee, Illinois, United States, 2019-05-27 - 2019-05-27. (LA-UR-19-24759)

Posters

Filin, D., I. M. Savukov and J. P. Colgan. CI- MBPT calculations of the iodine line strengths. Presented at *DAMOP*, Milwaukee, Wisconsin, United States, 2019-05-27 - 2019-05-31. (LA-UR-19-24863)

Filin, D., J. P. Colgan and I. M. Savukov. Ab Initio CI-MBPT Energy Levels and Line Strengths of the Sn XIII-Sn XVI Ions for 13-14 nm Lithography. Presented at *International Conference on Numerical Simulation of Plasmas*, Santa Fe, New Mexico, United States, 2019-09-03 - 2019-09-05. (LA-UR-19-28863)

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

Journal Articles

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)

Conference Papers

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)

Sidebottom, R. B., E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill, D. Tupa and M. A. Espy. Assessment of proton radiographic sensitivity limits for gold nanoparticle tagged tumors using gold leaf phantoms. Presented at *SPIE Medical Imaging*. (Houston, Texas, United States, 2020-02-16 - 2020-02-16). (LA-UR-20-20414)

Reports

Sidebottom, R. B. Gold-leaf phantoms of Au-tagged tumors to assess proton radiography for image guided proton therapy. Unpublished report. (LA-UR-19-23315)

Presentation Slides

Espy, M. A. How to look at a brain. Presented at *NogginFest*, portland, Oregon, United States, 2018-10-19 - 2018-10-20. (LA-UR-18-29895)

Freeman, M. S. Magnetic focused proton radiography and its implications for proton beam guidance, anatomical alignment and adaptive therapy. Presented at *Annual Rocky Mountain Chapter Meeting of the American Association of Physicists in Medicine*, Colorado Springs, Colorado, United States, 2018-06-09 - 2018-06-09. (LA-UR-18-24975)

Freeman, M. S. Instantaneous Full Field Proton Radiography For Image Guidance. Presented at *American Association of Physicists in Medicine*, Nashville, Tennessee, United States, 2018-07-29 - 2018-08-02. (LA-UR-18-25530)

Freeman, M. S. Proton Radiography for Treatment Planning and Guidance. Presented at *UNM Medical Physics Symposium*, Albuquerque, New Mexico, United States, 2018-11-16 - 2018-11-16. (LA-UR-19-20477)

Freeman, M. S. Flash Proton Radiography for the Clinic: Real-Time Adaptive Therapy and a Proton-Based Estimate of Water-Equivalent Thickness. . (LA-UR-19-23520)

Freeman, M. S. Proton Radiography for Dense Dynamic Systems: a Capabilities Overview. Presented at *Mesoscale Science at Extreme Conditions*, Santa Fe, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-31068)

Freeman, M. S. Hyperpolarized 129Xe MRI: Visualizing Lung Anatomy and Function. . (LA-UR-19-31585)

Freeman, M. S., E. F. Aulwes, L. Dong, T. Li, P. E. Magnelind, F. E. Merrill, L. P. Neukirch, R. Selwyn, R. Serda, R. B.

Sidebottom, Z. Tang, K. Teo, D. Tupa, C. H. Wilde and M. A. Espy. Scaling the Ultra-Fast LANL System to Medical Energies. Presented at *58th Annual Meeting of the Particle Therapy Co-Operative Group*, Manchester, United Kingdom, 2019-06-10 - 2019-06-10. (LA-UR-19-25360)

Freeman, M. S., E. F. Aulwes, L. Dong, T. Li, P. E. Magnelind, F. E. Merrill, R. Selwyn, R. Serda, R. B. Sidebottom, K. Teo, D. Tupa and M. A. Espy. Residual-Energy Lens Focused Proton Radiography at Clinical Energies. Presented at *Annual Meeting of the American Association of Physicists in Medicine*, San Antonio, Texas, United States, 2019-07-14 - 2019-07-14. (LA-UR-19-26544)

Freeman, M. S., J. C. Allison, M. A. Espy, J. J. I. Goett, J. D. Lopez, P. E. Magnelind, F. G. Mariam, J. J. Medina, F. E. Merrill, C. Morris, L. P. Neukirch, A. Saunders, A. M. Tainter, Z. Tang, F. R. Trouw, D. Tupa, J. L. Tybo and C. H. Wilde. Instantaneous Full Field Proton Radiography for Image Guidance. Presented at *Annual Meeting of the American Association of Physicists in Medicine*, Nashville, Tennessee, United States, 2018-07-22 - 2018-07-22. (LA-UR-18-26984)

Freeman, M. S., M. A. Espy, P. E. Magnelind, F. E. Merrill and D. Tupa. Proton Radiography and Therapy. . (LA-UR-18-22459)

Magnelind, P. E. Ultra-low field MRI and MEG. . (LA-UR-19-31476)

Posters

Aulwes, E. F., M. S. Freeman, F. E. Merrill, R. B. Sidebottom, D. Tupa and M. A. Espy. Developing a Treatment Planning Method for High-Energy Proton Therapy. . (LA-UR-19-27480)

Broder, B. A. and M. S. Freeman. TOPAS Model for Simulating Proton Radiography. Presented at *Research Computing Expo and Symposium*, chicago, Illinois, United States, 2019-11-05 - 2019-11-05. (LA-UR-19-30818)

Freeman, M. S., E. F. Aulwes, P. E. Magnelind, F. E. Merrill, L. P. Neukirch, R. B. Sidebottom, Z. Tang, D. Tupa and C. H. Wilde. Water Equivalent Thickness from Instantaneous Proton Radiographic Transmission Measurements. Presented at *International Meeting of the Particle Therapy Co-Operative Group*, Manchester, United Kingdom, 2019-06-10 - 2019-06-10. (LA-UR-19-25169)

Freeman, M. S., M. A. Espy, J. J. I. Goett, P. E. Magnelind, F. G. Mariam, F. E. Merrill, R. B. Sidebottom, F. R. Trouw, D. Tupa and C. H. Wilde. Lens-Refocused Proton Radiography for Proton Beam Guidance. Presented at *Annual Meeting 57 of the Proton Therapy Co-Operative Group*, Cincinnati, Ohio, United States, 2018-05-21 - 2018-05-26. (LA-UR-18-23884)

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 2018*, Houston, Texas, United States, 2018-02-12 - 2018-02-16. (LA-UR-18-20846)

Sidebottom, R. B., D. Tupa, E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill and M. A. Espy. Gold-leaf phantoms of AuNP-tagged tumors to assess proton radiography for image-guided proton therapy. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27565)

Sidebottom, R. B., D. Tupa, E. F. Aulwes, M. S. Freeman, P. E. Magnelind, F. E. Merrill and M. A. Espy. Assessment of proton radiographic sensitivity limits for gold nanoparticle tagged tumors using gold leaf phantoms. Presented at *SPIE Medical Imaging*, Houston, Texas, United States, 2020-02-16 - 2020-02-16. (LA-UR-20-20412)

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.

Publications

Presentation Slides

Ganguly, K., P. J. Gasda, C. D. Gleasner, C. Mensah, S. H. Adikari, H. M. Quinn, A. C. Watkins, S. P. Love, A. Misra, T. Acosta-Mayda, S. K. Sarma and R. C. Wiens. Survival, Genetic Modification, and Time-Resolved Laser-Induced Fluorescence Analysis of Bacteria Exposed to High-Dose Radiation Simulating Europa's Surface. Presented at *Europa Workshop*, Houston, Texas, United States, 2018-10-09 - 2018-10-12. (LA-UR-18-29555)

Watkins, A. C. and H. M. Quinn. Evaluation of Electronic Performance in the Europa Environment. Presented at *20th Topical Meeting of the Radiation and Protection Shielding Division*, Santa Fe, New Mexico, United States, 2018-08-26 - 2018-08-26. (LA-UR-18-28218)

Posters

Wiens, R. C., P. J. Gasda, A. K. Misra, T. E. Acosta-Maeda, S. K. Sharma, H. M. Quinn, K. Ganguly, R. T. Newell, S. M. Clegg, S. Maurice, C. Virmontois, S. P. Love, A. E. Nelson, L. A. Ott and B. F. Sandoval. Organicam: A Lightweight Time-Resolved Fluorescence Imager and Raman Spectrometer for Organic Detection and Characterization. Presented at *LANL Engineering Week*, Los Alamos, NM, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21405)

Wiens, R. C., P. J. Gasda, A. Misra, T. Acosta-Maeda, S. Sharma, H. M. Quinn, K. Ganguly, S. P. Love, A. E. Nelson, R. T. Newell, S. M. Clegg, S. Maurice, C. Virmontois, L. A. Ott and B. F. Sandoval. Organicam: a lightweight time-resolved fluorescence imager and raman spectrometer for icy world organic detection and characterization. Presented at *50th LPSC*, The Woodlands, Texas, United States, 2019-03-18 - 2019-03-22. (LA-UR-19-22356)

Wiens, R. C., P. J. Gasda, H. M. Quinn, K. Ganguly, R. T. Newell, S. M. Clegg, S. P. Love, L. A. Ott, B. F. Sandoval, S. Maurice, C. Virmontois, A. K. Misra, T. E. Acosta-Maeda and S. K. Sharma. Organicam: A Lightweight Time-Resolved Fluorescence Imager and Raman Spectrometer for Organic Detection and Characterization. Presented at *American Geophysical Union Fall Conference*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32186)

Early Detection of Explosive Volcanic Eruptions Using Very High Frequency (VHF) Radiation from Vent Discharges

Sonja Behnke
20190107ER

Project Description

Volcanic ash from an explosive volcanic eruption can rise to aircraft cruising altitudes within 5 minutes of eruption onset, posing a serious threat to aircraft. Thus, timely detection of explosive eruptions and rapid characterization of the resulting ash cloud is a priority for volcano observatories in the United States. The goals of this project are to identify the signal characteristics of a class of volcanic lightning discharges ("vent discharges") that commonly occur in ash plumes and determine how to exploit these characteristics in a radio frequency-based volcanic eruption monitoring system. This work will advance the state of the art of volcano monitoring and address gaps in current methods. In addition, the knowledge gained about the signal characteristics of vent discharges and the methods to discriminate them from other types of lightning and other radio frequency transients can be applied to mission areas that are of interest to the National Counter Proliferation Center. For example, vent discharges are similar to electrical discharges produced by chemical explosions; the scientific understanding gained from this work can help inform a science-based simulation framework to model the characteristics and signatures of a non-nuclear test device, from early detonation to late time combustion.

Publications

Posters

Behnke, S. A., H. E. Edens, S. Senay, J. B. Johnson, K. B. Eack, M. P. Caffrey, J. P. Theiler, A. R. Van Eaton, D. J. Schneider, M. Iguchi and D. Miki. Early Detection of Explosive Volcanic Eruptions Using VHF Radiation from Vent Discharges. Presented at *American Geophysical Union Fall Meeting 2019*, San Francisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32189)

Behnke, S. A., H. E. Edens and J. P. Theiler. Vent Discharges Produced by Explosive Volcanic Eruptions: Characteristics, Signatures, and Volcano Monitoring Applications. Presented at *American Geophysical Union Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31441)

Boron and Ribose in Clay: a Precursor for Life on Earth and Mars?

Nina Lanza
20190238ER

Project Description

On Earth, there is a close association between life and the presence of clay minerals and boron. Clays and borates, separately, have been invoked as possible components for the origin of life on Earth. Our goal is to understand the signatures of boron-bearing clays so that they may be identified on Mars by rovers. 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.

Publications

Posters

Nellessen, M., L. Crossey, P. J. Gasda, E. Peterson, N. L. Lanza, C. M. Yeager, A. Labouriau, R. C. Wiens and S. M. Clegg. Boron Adsorption In Clay Minerals: Implications For Martian Groundwater Chemistry And Prebiotic Processes. Presented at *Los Alamos Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-26618)

Reduced-profile Current-sheet Array (CSA) Antenna with Simpler Drive and Better Antenna Efficiency

MD Zuboraj
20190268ER

Project Description

The best antenna architecture for satellites today (the current-sheet array, or CSA) is not well suited for cubesat applications because the current CSA architecture has been optimized for ultra-high bandwidths (i.e., up to 900%) but not for compact size or aperture efficiency. Future cubesat-based national security missions will likely only need ~ 20% bandwidths, which allow us to reoptimize the CSA architecture with improved efficiency and smaller size. The impact of this technology development will be higher bandwidth communications on cubesats with greater directivity.

Publications

Posters

A. Zuboraj, M. R. and B. E. Carlsten. Beam-Current Loss in Emittance-Dominated High-Frequency Tubes. Presented at *IEEE Pulsed Power and Plasma Science Conference*, Orlando, Florida, United States, 2019-06-23 - 2019-06-28. (LA-UR-19-25558)

Quantum Metrology with an Atom Superconducting Quantum Interference Device (SQUID)

Changhyun Ryu
20190334ER

Project Description

Inertial sensing is essential in many critical national security missions. Although global positioning system (GPS)-based navigation can be used in ideal situations, when GPS service is denied or unavailable, an independent, accurate, inertial sensor is needed. Quantum metrology with an atom superconducting quantum interference device (SQUID) can increase the sensitivity in rotation sensing dramatically by utilizing macroscopic entanglement between angular momentum states. The successful completion of this project will demonstrate the revolutionary increase in rotation sensitivity from the macroscopic entanglement. This will make it possible to develop a portable inertial sensor with the highest sensitivity for critical national security missions. This research is relevant to Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions of national security science in developing novel sensing technologies.

Publications

Presentation Slides

Ryu, C. Quantum Metrology with an Atom SQUID. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31465)

Novel, Fast Enhancements to Bragg Ptychography

Kevin Mertes
20190373ER

Project Description

The ability to rapidly produce non-destructive, three-dimensional (3D) images of crystalline nanostructures with nanometer resolution is directly relevant to our nation's national security. This research will provide a versatile tool that meets the needs of Department of Energy-Basic Energy Sciences, Weapons Science and Global Security Intelligence and Emerging Threats.

Publications

Posters

Burdet, N. G., A. V. Carr, J. M. Bowlan, K. M. Mertes, J. D. Nguyen, R. Tobey, X. Ding, S. Lin, C. S. Walker, B. A. Pound, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins , V. Zapf, C. Mazzoli and R. L. Sandberg. Towards spatially mapping domain dynamics in Antiferromagnetic materials with soft x-ray scattering at NSLS-II. Presented at *SLAC Users Meeting*, Standford, California, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-25092)

Viral Mosaic Biosensor

Karina Yusim
20190392ER

Project Description

Influenza is a rapidly evolving viral pathogen that infects up to 5 million people annually. The early diagnosis and treatment of influenza infections can greatly reduce mortality. However, the currently available rapid influenza tests are unreliable and leave many infections undiagnosed. There is an urgent need for a highly sensitive influenza diagnostic test to be used in point-of-care settings. We will combine theoretical mosaic sequence design and the biosensor technology capabilities developed at Los Alamos National Laboratory to develop a rapid ultra-sensitive influenza biosensor using computationally-derived novel sequence probes that encompass a wide variety of influenza viruses to detect not only presently circulating viruses but potentially also future pandemic strains that will evolve through mutations and rearrangement. The resulting novel, inexpensive and highly sensitive diagnostic tool will be easily expandable to other pathogens, with influenza serving as a proof-of-principle. This work directly supports the Laboratory's Science of Signatures Pillar in threat reduction, biosurveillance and global health security and the missions of the DOE Office of Science Biological and Environmental Research (BER), as well as DHHS (NIH and CDC) missions to prevent, detect, diagnose, confront and treat disease, and is related to missions of DHS, DOD, and other federal agencies.

Publications

Posters

Kubicek-Sutherland, J. Z., J. P. Theiler, K. Yusim, B. T. Foley, C. A. Lopez Bautista, S. Gnanakaran and H. Mukundan. Targeting Amphiphilic Biomarkers from Emerging Pathogens for Detection and Therapeutic Applications. Presented at *2019 Chemical and Biological Defense Science & Technology (CBD S&T) Conference*, Cincinnati, Ohio, United States, 2019-11-18 - 2019-11-21. (LA-UR-19-31352)

Emulating Quantum Magnetism with Rydberg Atoms

Michael Martin
20190494ER

Project Description

The goal of this project to create a reconfigurable and tunable system for quantum emulation, based on dynamically-configurable arrays of individually-trapped ultracold rubidium atoms. The character, range and strength of the interaction between the atoms will be tuned by the geometry of the arrays, and by external laser parameters. This complete set of capabilities will be the first highly scalable, neutral atom-based platform for tackling a broad range of models in quantum magnetism. By exploring system behavior, such as spin correlations and ground states, we will improve understanding of important quantum many-body models. Further, we will study coherent quantum annealing as an approach to quantum optimization problems, which will inform ongoing research on the properties of commercially-available quantum devices, for which the exact role of entanglement and coherence is poorly understood. This work will impact basic understanding of materials, by elucidating the role of entanglement in material properties, such as the so-called quantum spin liquid ground state; information science/technology, by establishing a testbed for solving complex optimization problems through a process known as coherent quantum annealing; and advanced quantum sensing, where control over interactions yields robust quantum states for sensing beyond classical limits.

Publications

Reports

Martin, M. J., M. C. Revelle and G. W. Biedermann. A platform for quantum information and large-scale entanglement with Rydberg atoms in programmable optical potentials. Unpublished report. (LA-UR-18-31881)

Mitra, A., P. M. Poggi, M. J. Martin, A. V. Marino, G. W. Biedermann and I. H. Deutsch. Robust Molmer-Sorenson gate for neutral atoms using rapid adiabatic Rydberg dressing. Unpublished report. (LA-UR-19-31221)

Presentation Slides

Martin, M. J. Emulating quantum magnetism with Rydberg atoms. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31519)

Martin, M. J. Emulating quantum magnetism with Rydberg atoms. Presented at *LANL Quantum Day*, Los Alamos, New Mexico, United States, 2018-12-11 - 2018-12-11. (LA-UR-18-31484)

Martin, M. J. Neutral atom tools for quantum information science. Presented at *Meeting at Argonne Natl. Lab*, Lemont, Illinois, United States, 2019-03-25 - 2019-03-25. (LA-UR-19-22592)

Martin, M. J., C. Ryu and M. G. Boshier. Quantum technologies with ultracold atoms. Presented at *UC Quantum Information Science Research Workshop*, Berkeley, California, United States, 2019-05-08 - 2019-05-08. (LA-UR-19-24127)

Discovering the 3D Structure and Dynamics of the Sun-Interstellar Medium System on a Global Scale

Daniel Reisenfeld
20190498ER

Project Description

The primary goal of this project is to understand the structure and dynamics of the Sun's space environment (the heliosphere) and its ability to screen the Earth from damaging radiation that is ubiquitous in the interstellar medium. Notably, this radiation, particularly cosmic rays, has a strong solar cycle variation; it also represents the greatest risk to interplanetary travel by humans as well as one of the largest backgrounds in National Nuclear Security Administration-sponsored, Los Alamos-built space instruments that detect nuclear explosions around the globe. The project exploits data from the Los Alamos-led energetic neutral atom (ENA) imager on the National Aeronautics Space Administration Interstellar Boundary Explorer (IBEX) mission to "sound" the three-dimensional extent of the heliosphere by monitoring over time the response of the outer heliosphere (via ENA emission) to bursts of plasma originally ejected from the Sun. By imaging the outer heliospheric response over time, we can understand the plasma flows and thus the underlying physical processes that govern heliospheric dynamics over the solar cycle. This research builds leadership capabilities in space weather and informs the optimization of the ENA imager that Los Alamos will lead for NASA's upcoming IMAP mission.

Publications

Journal Articles

*Reisenfeld, D. B., M. Bzowski, H. O. Funsten, P. H. Janzen, N. Karna, M. A. Kubiak, D. J. McComas, N. A. Schwadron and J. M. Sokol. The Influence of Polar Coronal Holes on the Polar ENA Flux Observed by IBEX. 2019. *Astrophysical Journal Letters*. **879** (1): 1. (LA-UR-19-22264 DOI: 10.3847/1538-4357/ab22c0)

Posters

Reisenfeld, D. B., M. Bzowski, H. O. I. Funsten, P. H. Janzen, M. A. Kubiak, D. J. McComas, N. A. Schwadron and J. Sokol. Sounding The Dimensions of the Heliosphere Using the Time-Correlation Between IBEX ENA Observations and the Solar Wind Dynamic Pressure. Presented at *2019 Fall Meeting of the American Geophysical Union*, San Francisco, California, United States, 2019-12-09 - 2019-12-09. (LA-UR-19-32234)

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 results 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.

Technical Outcomes

The outcomes of this ER project are: (1) a Finite-Element-Discrete-Element model of the response of unconsolidated geomaterial to impacts; (2) new methods to establish material models; (3) numerical modeling of the Chelyabinsk air burst with the coupling between the ground and the atmosphere; (4) seismic models of Mars and first parametric study of these models; (5) modeling of scattering due to the high level of heterogeneity in the Moon's crust.

Publications

Journal Articles

*Karakostas, F., V. Rakoto, P. Lognonne, C. Larmat, I. Daubar and K. Miljkovic. Inversion of Meteor Rayleigh Waves on Earth and Modeling of Air Coupled Rayleigh Waves on Mars. 2018. *Space Science Reviews*. **214** (8): 127. (LA-UR-18-25160 DOI: 10.1007/s11214-018-0566-6)

Lei, Z., C. R. Bradley, A. Munjiza, E. Rougier, B. J. Euser and E. E. Knight. A NOVEL FRAMEWORK FOR ELASTOPLASTIC BEHAVIOR OF ANISOTROPIC SOLIDS. Submitted to *Computational Particle Mechanics*. (LA-UR-20-20240)

Munjiza, A., E. Rougier, Z. Lei and E. E. Knight. FSIS – A novel Fluid-Solid Interaction Solver for Fracturing and Fragmenting Solids. Submitted to *Computer Methods in Applied Mechanics and Engineering*. (LA-UR-19-24666)

Books/Chapters

Larmat, C. Time Reversal in Seismology. (LA-UR-19-27801)

Reports

Froment, M. REPORT 29 MARCH 2019 - LEARNING HOSS AND DEVELOPING A MATERIAL MODEL FOR SAND AND PUMICE. Unpublished report. (LA-UR-19-22851)

Froment, M. Internship Report: Numerical modelling of impact seismic signals on regolith. Unpublished report. (LA-UR-19-25117)

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)

Presentation Slides

Cooley, J. H., E. E. Knight, E. Rougier and B. J. Euser. HOSS HDBT Assured Weapons Lethality Assessment. . (LA-UR-18-30894)

Froment, M., B. J. Euser, Z. Lei, E. Rougier, C. Larmat, S. Kedar, T. Kawamura and P. Lognonn\xc3\xa9. Lagrangian-based simulations of hypervelocity impacts experiments on Mars regolith proxy. . (LA-UR-19-29583)

Froment, M., P. Lognonn\xc3\xa9, T. Kawaruma, C. Larmat, E. Rougier, Z. Lei, B. J. Euser and S. Kedar. Numerical modelling of impact seismic signals on regolith. . (LA-UR-19-25991)

Knight, E. E., E. Rougier, Z. Lei, B. J. Euser and V. T. Chau. HOSS Overview Latest Advancements. . (LA-UR-19-31536)

Larmat, C. Fundamentals of numerical methods. Presented at *CIG LLNL workshop*, Livermore, California, United States, 2017-09-18 - 2017-09-22. (LA-UR-17-28498)

Larmat, C., E. E. Knight, E. Rougier and Z. Lei. Walking the road from impacts to seismic sources.. . (LA-UR-17-25076)

Larmat, C., E. E. Knight, K. M. Cleveland, Z. Lei, H. J. Patton, E. Rougier and C. R. Bradley. Seismic signals from explosions and impacts. Presented at *LANL-IPGP pre-AGU workshop*, Washington, District Of Columbia, United States, 2018-12-09 - 2018-12-09. (LA-UR-18-31439)

Larmat, C., R. Maguire, F. Karakostas and L. Rolland. InSight, 3D modeling CTX impact. . (LA-UR-19-26204)

Larmat, C., Z. Lei, E. E. Knight and E. Rougier. w17_seismicsources "Walking the road from impacts to seismic sources for celestial bodies.". . (LA-UR-18-21120)

Larmat, C., Z. Lei, E. E. Knight and E. Rougier. w17_seismicsources “Walking the road from Impacts to Seismic Sources for celestial bodies”. . (LA-UR-19-22151)

Lee, Y. Geo-material Modelling: Parameters Identification and Multiscale Simulation. . (LA-UR-19-29922)

Lei, Z., E. E. Knight, E. Rougier and B. J. Euser. HOSS Training Material Modelling in HOSS - Part I. . (LA-UR-17-31215)

Lei, Z., E. E. Knight, E. Rougier and B. J. Euser. HOSS Training Contact & Fracture. . (LA-UR-17-31216)

Lei, Z., E. E. Knight, E. Rougier and B. J. Euser. HOSS Training Material Modelling in HOSS - Part II. . (LA-UR-17-31219)

Lei, Z., E. Rougier, E. E. Knight and A. Munjiza. The Combined Finite-Discrete Element Method (FDEM): Its Theory. . (LA-UR-19-23606)

Li, X. and C. Larmat. machine learning solutions to revealing the hidden seismicity of Mars. . (LA-UR-18-27327)

Mehta, R. S. and E. Rougier. Prediction of Rocket Plume Induced Rock Fracture for Landers. . (LA-UR-18-30076)

Rougier, E., Z. Lei, B. J. Euser, E. E. Knight and A. Munjiza. Fluid-Structure Interaction Problems via the Combined Finite-Discrete Element Method. Presented at *SES 2019 – Society of Engineering Science*, St. Louis, Missouri, United States, 2019-10-13 - 2019-10-13. (LA-UR-19-30330)

Rougier, E. and E. E. Knight. LANL HOSS Modeling Capabilities General Briefing. . (LA-UR-18-29674)

Posters

Froment, M., Z. Lei, B. J. Euser, J. E. Richardson, S. Kedar, C. Larmat, E. Rougier, P. Lognonn\xc3\xa9, T. Kawamura and B. W. Banerdt. Numerical Modeling of Impact Seismic Signal on Mars Regolith. Presented at *AGU*, San Fransisco, California, United States, 2019-12-09 - 2019-12-13. (LA-UR-19-32064)

Froment, M., Z. Lei, B. J. Euser, S. Kedar, C. Larmat, E. Rougier, P. Lognonn\xc3\xa9, T. Kawamura and B. W. Banerdt. Lagrangian based simulations of hypervelocity impacts on Martian regolith. Presented at *InSight Science Team Meeting*, Los Angeles, California, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30626)

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Froment, M., Z. Lei, S. Kedar, C. Larmat, E. Rougier, P. Lognonne and T. Kawamura. Internship: Modeling impacts on Martian stratified regolith. . (LA-UR-19-21304)

Karakostas, F., C. Larmat and P. Lognonne. Source inversion of Chelyabinsk and perspective for inversion of Mars airburst. Presented at *Insight Science team meeting*, Buellton, California, United States, 2018-05-04 - 2018-05-06. (LA-UR-18-23850)

Karakostas, F., R. Maguire, C. Larmat, Q. Huang, N. Schmerr, P. Lognonn\xc3\xa9 and I. Daubar. Update on Martian impacts modeling, after almost one year of Martian seismic data recordings.. Presented at *InSight Science Team Meeting*, Pasadena, California, United States, 2019-10-21 - 2019-10-25. (LA-UR-19-30628)

Karakostas, F., V. Rakoto, P. Lognonne, C. Larmat, I. Daubar and K. Miljkovic. Inversion of meteor Rayleigh waves on Earth and Modeling of Air Coupled Rayleigh Waves on Mars. Presented at *2018 AGU Fall meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31396)

Larmat, C., J. K. Maccarthy and W. S. Phillips. Development and validation of Statistical models of small-scale heterogeneities. Presented at *2018 SSA meeting*, Miami, Florida, United States, 2018-05-14 - 2018-05-17. (LA-UR-18-24138)

Larmat, C. and X. Li. Detecting the hidden seismicity of Mars. Presented at *2018 AGU Fall meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-14. (LA-UR-18-31418)

Lee, Y., Z. Lei and R. Regueiro. Hierarchical Multi-scale FEM-DEM Modeling of Biaxial Compression test and RVE size study. . (LA-UR-19-31125)

E. Neal, K. A., V. D. Shah, Z. Lei and C. Larmat. Modeling Seismic Wave Propagation Generated by Explosive Sources. . (LA-UR-17-27118)

Rolland, L., C. Larmat, R. Garcia, L. Martire, A. Spiga and P. Lognonn\xc3\xa9. Infrasounds propagation on Mars. Presented at *Insight Science meeting*, Paris, France, 2019-06-17 - 2019-06-21. (LA-UR-19-25739)

Rougier, E., Z. Lei, B. J. Euser, M. Froment, S. Kedar, E. E. Knight and C. Larmat. THE NUMERICAL ROAD TO DETERMINATION OF FRACTURE ROLE ON IMPACTS AS SEISMIC SOURCES:

FINITE-DISCRETE MODELING OF IMPACTS. Presented at *50th Lunar and Planetary Science Conference*, The Woodlands, Texas, United States, 2019-03-18 - 2019-03-22. (LA-UR-19-22407)

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.

Technical Outcomes

We investigated two new approaches for chemically specific 3D imaging based on nuclear quadrupole resonance. While other imaging techniques are well established their ability to identify specific chemicals is severely limited. Our approaches were tested experimentally and computationally to demonstrate their feasibility. This will have applications in both narcotics and explosives detection.

Publications

Presentation Slides

Espy, M. A., J. F. Hunter, M. T. Janicke, D. Kaseman, P. E. Magnelind, M. Malone, P. Nath, L. J. Schultz, A. V. Urbaitis, P. L. Volegov, S. Widgeon, J. L. Yoder and R. F. Williams. Ultra-low Field NMR for detection of threat materials. Presented at *3rd Annual Workshop on Concealed Explosives Detection*, Santa Fe, New Mexico, United States, 2018-08-27 - 2018-08-31. (LA-UR-18-28124)

Malone, M. Targeted Relaxation for Nuclear Quadrupole Resonance Imaging. Presented at *Workshop on Low Field Magnetic Resonance*, Boulder, Colorado, United States, 2019-08-11 - 2019-08-13. (LA-UR-19-28008)

Malone, M. and P. L. Volegov. Targeted Relaxation for Nuclear Quadrupole Resonance Imaging. Presented at *60th Experimental Nuclear Magnetic Resonance Conference*, Pacific Grove, California, United States, 2019-04-07 - 2019-04-12. (LA-UR-19-22102)

Posters

Malone, M. and P. L. Volegov. Targeted Relaxation for Nuclear Quadrupole Resonance Imaging. Presented at *60th Experimental NMR Conference*, Pacific Grove, California, United States, 2019-04-07 - 2019-04-12. (LA-UR-19-23050)

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).

Technical Outcomes

We have developed new methods and instrumentation for conducting radiochronometry by laser absorption spectroscopy, which takes advantage of the fact that different isotopes of a given element exhibit slightly different electronic transition energies. We have determined isotope ratios of uranium and plutonium samples, from which the age of last purification can be obtained.

Publications

Posters

Castro, A. Actinide Isotopic Analysis by Atomic Beam Laser Absorption Spectroscopy. . (LA-UR-18-24123)

Castro, A., J. Bartlett and S. Lebedev. Fieldable Atomic Beam Laser Spectrometer for Isotopic Analysis. . (LA-UR-18-23253)

Castro, A., J. Bartlett and V. Lebedev. Generation of Atomic Beams of Highly Refractory Elements for Laser Spectroscopy. Presented at *ICAP 2018*, Barcelona, Spain, 2018-07-22 - 2018-07-22. (LA-UR-18-26335)

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.

Technical Outcomes

We have developed novel plane-wave and fan-beam ultrasound tomography techniques for prostate cancer imaging. We have designed and built a new transrectal ultrasound tomography prototype, and tested the prototype using a prostate phantom. Our clinical collaborators have used the prototype to image the prostates for 19 patients. Our preliminary clinical imaging results show that our fan-beam transrectal ultrasound imaging technique produces higher-resolution images with more even illumination of the prostate than other ultrasound techniques do.

Publications

Journal Articles

Shin, J., L. Huang and J. T. Yen. Spatial Prediction Filtering for Medical Ultrasound in Aberration and Random Noise. 2018. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*. **65** (10): 1845-1856. (LA-UR-17-30593 DOI: 10.1109/TUFFC.2018.2860962)

Conference Papers

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., 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)

Presentation Slides

Huang, L. Transrectal Ultrasound Tomography for Prostate Cancer Imaging. . (LA-UR-19-22349)

Huang, L. Super-Resolution Imaging: From Subsurface Fracture Detection to Cancer Characterization. . (LA-UR-19-22639)

Huang, L., K. Gao, B. Chi and Y. Huang. Ultrasound-Waveform Tomography Using Speckle Diffraction. Presented at *2019 UITC Symposium*, Arlington, Virginia, United States, 2019-06-04 - 2019-06-07. (LA-UR-19-25314)

Huang, L., K. Gao, Y. Huang and K. G. Wen. Transrectal Ultrasound Tomography with Plane-Wave Ultrasound-Waveform Inversion. Presented at *2018 UITC Symposium*, Arlington, Virginia, United States, 2018-05-30 - 2018-06-01. (LA-UR-18-24754)

Huang, L., Y. Huang and K. Gao. Transrectal Plane-Wave Ultrasound Tomography for Prostate Cancer Imaging. Presented at *2019 AIUM Annual Convention*, Orlando, Florida, United States, 2019-04-06 - 2019-04-06. (LA-UR-19-23237)

Posters

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 Meeting*, Houston, Texas, United States, 2018-02-12 - 2018-02-15. (LA-UR-18-21058)

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-19-21237)

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, DC, District Of Columbia, United States, 2017-09-05 - 2017-09-09. (LA-UR-17-28496)

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 Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions of national security science in developing novel sensing technologies for national security missions.

Technical Outcomes

In this project, we developed a novel waveguide atom interferometer with a Bose-Einstein condensate BEC which can sense rotation and acceleration. A linear waveguide was moved during the interrogation to create an enclosed area for sensing of rotation and by using a double reflection scheme, an waveguide atom interferomter gyroscope with a BEC immune to acceleration noise was demonstrated for the first time.

Publications

Presentation Slides

Samson, E. C., C. Ryu and M. G. Boshier. Development of Quantum Inertial Sensors Using Painted Potentials. . (LA-UR-17-21882)

Posters

Ryu, C. and M. G. Boshier. Experiments with matter wave circuits. Presented at *DAMOP 2018*, Fort Lauderdale, Florida, United States, 2018-05-28 - 2018-06-01. (LA-UR-18-24505)

Ryu, C. and M. G. Boshier. Experiments with matter wave circuits. Presented at *DAMOP 2018*, Fort Lauderdale, Florida, United States, 2018-05-28 - 2018-06-01. (LA-UR-18-24859)

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, howver they have historically been difficult to study. Here we explore how the new generation of magnetic field and X-ray technologies at Department of Energy(DOE)/National Nuclear Security Administration(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.

Technical Outcomes

We have successfully measured the dynamic behavior of domains in three antiferromagnets at the National High Magnetic Field Laboratory and the Center for Integrated Nanotechnology at Los Alamos, and at the National Synchrotron Light Source II at Brookhaven National Lab. We tested and and advanced classic theories of dynamic behavior in antiferromagnets.

Publications

Journal Articles

*Jae, W. K., E. D. Mun, X. Ding, A. Hansen, M. Jaime, N. Harrison, H. T. Yi, Y. Chai, Y. Sun, S. W. Cheong and V. S. Zapf. Metastable states in the frustrated triangular compounds Ca3Co2−xMnxO6 and Ca3Co2O6. 2018. *Physical Review B*. **98** (2): 024407. (LA-UR-17-28067 DOI: 10.1103/PhysRevB.98.024407)

Lei, S., S. Chikara, J. Peng, Y. Wang, M. Zhu, D. Puggioni, M. Gu, W. Zhao, Y. Yuan, H. Akamatsu, M. H. W. Chan, J. M. Rondinelli, X. Ke, Z. Mao, M. Jaime, J. Singleton, D. F. Weickert, V. Zapf and V. Gopalan. Comprehensive magnetic phase diagrams of the polar metal, Ca3(Ru0.95Fe0.05)2O7. Submitted to *Physical Review B*. (LA-UR-18-30772)

*Rai, B. K., S. Chikara, X. Ding, I. W. H. Oswald, R. Schonemann, V. Loganathan, A. M. Hallas, H. B. Cao, M. Stavinoha, T. Chen, H. Man, S. Carr, J. Singleton, V. Zapf, K. A. 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, H. C. Walker, D. T. Adroja, P. Dai, A. H. Nevidomskyy, C. -. Huang and E. Morosan. Anomalous Metamagnetism in the Low Carrier Density Kondo Lattice. 2018. *Physical Review X*. **8** (4): 041047. (LA-UR-18-30067 DOI: 10.1103/PhysRevX.8.041047)

Reports

Zapf, V. Multiferroic Metal-Organic Materials. Unpublished report. (LA-UR-18-21705)

Posters

Burdet, N. G., A. V. Carr, J. M. Bowlan, K. M. Mertes, J. D. Nguyen, R. Tobey, X. Ding, S. Lin, C. S. Walker, B. A. Pound, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins , V. Zapf, C. Mazzoli and R. L. Sandberg. Towards spatially mapping domain dynamics in Antiferromagnetic materials with soft x-ray scattering at NSLS-II. Presented at *SLAC Users Meeting*, Standford, California, United States, 2019-09-24 - 2019-09-27. (LA-UR-19-25092)

Chikara, S., V. Zapf, J. Singleton, B. L. Scott, N. C. Smythe, J. Eckert, E. Krenkel, S. Lin, C. Batista, X. Gu, H. Cheng and X. Zhang. Using spin state transitions to create multiferroic-like behavior. Presented at *Gordon Conference on Multiferroics*, Bates, Maine, United States, 2018-08-06 - 2018-08-06. (LA-UR-18-26740)

Pound, B. A., H. I. Garland, J. Hendriks and R. L. Sandberg. Ptychography: a versatile imaging tool. Presented at *Los Alamos National Laboratory Student Symposium*, Los Alamos, New Mexico, United States, 2017-08-09 - 2017-08-09. (LA-UR-17-26887)

Sandberg, R. L., V. Zapf, J. M. Bowlan, X. Ding, C. Walker, N. Lee, Y. J. Choi, A. Barbour, W. Hu, S. Wilkins and C. Mazzoli. Using soft X-ray photon correlation spectroscopy to probe fluctuating antiferromagnetic domains. Presented at *Coherence 2018: International Workshop on Phase Retrieval and Coherent Scattering*, Port Jefferson, New York, United States, 2018-06-25 - 2018-06-28. (LA-UR-18-25595)

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.

Technical Outcomes

A core group of radiation and desiccation-tolerant cyanobacteria and associated heterotrophic bacteria was found to comprise the central hub of the varnish community. These organisms accumulate and concentrate Mn to protect against radiation damage and secrete siderophores, which coat the rock surface as a long-lived catalyst for Mn oxidation. By establishing these two completely novel mechanisms for biogenic varnish formation, we have identified organic/ inorganic biosignatures to distinguish biogenic and abiogenic origins of Mn-rich surfaces.

Publications

Journal Articles

Lingappa, U., C. M. Yeager, A. Sharma, N. L. Lanza, D. P. Morales, G. Xie, A. D. Atencio, G. Chadwick, D. Monteverde, J. Magyar, S. M. Webb, J. Valentine, B. Hoffman and W. W. Fischer. Manganese in rock varnish derives from Cyanobacteria. Submitted to *Nature*. (LA-UR-20-22090)

Reports

Yeager, C. M. Life on the Edge: Microbes in Rock Varnish. Unpublished report. (LA-UR-19-30329)

Presentation Slides

Marti-Arbona, R., S. P. Hennelly and S. N. Micheva-Viteva. Novel RNA Based Approach to High Throughput Discovery and Validation of New Drug Targets. Presented at *017 Chemical and Biological Defense Science & Technology Conference*, Long Beach, California, United States, 2017-11-27 - 2017-12-01. (LA-UR-17-30136)

Posters

Burns, E., M. Teshima, R. Marti-Arbona, N. L. Lanza and C. M. Yeager. Rock Varnish as a Source of Biosignatures for Mars Extant Life. Presented at *The Annual Biomedical Research Conference for Minority Students (ABRCMS) 2019*, Anaheim, California, United States, 2019-11-13 - 2019-11-16. (LA-UR-19-28269)

Yeager, C. M. Microbial Inhabitants of Rock Varnish: Visitors or Niche Specialists. Presented at *Goldschmidt 2019*, Boston, Massachusetts, United States, 2018-08-13 - 2018-08-13. (LA-UR-18-27675)

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.

Technical Outcomes

Some of the world's fastest infrared photodetectors have been demonstrated here using semiconductor quantum dots as photoactive media. Photodetector temporal response on the order of tens of picoseconds has been achieved with infrared sensitivity at wavelengths up to 4 micrometers and a tunable onset of photoresponse to wavelengths between 1 and 4 micrometers. Other advantages include solution-based synthesis and deposition of nanomaterials, room-temperature operation, and sensitivity in the ultraviolet, visible, and infrared spectral regions.

Publications

Presentation Slides

Robel, I. Photoionization in Doped and Undoped Semiconductor Quantum Dots. Presented at *235th Electrochemical Society Meeting*, Dallas, Texas, United States, 2019-05-26 - 2019-05-31. (LA-UR-18-31679)

Robel, I. Controlling Carrier Dynamics in Mesoscale Quantum Dot Assemblies: From Efficient Solar Cells to Ultrafast Photodetectors. Presented at *233rd Meeting of the Electrochemical Society*, Seattle, Washington, United States, 2018-05-13 - 2018-05-17. (LA-UR-18-23817)

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.

Technical Outcomes

We successfully matured the EPICS concept into a producible design through simulation, testing of key components, and building and testing a prototype. This demonstrates the potential of combined neutron and gamma-ray spectroscopy within a single detector and paves the way for future high-profile planetary science missions. The performance testing performed under this project is critical to evaluating the key enabling technologies of EPICS for future planetary science and national security missions in space.

Publications

Journal Articles

Bartlett, K. D., D. D. S. Coupland, D. T. Beckman and K. E. Mesick. Proton Irradiation Damage and Annealing Effects in ON Semiconductor J-Series Silicon Photomultipiers. Submitted to *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. (LA-UR-19-31419)

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)

Mesick, K. E., K. D. Bartlett, D. D. S. Coupland and L. C. Stonehill. Effects of proton-induced radiation damage on CLYC and CLLBC performance. 2019. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **948**: 162774. (LA-UR-19-26719 DOI: 10.1016/j.nima.2019.162774)

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)

Watts, M. M., K. E. Mesick, K. D. Bartlett and D. D. S. Coupland. Thermal Characterization of Tl_2LiYCl_6:Ce (TLYC). Submitted to *IEEE Transactions on Nuclear Science*. (LA-UR-19-30413)

West, S., D. Beckman, D. Coupland, N. Dallmann, C. Hardgrove, K. Mesick and L. Stonehill. Compact readout of large CLYC scintillators with silicon photomultipler arrays. 2020. *Nuclear Instruments & Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment*. **951**: 162928. (LA-UR-19-24732 DOI: 10.1016/j.nima.2019.162928)

Conference Papers

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., L. C. Stonehill, D. D. S. Coupland, D. T. Beckman, S. T. West, S. F. Nowicki, N. Dallmann, S. A. Storms and W. Feldman. 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)

Presentation Slides

S. Coupland, D. D., K. D. Bartlett and K. E. Mesick. EPICS: Prototype Development Status. Presented at *LANL/ASU Planetary Neutrons Workshop*, Los Alamos, New Mexico, United States, 2019-05-20 - 2019-05-20. (LA-UR-19-24713)

S. Coupland, D. D., K. E. Mesick, A. M. Ollila, C. Hardgrove, K. D. Bartlett, D. T. Beckman, N. Dallmann, D. K. Hemsing, L. A. Ott and S. A. Storms. EPICS-LITE: Elpasolite Planetary Ice and Composition Spectrometer for Lunar In-situ deTectionof Elements. Presented at *Microsymposium 60 Forward to the Moon to Stay: Undertaking Transformative Lunar Science with Commercial Partners*, The Woodlands, Texas, United States, 2019-03-16 - 2019-03-16. (LA-UR-19-22268)

Mesick, K. E. Nuclear Physics and Planetary Exploration. Presented at *2019 APS Division of Nuclear Physics*, Crystal City, Virginia, United States, 2019-10-14 - 2019-10-14. (LA-UR-19-30362)

Nowicki, S. F., K. E. Mesick, D. D. S. Coupland, N. Dallmann, W. C. Feldman, L. C. Stonehill, S. A. Storms, C. Hardgrove, S. Dibb, T. Gabriel and S. West. Constraining the origin of Phobos with the Elpasolite Planetary Ice and Composition Spectrometer (EPICS) – Simulated Performance. Presented at *AGU Fall meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-11. (LA-UR-17-30981)

Nowicki, S. F., L. C. Stonehill, D. D. S. Coupland, K. E. Mesick and A. M. Parsons. Neutron Gamma Detector Systems for Planetary Science Applications. . (LA-UR-17-22278)

Posters

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 *2017 IEEE Nuclear Science Symposium*, Atlanta, Georgia, United States, 2017-10-23 - 2017-10-23. (LA-UR-17-29542)

S. Coupland, D. D., L. C. Stonehill, K. E. Mesick, D. T. Beckman, S. T. West, N. Dallmann, S. A. Storms and W. C. Feldman. Elpasolite Planetary Ice and Composition Spectrometer (EPICS): A Low-Resource Combined Gamma-Ray and Neutron Spectrometer for Planetary Science. Presented at *AGU 2018 Fall Meeting*, Washington, District Of Columbia, United States, 2018-12-10 - 2018-12-10. (LA-UR-18-31371)

S. Coupland, D. D., L. C. Stonehill, K. E. Mesick, K. D. Bartlett, D. T. Beckman, S. T. West, S. F. Nowicki, N. Dallmann, S. A. Storms and W. C. Feldman. Elpasolite Planetary Ice and Composition Spectrometer (EPICS): A Low-Resource Combined Gamma-Ray and Neutron Spectrometer for Planetary Science. Presented at *50th Lunar and Planetary Science Conference*, The Woodlands, Texas, United States, 2019-03-18 - 2019-03-18. (LA-UR-19-22338)

Dallmann, N., B. E. Carlsten, R. M. Holmes and L. C. Stonehill. A Model Based Deconvolution Approach for Creating Surface Composition Maps of Irregularly Shaped Bodies from Limited Orbiting Nuclear Spectrometer Measurements. Presented at *American Geophysical Union (AGU) Fall meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-31113)

Mesick, K. E. Elpasolites for Dual Neutron and Gamma-Ray Detection. . (LA-UR-18-23068)

Mesick, K. E., D. D. S. Coupland, S. F. Nowicki and L. C. Stonehill. The effects of radiation damage on CLYC performance. Presented at *2017 IEEE Nuclear Science Symposium*, Atlanta, Georgia, United States, 2017-10-23 - 2017-10-27. (LA-UR-17-29525)

Mesick, K. E., L. C. Stonehill, D. D. S. Coupland, D. T. Beckman, S. T. West, N. Dallmann, S. F. Nowicki, W. C. Feldman and S. A. Storms. Elpasolite Planetary Ice and Composition Spectrometer (EPICS): A low resource combined neutron and gamma-ray spectrometer for planetary science. Presented at *2018 IEEE NSS*, Sydney, Austria, 2018-11-10 - 2018-11-16. (LA-UR-18-30380)

Stonehill, L. C., D. D. S. Coupland, K. E. Mesick and S. F. Nowicki. Development of an Elpasolite Planetary Science Instrument. Presented at *IEEE Nuclear Science Symposium*, Strasbourg, France, 2016-10-31 - 2016-10-31. (LA-UR-16-28153)

Stonehill, L. C., D. D. S. Coupland, N. Dallmann, W. C. Feldman, K. E. Mesick, S. F. Nowicki 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 *American Geophysical Union Fall Meeting*, New Orleans, Louisiana, United States, 2017-12-11 - 2017-12-15. (LA-UR-17-30941)

West, S. T., K. E. Mesick, D. D. S. Coupland, L. C. Stonehill, D. T. Beckman and N. Dallmann. Readout Electronics and Data Processing for Planetary Nuclear Spectrometers. Presented at *LANL Annual Student Symposium*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-26967)

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.

Technical Outcomes

We have developed a novel, low-cost, portable, high-sensitivity 16-channel atomic magnetometer in order to accelerate magnetic measurements in various fields, such as neuroscience and biomedical research, and improve the current technologies. The decrease in the cost of sensors by an order of magnitude is achieved by the 16-channel operation realized in a single module using a single large rubidium vapor cell, broad laser beams, and a 16-channel photodiode array. We demonstrated its applications in magnetocardiography.

Publications

Journal Articles

*Kim, Y. J., I. Savukov and S. Newman. Magnetocardiography with a 16-channel fiber-coupled single-cell Rb optically pumped magnetometer. 2019. *Applied Physics Letters*. **114** (14): 143702. (LA-UR-19-21746 DOI: 10.1063/1.5094339)

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*. **7** (10): 54-57. (LA-UR-18-28670)

Zhu, Y., I. M. Savukov, Y. Gao and C. Hilty. Multinuclear Detection of Nuclear Spin Optical Rotation at Low Field. 2018. *The Journal of Physical Chemistry Letters*. **9** (12): 3323-3327. (LA-UR-18-22153 DOI: 10.1021/acs.jpclett.8b01053)

Conference Papers

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)

Presentation Slides

Kim, Y. J. Precision Magnetic Measurements: From Dark Matter Search to Biomagnetism. Presented at *2019 Joint KPS-AKPA Symposium*, Boston, Massachusetts, United States, 2019-03-03 - 2019-03-03. (LA-UR-19-21745)

Kim, Y. J. and I. M. Savukov. Highly sensitive multi-channel atomic magnetometer. Presented at *2018 IEEE Sensors Applications Symposium (SAS)*, Seoul, Korea, South, 2018-03-12 - 2018-03-12. (LA-UR-18-21595)

Kim, Y. J. and I. M. Savukov. A high-sensitivity 16-channel magnetic sensor for magnetocardiographic experiments. Presented at *APS March Meeting*, Boston, Massachusetts, United States, 2019-03-04 - 2019-03-04. (LA-UR-19-21744)

Savukov, I. M. and Y. J. Kim. Highly sensitive multi-channel atomic magnetometer for MEG and MRI. Presented at *SBMT*, Los Angeles, California, United States, 2018-04-13 - 2018-04-15. (LA-UR-18-23092)

Savukov, I. M. and Y. J. Kim. Highly sensitive multi-channel atomic magnetometer for MEG and MRI. Presented at *SBMT*, Los Angeles, California, United States, 2018-04-13 - 2018-04-13. (LA-UR-18-23133)

Savukov, I. M. and Y. J. Kim. Highly sensitive multi-channel atomic magnetometer. Presented at *Workshop on Optically Pumped Magnetometers*, Mainz, Germany, 2019-08-14 - 2019-08-16. (LA-UR-19-27962)

Posters

Savukov, I. M., Y. J. Kim and P. Chu. Atomic magnetometer research at Los Alamos. Presented at *Heraeus-Workshop: Quantum Sensing & Magnetometry / August 2019*, Bad Honnef, Germany, 2019-08-12 - 2019-08-14. (LA-UR-19-27961)

Savukov, I. M. and Y. J. Kim. Applications of atomic magnetometers in NMR and MRI. Presented at *PANIC*, Hilton Head Island, South Carolina, United States, 2019-03-03 - 2019-03-03. (LA-UR-19-21337)

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.

Technical Outcomes

This project engineered a fieldable miniaturized optical biosensor platform, and fabricated and validated the mirofluidics chip for the sample processing.

Publications

Journal Articles

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)

Reports

Smith, J. E. Rapid Detection of Bacteremia in Human Blood. Unpublished report. (LA-UR-19-24567)

Presentation Slides

Kubicek-Sutherland, J. Z. Towards a Fieldable Biosensor for Detecting Bacterial Select Agent Pathogens. Presented at *2019 ASM Biothreats*, Arlington, Virginia, United States, 2019-01-29 - 2019-01-29. (LA-UR-19-20579)

Kubicek-Sutherland, J. Z., A. S. Anderson and H. Mukundan. NNSA/LDRD program manager briefing. Presented at *NNSA/LDRD program manager briefing*, Los Alamos, New Mexico, United States, 2018-05-30 - 2018-05-30. (LA-UR-18-24783)

Lenz, K. D. A Microfluidics-Based Cross-Flow Filtration Platform for Rapid Processing of Amphiphilic Biomarkers from Blood. Presented at *UNM Thesis defense meeting*, Los Alamos, New Mexico, United States, 2019-04-05 - 2019-04-05. (LA-UR-19-23087)

Mukundan, H. The Microbe Strikes Back: Emerging infectious Diseases and the need for point of care diagnostics. . (LA-UR-18-30804)

Mukundan, H. Universal Diagnostics: dream or reality. Presented at *triage diagnostics working group: Foundation for innovative new diagnostics*, Geneva, Switzerland, 2019-03-26 - 2019-03-27. (LA-UR-19-22543)

Mukundan, H. Universal Diagnostics- Dream or Reality. Presented at *Biodefense World Summit*, Bethesda, Maryland, United States, 2019-06-18 - 2019-06-19. (LA-UR-19-25590)

Mukundan, H. Fieldable Automated Biosensor for Rapid Detection of Select Agent Pathogens. . (LA-CP-19-20055)

Posters

Hjelvik, E. A., A. S. Anderson and H. Mukundan. Optimized plastic functionalization for applications in biosensors. . (LA-UR-18-27033)

Hjelvik, E. A., A. S. Anderson and H. Mukundan. Functional thin films on plastic surfaces for applications in bacterial biosensor. Presented at *American Chemical Society Spring 2019 National Meeting*, Orlando, Florida, United States, 2019-03-31 - 2019-03-31. (LA-UR-19-22735)

Lenz, K. D., A. N. Mercer, J. Z. Kubicek-Sutherland, A. S. Anderson, P. Nath and H. Mukundan. Adaptation of centrifugal microfluidic techniques for blood sample processing to detect Francisella tularensis. Presented at *LANL Student Symposium 2018*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27137)

Lenz, K. D., A. N. Mercer, J. Z. Kubicek-Sutherland, A. S. Anderson, P. Nath and H. Mukundan. Adaptation of centrifugal microfluidic techniques for blood sample processing to detect bacterial pathogens. Presented at *SelectBio Lab-on-a-Chip and Microfluidics World Congress 2018*, Coronado, California, United States, 2018-10-01 - 2018-10-03. (LA-UR-18-29216)

Lenz, K. D., A. S. Anderson, S. Jakhar, P. Nath, H. Mukundan and J. Z. Kubicek-Sutherland. Automation of sample processing for point-of-care diagnostics using microfluidics-based technologies. Presented at *Sensors Summit 2019*, San Diego, California, United States, 2019-12-10 - 2019-12-12. (LA-UR-19-31983)

Mercer, A. N., J. Z. Kubicek-Sutherland, K. D. Lenz, A. S. Anderson, P. Nath and H. Mukundan. Host-Pathogen Interactions that Affect the Detection of Francisella tularensis in Blood. Presented at *2019 ASM Biothreats*, Arlington, Virginia, United States, 2019-01-29 - 2019-01-31. (LA-UR-19-20575)

Mukundan, H. Integrative Biosurveillance for Development and deployment of effective surveillance. Presented at *Sos capability review*, los alamos, New Mexico, United States, 2018-04-23 - 2018-04-27. (LA-UR-18-23725)

Mukundan, H. Trafficking and Innate Immune Recognition of Amphiphilic Bacterial PAMPs Strategies for Blood-based Diagnosis. Presented at *Keystone Symposia on Tuberculosis*, Santa Fe, New Mexico, United States, 2020-01-17 - 2020-01-20. (LA-UR-20-20506)

Mukundan, H., A. S. Anderson, J. Z. Kubicek-Sutherland, A. A. Bitzer, L. R. Stromberg, L. M. Lilley, P. Nath, J. E. Morales Garcia, D. D. L. Mascarenas, J. F. Harris, K. Bayles, M. Larson and S. Jakhar. Fieldable Universal Diagnostics for Bacterial Pathogens. Presented at *DTRA CHEMBIO CONFERENCE*, CINCINNATI, Ohio, United States, 2019-11-18 - 2019-11-22. (LA-UR-19-31636)

Pedersen, C. A. Application of Long-Term Air-Stable Lipid Bilayers for Waveguide-Based Biosensors. Presented at *LANL Student Symposium 2018*, Los Alamos, New Mexico, United States, 2018-07-31 - 2018-08-02. (LA-UR-18-27102)

Pedersen, C. A., H. Mukundan, A. S. Anderson, J. Z. Kubicek-Sutherland and L. R. Stromberg. Application of Long-Term Air-Stable Lipid Bilayers for Waveguide-Based Biosensors. Presented at *Biophysical Society Conference*, Baltimore, Maryland, United States, 2019-03-01 - 2019-03-07. (LA-UR-19-21678)

Yeong, L. R., A. S. N. Liao, J. E. Morales Garcia, B. Martinez, D. D. L. Mascarenas, P. Nath, A. S. Anderson and H. Mukundan. Engineering the Universal Bacterial Sensor. Presented at *2018 Los Alamos National Laboratory Student Symposium*, Los Alamos, New Mexico, United States, 2018-08-01 - 2018-08-01. (LA-UR-18-27092)

Chiroptical Characterization and Photocatalytic Destruction of Organophosphorus Nerve Agents

Amanda Evans
20190602ER

Project Description

Department of Energy(DOE)/National Nuclear Security Administration(NNSA) missions include preventing, countering, and responding to terrorist and other adversarial threats to the United States. Effective detection and destruction of chemical agent threats remain National and Global Security challenges that this research will address. Light-based approaches for agent destruction offer distinct advantages that other chemical/biochemical approaches cannot provide, including improved operational safety and scalability and tuned selectivity, while light-based characterization/ detection strategies for small molecules can offer unique characterization technologies that can be miniaturized for improved portability. This research will demonstrate light-based characterization of chemical agent analogs and selective light-based destruction of chemical agent analogs.

Technical Outcomes

Organophosphorus (OP) compounds are neurotoxic compounds found in pesticides and chemical warfare (CW) agents that present detection/degradation challenges. Chiral at the phosphorus atom, these compounds have unique spectral signals that can be detected in the presence of other chiral phenomena such as circularly polarized light. This project has established new means for detecting the chiral spectral signals of OPs. A continuous light-based destruction technology for OP CW analogs has also been demonstrated.

Publications

Conference Papers

Evans, A. C. Tunable Chiroptical Induction/Destruction Using Synchrotron-Sourced Circularly Polarized Light. Presented at *Microfluidics and Flow Chemistry 2019, SelectBio*. (Coronado Island, California, United States, 2019-10-08 - 2019-10-09). (LA-UR-19-29964)

Evans, A. C. “Tunable Chiroptical Induction and Photolysis in Flow". Presented at *American Chemical Society National Fall Meeting*. (Sand Diego, California, United States, 2019-08-25 - 2019-08-25). (LA-UR-19-28451)

Evans, A. C. Tunable chiroptical induction and photolysis in flow. Presented at *Gordon Research Conference Self-Assembly and Supramolecular Chemistry*. (Les Diablerets, Switzerland, 2019-05-19 - 2019-05-24). (LA-UR-19-24164)

Evans, A. C. Chiroptical Signatures & Photocatalytic Destruction of Organophosphorus Nerve Agents. Presented at *DTRA Tech Watch*. (Washington, District Of Columbia, United States, 2019-04-18 - 2019-04-24). (LA-UR-19-23541)

Evans, A. C. “Continuous Biocatalytic/Chiroptical Manufacturing Approaches for Making Useful Molecules". Presented at *Research Talk at UC Irvine (Host: Greg Weiss)*. (Irvine, California, United States, 2019-08-29 - 2019-08-29). (LA-UR-19-28547)

Presentation Slides

Evans, A. C. Continuous Chiroptical/Biocatalytic/Microgravity Manufacturing Approaches for Making Useful Molecules. Presented at *Betsy Cantwell Visit to LANL*, Los Alamos, New Mexico, United States, 2020-03-17 - 2020-03-17. (LA-UR-20-22387)

Plutonium Hydriding Dynamics (U)

Brian Scott
20190604ER

Project Description

This work will provide signatures for monitoring 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.

Technical Outcomes

This project made progress on two tasks. First, a Plutonium coupon was hydrided, and Raman and IR spectra were collected and compared to theoretical calculations to determine hydride and oxide speciation. Second, a laser ablation cell was designed and fabricated. Forty-one laser ablation shots were performed on tin metal targets of different thicknesses and in different atmospheres (air, hydrogen, vacuum). Temperature of the plume and emission spectra were successfully measured for each shot.

Publications

Reports

Scott, B. L. Plutonium Hydriding Dynamics. Unpublished report. (LA-UR-20-21385)

Presentation Slides

Scott, B. L., L. E. Wolfsberg, D. A. Yarotski, A. L. Pugmire, A. J. Gaunt, G. Wang, E. R. Batista and G. S. Goff. Raman spectroscopy and x-ray diffraction of plutonium oxide and hydride phases. . (LA-UR-20-21119)

Genomics to Facilitate a New Approach to Infections Disease Forecasting

Karen Davenport

20190627ER

Project Description

The overall goal is to enhance outbreak forecasting using genomic data by leveraging the integrated pair of tools, Genome Analytics for Biosurveillance (GenoSurv) and Analytics for Investigation of Disease Outbreaks (AIDO). We will build forecasting components using two different approaches. The approach through GenoSurv will build a phylogenetic tree for isolate/clinical sequence data obtained for a particular pathogen during a suspected outbreak and identify related locations where the pathogen strain is present. This information in turn will be used to select historical outbreaks from AIDO to forecast an outbreak curve for the user's outbreak. The second approach is through AIDO where a user can extract data about a particular strain of a pathogen from GenoSurv to develop a more robust similarity score, which in turn will be fed into the short term forecast feature for the unfolding situation. Real-time decision support through rapid, easy-to use, and easy to interpret analytics are much needed and this is what our project will aim to achieve. This project directly addresses the mission of global health security.

Technical Outcomes

This project resulted in the improvement of the forecast capability of AIDO and integration with a new data source, identification of pathogens from genomic data, through GenoSurv. Together this combined analytic builds the infrastructure for use of genomic data that is anticipated to become increasingly used in environmental and clinical surveillance of infectious diseases.

Publications

Posters

Kelly Graves, O. Disease Outbreak Analytics. Presented at *LAESF Mini Showcase*, Los Alamos, New Mexico, United States, 2019-08-05 - 2019-08-05. (LA-UR-19-27964)

Using Acoustic Signals from Laser-Induced Breakdown Spectroscopy Plasma Shock Waves to Identify Surface Coatings and Layers on Martian Rocks

Nina Lanza
20190628ER

Project Description

On Earth, there is a close association between life and the presence of rock coatings. As a result, coatings are an important material of interest to the National Aeronautics Space Administration's Mars 2020 rover mission. Part of the Mars 2020 mission is to identify and cache samples containing biosignatures that will be returned to Earth on a future mission. In pursuit of this goal, Mars 2020 will carry the SuperCam instrument suite, which includes a microphone for recording acoustic data from laser ablation analyses. This is a completely novel type of data with which to identify and understand rock coatings. Our goal in this project is to determine the signature of rock coatings in acoustic data to allow for a positive identification of rock coatings on Mars so that these materials may be cached for sample return and further study on Earth.

Technical Outcomes

We have found a unique acoustic signal from laser-induced breakdown spectroscopy (LIBS) analyses that can identify the presence of rock coatings under Mars conditions. This signature can be discerned at a standoff distance of ~1.3 m at a range of temperatures and laser powers. Results are applicable to future data sets from the NASA Mars 2020 rover and may be applicable to acoustic data from the Earth stratospheric environment and other laser-induced shock wave experiments.

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 the Department of Energy(DOE)/National Nuclear Security Administration(NNSA) and National Geospatial-Intelligence Agency (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

Journal Articles

Ren, C. X., A. Ziemann, J. P. Theiler and A. Durieux. Cycle-Consistent Adversarial Networks for Realistic Pervasive Change Generation in Remote Sensing Imagery. Submitted to *Proceedings of the IEEE arXiv*. (LA-UR-19-31936)

Theiler, J. P., A. Ziemann, S. Matteoli and M. Diani. Spectral variability of remotely-sensed target materials. Submitted to *IEEE Geoscience and Remote Sensing Magazine*. (LA-UR-19-25129)

Ziemann, A., C. X. Ren and J. P. Theiler. Multi-sensor anomalous change detection at scale. Submitted to *Proceedings of SPIE - the International Society for Optical Engineering*. (LA-UR-19-24295)

Conference Papers

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)

Books/Chapters

Ziemann, A. and S. Matteoli. Detection of Anomalous and Large-Scale Changes. (LA-UR-19-23173)

Ziemann, A. and S. Matteoli. Detection of Large-Scale and Anomalous Changes. (LA-UR-19-23681)

Presentation Slides

Theiler, J. P. Machine Learning for Background Estimation in Multispectral Imagery. . (LA-UR-18-30337)

Ziemann, A., C. X. Ren and J. P. Theiler. Multi-Sensor Anomalous Change Detection at Scale. . (LA-UR-19-23682)

Ziemann, A., G. Fairchild, J. R. Conrad, C. A. Manore, N. K. Parikh, S. Y. Del Valle and E. N. A. Generous. Predicting dengue incidence in Brazil using broad-scale spectral remote sensing imagery. Presented at *International Geoscience and Remote Sensing Symposium (IGARSS)*, Valencia, Spain, 2018-07-22 - 2018-07-27. (LA-UR-18-26809)

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.

Publications

Presentation Slides

Johnson, C. E., K. L. Van Buren, H. R. J. Anaya, L. J. Lynch, J. F. Vigil, E. J. Salazar and F. M. Hemez. Detonation Electric Effect Measurements in PBX 9501 and Comparison with Hydrocode Calculations. Presented at *APS SCCM 2019*, Portland, Oregon, United States, 2019-06-16 - 2019-06-21. (LA-UR-19-25524)

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.

Publications

Conference Papers

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius, N. A. Suvorova and D. M. Oschwald. Resolving the loss of crystallinity during a detonation with visible light scattering. Presented at *The APS topical meeting on Shock Compression of Condensed Matter*. (Portland, Oregon, United States, 2019-06-17 - 2019-06-17). (LA-UR-19-27100)

Presentation Slides

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius, N. A. Suvorova and D. M. (. Oschwald. Time resolving the loss of crystallinity during detonation in a secondary solid explosive. Presented at *APS March Meeting*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21854)

Bowlan, P. R., L. B. Smilowitz, B. F. Henson, D. K. Remelius, N. A. Suvorova and D. M. Oschwald. Resolving the ultrafast loss of crystallinity during a detonation with visible light scattering. Presented at *Shock Compression of Condensed Matter*, portland, Oregon, United States, 2019-06-17 - 2019-06-17. (LA-UR-19-25369)

High Efficiency Active Environmental Sampling of Chemical Traces

Sylvia Ann Junghans
20190517ECR

Project Description

The proposed work aims to deliver an active sampling matrix that enhances the Raman signature of a target analyte thereby enabling in-field analysis by handheld instruments. Successful completion of the proposed work could result in a disruptively new detection method for fast in-field analysis of traces of a multitude of Raman active chemicals (e.g. high explosives, hazardous chemicals, chemical and biological warfare agents) relevant for national security applications.

Publications

Posters

Junghans, S. A., S. Bajric, L. E. Wolfsberg, E. S. Davis, C. Pantea, G. S. Goff, B. L. Scott, R. E. Lakis and V. Henzl. High Efficiency Active Environmental Sampling of Chemical Traces. Presented at *LANL Global Security Symposium*, Los Alamos, New Mexico, United States, 2019-11-13 - 2019-11-13. (LA-UR-19-31344)

Granddaughter Radiochronometry for Nuclear Forensics

Joanna Denton
20190565ECR

Project Description

To date there have been more than 2800 cases of nuclear material being found out of regulatory control. The illegal trafficking of such nuclear material poses a serious risk to global safety and security. Once nuclear material is interdicted, the discipline of nuclear forensics, alongside traditional forensics, attempts to identify a source, destination, and suspected use for the materials. The age, of a material, obtained through radiochronometry, is a key predictive signature in a nuclear forensics investigation. Currently, the age of a material can be obtained through parent-daughter radiochronometry. This project aims to add parent-granddaughter radiochronometry to the Laboratory's nuclear forensics toolbox enabling the age of a material to become more tightly constrained. Additionally, the results of this project will shed light on the behavior of uranium decay products during material processing and production. This information can be used as vital reference points for seizures of unknown uranium materials.

Understanding the Wave Mechanics of Micro-architected Waveguides to Design Acoustic Quick Response Codes

Vamshi Chillara
20190568ECR

Project Description

This project develops a first of its kind acoustic Quick Response (QR) code system that can store information in the acoustic wave response characteristics of structures. Acoustic QR codes do not broadcast information and cannot be tampered/intruded/compromised with any existing wireless technologies. Thus, they can provide an additional layer of security for applications in nuclear proliferation and global security. The outcomes of this research effort will have applications in chemical/biomaterials characterization and energy security.

Publications

Posters

Hakoda, C. N., C. Pantea and V. Chillara. Investigation into form factors for mechanical-resonance-based methods of information storage. Presented at *APS March Meeting 2020*, Denver, Colorado, United States, 2020-03-02 - 2020-03-06. (LA-UR-20-21738)

In-Process, Full Part Defect Detection for Additive Manufacturing

Adam Wachtor
20190580ECR

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 may lead to active feedback and control of the additive manufacturing process and benefit quality control and part certification. 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.

Publications

Presentation Slides

Mellos, G. N., P. H. Fickenwirth, C. J. Montgomery, A. J. Wachtor and E. B. Flynn. Estimating Porosity of AM Constructed 304L SS Cylinders Using Process Parameters. . (LA-UR-19-26285)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, G. Guss, J. Forien, N. Calta and M. Matthews. In-Situ Process Monitoring for Defect Prediction in Laser Powder Bed Fusion. Presented at *Conference on Data Analysis*, Santa Fe, New Mexico, United States, 2020-02-25 - 2020-02-25. (LA-UR-20-21832)

Tempelman, J. R., A. J. Wachtor and E. B. Flynn. Feature Extraction of Acoustic Emissions. . (LA-UR-19-26291)

Wachtor, A. J. In-Process Quality Control of Additively Manufactured Parts. . (LA-UR-19-21711)

Wachtor, A. J., J. R. Tempelman, E. B. Flynn, G. Guss, J. Forien, N. Calta and M. Matthews. In-Situ Acoustic Monitoring of Metal Powder Bed Fusion Processes. Presented at *Cross-JOWOG on AM*, Livermore, California, United States, 2020-01-27 - 2020-01-27. (LA-CP-20-20093)

Posters

Fickenwirth, P. H., C. J. Montgomery, E. B. Flynn and A. J. Wachtor. In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing. Presented at *LANL Student Symposium*, Los Alamos, New Mexico, United States, 2019-08-06 - 2019-08-07. (LA-UR-19-27760)

Jacobson, E. M., P. H. Fickenwirth, A. J. Wachtor and E. B. Flynn. Damage Detection in Metallic Additively Manufactured Parts using In-Situ Steady-State Ultrasonic Response Data. Presented at *LANL Engineer's Week 2020*, Los Alamos, New Mexico, United States, 2020-02-20 - 2020-02-20. (LA-UR-20-21545)

Mellos, G. N., P. H. Fickenwirth, C. J. Montgomery, E. B. Flynn and A. J. Wachtor. In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing. Presented at *LANL E-Week Poster Session*, Los Alamos, New Mexico, United States, 2019-02-20 - 2019-02-20. (LA-UR-19-21306)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. . (LA-UR-19-27835)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. . (LA-UR-19-27862)

Tempelman, J. R., A. J. Wachtor, E. B. Flynn, F. Khasawneh, G. Guss, J. Forien, N. Calta and M. Matthews. Process Monitoring of Powder-bed Laser Sintering via Acoustic Signals. Presented at *Solid Free form Fabrication*, Austin, Texas, United States, 2019-08-12 - 2019-08-15. (LA-UR-19-28147)

Persistent Signatures of Neutron Fluence in Structural Materials (U)

Anthony Pollington
20190595ECR

Project Description

To this date, all nuclear weapons states including the United States of America have followed relatively similar paths to achieving a working arsenal. One of the steps that is common to all known nuclear weapons programs is the testing of material in criticality experiments. These experiments impart chemical signatures on the material around them (concrete, dirt, steel, etc.), which can potentially be measured and can be used to infer what types of activities occurred. The aim of this project is to develop and demonstrate a new capability for determining these signatures and inferring activities around critical assemblies. This will have a direct impact on the US government's nonproliferation, stockpile stewardship and nuclear forensics missions.

Technical Outcomes

This project successfully measured isotopic perturbations in uranium ores, demonstrating that they had experienced a natural neutron flux higher than that typically seen on earth. Irradiations were also carried out at the NIST Center for Neutron Research of concretes to attempt to generate similar isotopic perturbations under controlled conditions. This work was facilitated by improved analytical methods refined under this project.

Publications

Posters

Pollington, A. D., J. D. Inglis and S. M. K. Hanson. A new method for high-precision Sm isotope analyses: applications to natural and perturbed samples. Presented at *Goldschmidt Conference*, Barcelona, Spain, 2019-08-19 - 2019-08-19. (LA-UR-19-28231)

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

We 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.

Publications

Posters

Graf, S. M. and L. M. Winter. Stellar Activity from X-Ray Observations of Solar Analog Stars. Presented at *Cool Stars*, Cambridge, Massachusetts, United States, 2018-07-29 - 2018-07-29. (LA-UR-18-27050)

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.

Publications

Journal Articles

Bartlow, A. W., C. Machalaba, W. Karesh and J. M. Fair. Biodiversity and Global Health: Intersection of Health, Security and the Environment. Submitted to *Med One*. (LA-UR-19-32341)

*Bartlow, A. W., C. Manore, C. Xu, K. A. Kaufeld, S. D. Valle, A. Ziemann, G. Fairchild and J. M. Fair. Forecasting Zoonotic Infectious Disease Response to Climate Change: Mosquito Vectors and a Changing Environment. 2019. *Veterinary Sciences*. **6** (2): 40. (LA-UR-19-22170 DOI: 10.3390/vetsci6020040)

*Musgrave, K., A. W. Bartlow and J. M. Fair. Long-term variation in environmental conditions influences host–parasite fitness. 2019. *Ecology and Evolution*. **9** (13): 7688-7703. (LA-UR-18-31593 DOI: 10.1002/ece3.5321)

Wysner, T. E., A. W. Bartlow, C. D. Hathcock and J. M. Fair. Long-term phenology of two North American secondary cavity-nesters in response to changing climate conditions. 2019. *The Science of Nature*. **106** (9-10): 54. (LA-UR-18-30750 DOI: 10.1007/s00114-019-1650-9)

Presentation Slides

Fair, J. M. Bird communities and climate change. Presented at *Bird communities and climate change*, Los Alamos, New Mexico, United States, 2018-11-06 - 2018-11-07. (LA-UR-18-30737)

Fair, J. M., L. L. Jacobs, A. W. Bartlow, N. W. Hengartner, J. D. Cohn and J. L. Longmire. Phylogenetic and Functional Information Provided by Metagenomic Sequencing of California Condor Fecal and Cloacal Microbiomes. . (LA-UR-17-26676)

Improving Public Health by Linking Virus Genetic Evolution and Epidemic Spread

Arshan Nasir
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 human immunodeficiency virus (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 Department of Energy(DOE)/ National Nuclear Security Administration(NNSA) National Security mission of forecasting and predicting biological threats. We focus specifically on the US HIV epidemic, working togheter 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).

Publications

Journal Articles

Bokhari, R. H., N. NA, H. Jeong, K. M. Kim, G. Caetano-Anolles and A. Nasir. The origin and evolution of bacterial candidate phyla radiation as revealed by a phylogenomic study of protein domain structures. Submitted to *eLife*. (LA-UR-19-24949)

Nasir, A. Genetic Promiscuity in the Human Microbiome. Submitted to *Science*. (LA-UR-20-20701)

Books/Chapters

Nasir, A. and G. Caetano-Anolles. An early cellular origin of viruses. (LA-UR-19-24950)

Reports

Nasir, A., G. Caetano-Anolles and J. Claverie. Editorial: Viruses, Genetic Exchange, and the Tree of Life. Unpublished report. (LA-UR-19-28355)

Posters

Nasir, A., T. K. Leitner and E. Romero-Severson. Improving Public Health by Linking HIV Genetic Evolution and Epidemic Spread. Presented at *Sandia National Lab's Annual Postdoc Technical Showcase*, Albuquerque, New Mexico, United States, 2019-12-18 - 2019-12-18. (LA-UR-19-32531)

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 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.

Publications

Posters

Kim, H., J. Ferreras Fuertes, K. A. Krzyzanowska, K. C. Henderson, C. Ryu, D. M. Kurkcuoglu and M. G. Boshier. Progress Toward Atomtronics Sagnac Interferometer. Presented at *2019 Postdoc Research Symposium and Career Fair*, Los Alamos, New Mexico, United States, 2019-08-27 - 2019-08-29. (LA-UR-19-28645)

Biophysical Interactions of Amphiphiles with Biomimetically Patterned Membranes

Loreen Stromberg
20190614PRD1

Project Description

Many of the biomarkers involved in infectious disease, cancer, and neurotraumatic conditions are lipids. The lipidic biochemistry is critical in determining the interaction of these biomarkers with membranes (which are also lipidic), blood, and other body fluids (which are aqueous). Yet, current methods for the measurement and detection of these biomarkers completely ignore their lipid biochemistry. Because of this, there is a significant failure rate in the adaptation of such technologies for real-world applications. Characterization, measurement, and understanding of these biomarkers in a physiological context can therefore revolutionize our ability to combat many conditions of relevance to human health. In this project, we will develop an ink-jet printing based method for the characterization and measurement of such lipidic biomarkers with membrane interactions, so as to enhance our understanding of human health without the need for animal models. This combines expertise in materials science, chemistry, modeling, and biological sciences and can provide new capabilities that can stretch beyond the biological sciences and influence materials science and environmental studies as well.

Publications

Posters

Stromberg, L. R., J. H. Werner, G. A. Montano and H. Mukundan. LPS-induced bilayer deformation is modulated with increasing lipid membrane complexity. Presented at *2019 CINT User Meeting*, Santa Fe, New Mexico, United States, 2019-09-22 - 2019-09-24. (LA-UR-19-29418)

Stromberg, L. R., J. H. Werner, G. A. Montano and H. Mukundan. LPS-Induced Bilayer Deformation is Modulated with Increasing Lipid Membrane Complexity. Presented at *Biophysical Society Meeting*, San Diego, California, United States, 2020-02-15 - 2020-02-19. (LA-UR-20-21298)

Disease Outcome Analysis for Improved Disease Interventions

Paul Fenimore
20190618PRD1

Project Description

This project addresses the need for radically improved multiplexing of both biothreat agent detection schemes and disease marker measurements (biothreat detection needs are exemplified by desired improvements to the Department of Homeland Security's Biowatch program). Improved instrumentation should address both problems. Quanlitatively better data is expected to lead to important advances in our analysis of multiple markers found in serious disease states and complex biothreat monitoring samples.

Smart Mobile Sensor Platform Development for Radiological Mapping of Large-Scale Areas

Suzanne Nowicki
20190625PRD2

Project Description

With the recent developments in drone technology and relatively low-cost radiation sensors (e.g., neutron and gamma-ray sensitive sensors) coupled with well-established statistical techniques, it is possible to implement an intelligent mobile sensor platform that exhibits an active learning methodology through continuous real-time observations of radiological signatures. We propose to develop a smart mobile sensor platform composed of several drones equipped with low-cost radiation sensors to develop a network of detectors that can efficiently survey and create high-fidelity radiological maps of large-scale areas. This work will demonstrate the potential benefits of utilizing technological advancements in drone technology and low-cost radiation sensors in conjunction with advanced active learning algorithms for radiological mapping of large-scale areas. It will demonstrate how the advanced active learning framework can be developed to ultimately improve on the speed and accuracy of the results. While this research will help improve on current radiological mapping capabilities, it will more generally explore how active learning algorithms can improve any decision making process, thus providing a versatile extension to other fields of interest.

Development and Implementation of a Portable Microfluidic J-Coupled Spectrometer for Rapid Detection and Identification of Emerging Chemical Threats

Robert Williams
20190641PRD3

Project Description

This project will invent and develop new approaches for the detection of chemical warfare agents, chemical threat agents, pesticides, and insecticides. The detector is designed as a portable system that can be implemented domestically and internationally to help combat terrorism. The overarching goal of this project is to optimize a portable, fieldable detector that only uses earth's very small magnetic field to detect and identify minute quantities of chemical threats. This will be accomplished by optimizing a microfluidics-based spectrometer with a new detection system that reduces, by 10-fold, the total volume of sample required and the amount of sample in the volume by 1000-fold. This project ties into other Department of Energy national security missions by developing a unique technique for signature based, portable chemical sensing, which has important applications for military defense and homeland security.

Publications

Journal Articles

Kaseman, D., M. T. Janicke, R. K. Frankle, T. R. Nelson, G. F. Angles-Tamayo, R. J. Batrice, P. E. Magnelind, M. A. Espy and R. F. Williams. Structural Analysis of Fluorobenzenes via J-Coupled Spectroscopy at Earth's Magnetic Field. Submitted to *Journal of the American Chemical Society*. (LA-UR-19-30126)

Presentation Slides

Kaseman, D. Nuclear Magnetic Resonance of Complex Material Systems: From Glasses to Chemical Warfare Agents. . (LA-UR-19-31588)

Kaseman, D. Chemical Warfare Agents Detection via Portable Low-Field Nuclear Magnetic Resonance. Presented at *Techwatch*, Washington D.C., Virginia, United States, 2020-03-11 - 2020-03-11. (LA-UR-20-22174)

Posters

Kaseman, D., P. E. Magnelind, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. New Frontiers in Nuclear Magnetic Resonance using Earth's Magnetic Field. . (LA-UR-19-28901)

Kaseman, D., P. E. Magnelind, S. Widgeon Paisner, J. L. Yoder, A. V. Urbaitis, M. T. Janicke, M. A. Espy and R. F. Williams. A Fieldable Spectrometer Using Earth's Magnetic Field for Detection of Organophosphorus Nerve Agents. Presented at *Chemical and Biological Defense Science & Technology*, Cincinatti, Ohio, United States, 2019-11-17 - 2019-11-21. (LA-UR-19-31201)

Unraveling Lipoprotein Signatures for Tick-Borne Pathogens

Harshini Mukundan
20190655PRD4

Project Description

Vector borne pathogens present with different immunological signatures in the vector vs. the human host. These signatures are often the key towards unraveling their mode of action - be it immune evasion or activation- and lipidic molecules produced by the pathogen have a critical role to play in this response. In this project, we will use novel sensor technology together with lipoprotein measurement strategies in order to identify and unmask these critical signatures of Borrelia surface proteins, the causative agent of Lyme disease, in order to develop methods for rapid diagnostics and treatment of the infection.

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.

Technical Outcomes

We developed an additive manufacturing procedure for scintillating glass particle composites and demonstrated robotic fabrication of such a composite; this is a new capability to produce gamma-insensitive neutron detectors that can match or exceed the performance of more expensive He-3 gas tubes. We determined the impact of particle geometry, size, inter-particle separation, and volume fraction on scintillating glass particle composite performance. We investigated wavelength shifting coatings and determined the impact of fast neutron damage.

Publications

Journal Articles

*Wiggins, B. W., A. Favalli, M. L. Iliev, K. D. Ianakiev and M. P. Hehlen. Computational investigation of arranged scintillating particle composites for fast neutron detection. 2019. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. **915**: 17-23. (LA-UR-18-21568 DOI: 10.1016/j.nima.2018.10.165)

Wiggins, B. W., M. P. Hehlen, R. O. Nelson and C. G. Richards. Optical transport simulations in radiation damaged scintillating particle composite systems. Submitted to *Journal of Applied Physics*. (LA-UR-19-29565)

Conference Papers

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)

Presentation Slides

Wiggins, B. W., M. Iliev, A. Favalli, K. D. Ianakiev and M. P. Hehlen. Developments in additive manufacturing of arranged scintillating particle composites for neutron detection. Presented at *SPIE optics + photonics*, San Diego, California, United States, 2018-08-19 - 2018-08-24. (LA-UR-18-27880)

Full-Field Characterization of the Micromechanical Cues Associated with the Breakdown of the Cytoskeleton During Cancer Metastasis

Harshini Mukundan
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 signifigant 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.

Technical Outcomes

Dr. Martinez was able to develop the imaging system, and demonstrate preliminary visualization of cells using this system. Because she left the Laboratory, this demonstration was not validated.

Publications

Journal Articles

Martinez, B., A. W. Green, M. F. Silva, Y. Yang and D. D. L. Mascarenas. Sparse and Random Sampling Techniques for High-Resolution, Full-Field, Video-Based Structural Dynamics Identification. Submitted to *Structural Control & Health Monitoring*. (LA-UR-19-30846)

Martinez, B., Y. Yang, A. S. N. Liao, C. R. Farrar, H. Mukundan, P. Nath and D. D. L. Mascarenas. Full-Field Mode Shape Identification of Vibrating Structures From Compressively Sampled Video. Submitted to *Mechanical Systems and Signal Processing*. (LA-UR-19-23277)

Martinez, B., Y. Yang, C. R. Farrar, 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)

Conference Papers

Martinez, B., Y. Yang, A. S. N. Liao, C. R. Farrar, H. Mukundan, P. Nath and D. D. L. Mascarenas. 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., Y. Yang, C. R. Farrar, H. Mukundan, P. Nath 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)

Presentation Slides

Martinez, B., Y. Yang, A. S. N. Liao, C. R. Farrar, H. Mukundan, P. Nath and D. D. L. Mascarenas. 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 - 2019-01-31. (LA-UR-19-20531)

Martinez, B., Y. Yang, C. R. Farrar, H. Mukundan, P. Nath and D. D. L. Mascarenas. Full-Field Mode Shape Identification of Vibrating Structures From Compressively Sampled Video-A Unique Approach to Cancer. . (LA-UR-19-21314)

Martinez, B., Y. Yang, C. R. Farrar, P. Nath, 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 - 2019-01-31. (LA-UR-19-20642)

Posters

Martinez, B., W. E. Scott, H. Jung, M. J. Adams, K. E. Coombs, J. F. Harris, P. Nath, Y. Yang and D. D. L. Mascarenas. Extraction of Full-Field, Vibration Mode Shapes for

Structural Health Assessment using Video. Presented at *Adaptive Optics Summer School*, Santa Cruz, California, United States, 2019-08-19 - 2019-08-19. (LA-UR-19-28150)

Martinez, B., Y. Yang, C. R. Farrar, H. Mukundan, P. Nath and D. D. L. Mascarenas. Experimental Structural Dynamics of Tumorigenesis and Cancer Metastasis. Presented at *Systems and Synthetic Biology Summer School*, Pisa, Italy, 2019-07-22 - 2019-07-22. (LA-UR-19-26839)