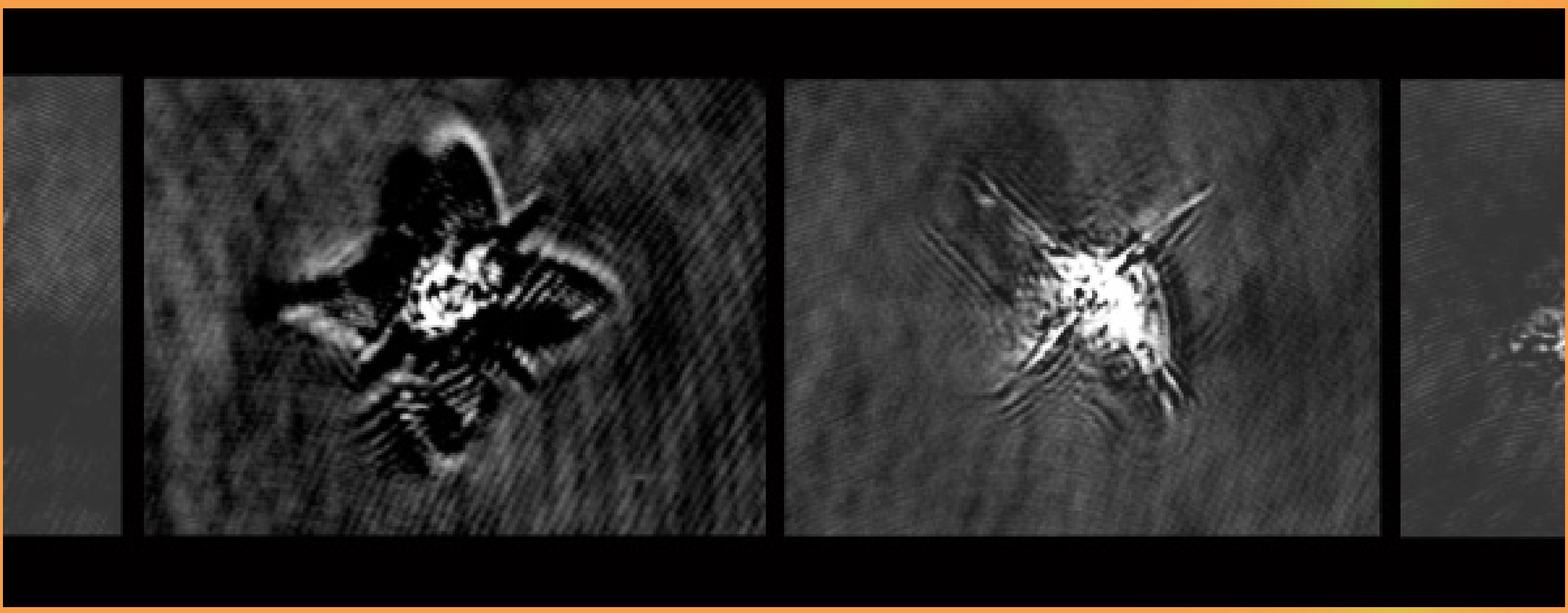
Science and Technology UPDATE

November/December 2012



A bulletin of achievements
at Lawrence Livermore National Laboratory

Published by the Office of the
Deputy Director for Science and Technology

LLNL-MI-608822

SECRETARY OF ENERGY AWARD WON FOR MARS MISSION SUPPORT

Steve Homann received a Secretary of Energy Achievement Award for his role as senior science adviser for radiological contingency planning for the Mars Science Laboratory Multi-Mission Radioisotope Thermal Generator (MMRTG) team. Steve played a lead role in deploying the MMRTG for NASA's Mars Science Laboratory **mission**, which launched on November 26, 2011, successfully delivering the rover *Curiosity* to the red planet on August 5. Ahead of the launch the MMRTG team deployed 30 air monitors in and around the Kennedy Space Center to look for the signature of plutonium-238 in the event of an emergency. (*Curiosity* has a radioisotope thermoelectric generator—a "nuclear battery"—that contains plutonium dioxide.) The monitor data was transmitted to NASA personnel and to Livermore's National Atmospheric Release Advisory Center, to generate impact assessments in the event of an accident. The Secretary of Energy Achievement Award is bestowed on a group or team of employees who together accomplished significant achievements on behalf of the Department of Energy. Steve and the rest of the MMRTG team received their awards in October via satellite broadcast as part of DOE's 35th anniversary celebration and Secretarial Honor Awards ceremony.

LAB WINS NATIONAL CYBERSECURITY AWARD

LLNL **won** a 2012 U.S. National Cybersecurity Innovation Award for proving that defenders can work together to improve security by combating advanced persistent threats through the real-time sharing of reputation data in an operational master block list (**MBL**), which is used to create filters—or "blocks"—against cyber attacks. Multiple DOE labs and plants actively share block information through the MBL tool, which was developed primarily at LLNL by a DOE team led by LLNL. The tool allows multiple DOE sites to automatically share up-to-the minute data on malicious websites and other cyber threats in real time. The MBL is currently being used by 10 agencies in DOE, and its user base is rapidly growing. The National Cybersecurity Innovation Awards recognize quickly scalable technologies that can reduce cyber risk for large numbers of people. The photo shows LLNL's Matt Myrick with NSA Information Assurance Director Debora Plunkett.

About the Cover

Different delay times between pump and probe laser shots yield different damage patterns in deuterated potassium dihydrogen phosphate optics, which are critical to fusion and other experiments on NIF. See "New Insight into Laser-Induced Crystal Damage," on page 16.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-7NA27344.

AT SUPERCOMPUTER CONFERENCE, A STRONG SHOWING BY LIVERMORE HPC, INCLUDING EDITOR'S CHOICE AWARD

The Laboratory's high-performance computing (HPC) made a strong showing among technical content and awards at Supercomputing Conference 2012 (**SC12**), held November 10–16 in Salt Lake City, Utah. A Best Student Paper Award was won by former Laboratory student Stephen Olivier, two of whose contributors were Livermore's Bronis de Supinski and Martin Schulz. Amanda Peters Randles, a Ph.D. student who worked at LLNL last summer under the DOE Computational Science Graduate Fellowship Program, received the prestigious George Michael Memorial HPC Fellowship Award. An all-female student team from the University of the Pacific—formed at the Laboratory's invitation and mentored by LLNL computational scientists—competed in the conference's Student Cluster Competition. The Laboratory's Michel McCoy (right in photo) was officially presented by HPCwire publisher Tom Tabor with the Editor's Choice Award that HPCwire gave to Sequoia in the "top supercomputing achievement" category of its 2012 **Readers' and Editor's Choice Awards**. The Laboratory's Trish Damkroger and John Grosh, who served as communications co-chair and communities chair, respectively, were among the many LLNL employees who helped organize the massive international confab.

RESEARCHER JOINS EARLY-GALAXY SEARCH USING COSMIC LENSES

Mark Ammons has joined a National Academies of Science–funded multi-institution **project** to use galaxy clusters as lenses to peer farther into the depths of space and farther back in time than any manmade telescope is capable of viewing—back to the time when the Universe's earliest stars and galaxies still were forming from the gravitational collapse of gas and dark matter. With a $600,000 grant from the National Science Foundation, University of Arizona Professor of Astronomy Ann Zabludoff and her team at Steward Observatory, along with Livermore's Mark Ammons and co-principal investigator Charles Keeton at Rutgers University, are working to find and analyze "cosmic lenses"—a lensing effect produced as light is bent by the gravity of a massive object in space.

PHYSICIST NAMED IEEE SENIOR MEMBER

Mark Rowland, a physicist in Global Security, has been named a senior member of the Institute of Electrical and Electronics Engineers (IEEE). Fewer than 8 percent of IEEE members attain this level. Mark joined LLNL in 1984 and has worked in the field of radiation detection for much of his career here. He has led Livermore teams that developed a pair of identification instruments—the Detective, to detect and measure gamma rays, and the Fission Meter, to detect and measure neutrons. These technologies, both licensed to Tennessee-based ORTEC, assist in meeting the challenges of inspecting cargo. In March 2011, when the tsunami-crippled Fukushima nuclear plant started leaking radiation, four Detective instruments were shipped to Japan within several days of the incident. The instruments were moved around the island nation and used to calibrate aerial measurement systems for about two months.

APS FELLOW ELECTED

PLS researcher Andris Dimits has been elected a fellow of the American Physical Society (APS) upon the recommendation of the APS Division of Plasma Physics. Andris was recognized for his "important insights and contributions to the theory and simulation of kinetic turbulent transport in magnetized plasmas, including the effects of self-consistent turbulence-induced velocity shear and Coulomb collisions."

CLIMATE SCIENTIST WINS AGU AWARD

PLS climate scientist Stephen Klein was one of the inaugural recipients of the American Geophysical Union (AGU) Atmospheric Sciences Section's Ascent Award "for elucidating the role of clouds in climate change and the fidelity with which climate models simulate clouds." The award was presented at the **fall AGU meeting**, held in San Francisco December 3–7. Established in 2012, the Atmospheric Sciences Ascent Award is intended to reward exceptional mid-career scientists in the fields of the atmospheric and climate sciences. The only criterion for the award is that the applicant must have demonstrated excellence in research and leadership in his or her field.

NANOLIPOPROTEIN PARTICLE TECHNOLOGY OPTIONED

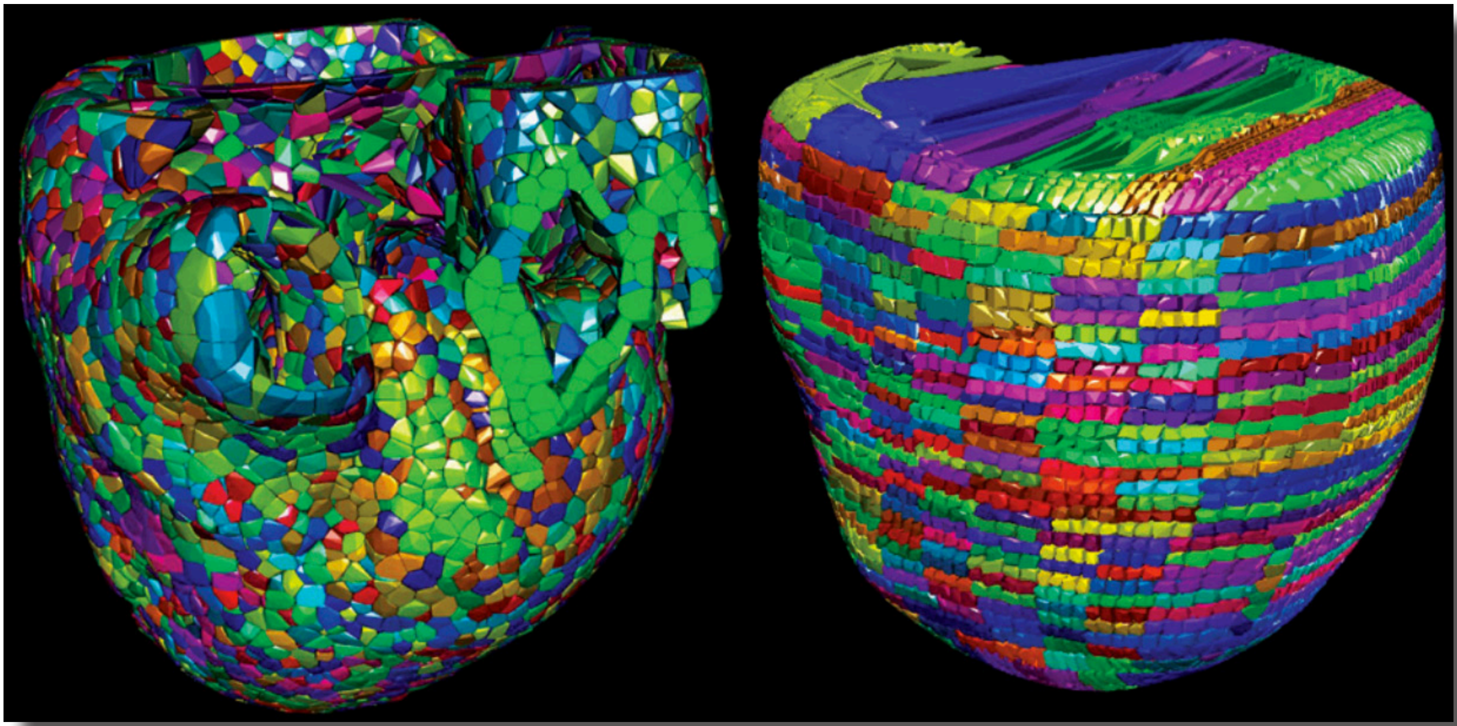
Nzyme2HC, LLC has optioned a Laboratory technology titled "Nanolipoprotein Particles for Hydrogen Production for Energy Applications." The option provides the company an exclusive, time-limited right to negotiate and execute a license agreement. Nzyme2HC, LLC is a small startup formed around LLNL technology and is based in San Clemente, California.

LAB GETS FUNDING FOR COAL GASIFICATION WORK

LLNL has received a two-year research grant to study water-quality hazard mitigation strategies for underground coal gasification (UCG) for the Department of Interior's Office of Surface Mining Reclamation and Enforcement (OSMRE). OSMRE is coordinating a working group of federal, state, and tribal regulators who are developing best-practices guidelines for granting permits for new projects. "We believe we understand the principles of clean operation," says Livermore's UCG Program Leader David Camp. "The information we develop under this $200,000 grant will help regulators do their job of assuring minimal environmental impacts." The project will be led by Joshua White, who says, "It will allow LLNL to share our significant experience and understanding of strategies to mitigate water quality hazards." According to OSMRE's Duane Matt, UCG Team Leader and Western Region applied science contact, "OSMRE is very pleased to be associated with such a laboratory like LLNL. Not only are we able to collaborate with LLNL on the development of UCG guidelines for our customers . . . but we are also able to learn more about an exciting new technology. This collaboration will serve the public by thoroughly examining this type of technology and helping them understand its possible uses."

HEART SIMULATION FEATURED IN *POPULAR MECHANICS*

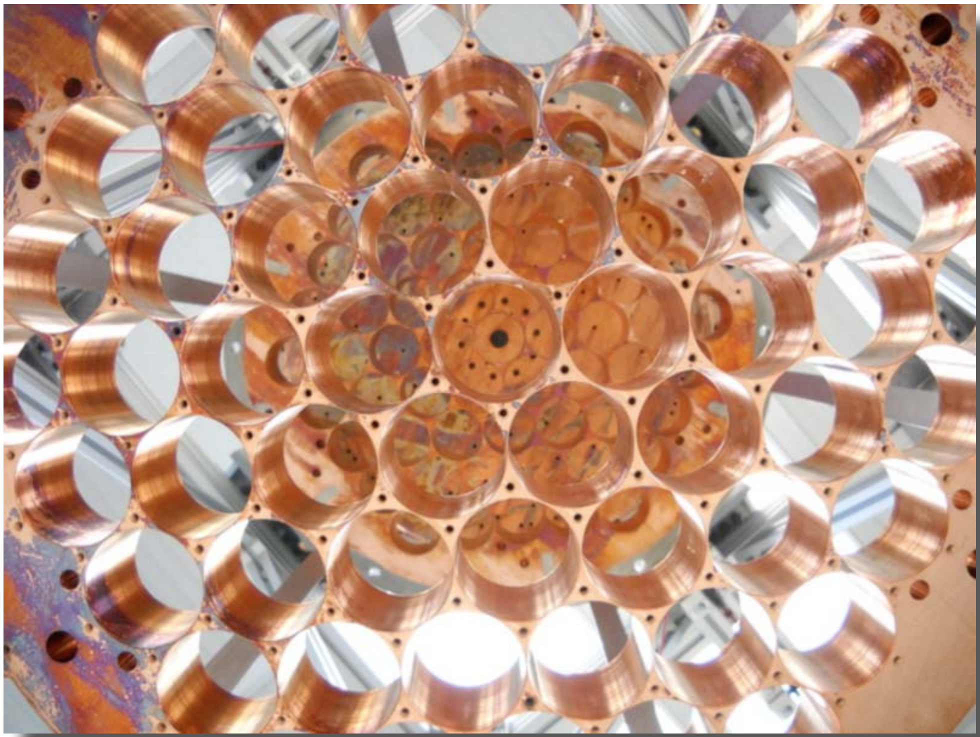
Popular Mechanics **reported** LLNL's creation of the world's fastest computer simulation of the human heart on the Sequoia supercomputer using a highly scalable code called **Cardioid**, which researchers including Art Mirin, Fred Streitz, and Dave Richards created along with IBM. Lab scientists have modeled the electrical signals travelling from cell to cell, triggering them to contract. Art et al. revealed their results publicly for the first time on November 13 at the **SC12** conference, where the team was one of five finalists for the Gordon Bell Prize. The figure below, used in the *Popular Mechanics* story, illustrates how Cardioid computationally divides the human heart into numerous subdomains.



DARK-MATTER DETECTOR LOWERED INTO POSITION—A MILE UNDERGROUND

In November, researchers at the Large Underground Xenon (LUX) experiment lowered the world's most sensitive dark matter detector into position nearly a mile underground in a former South Dakota gold mine that today is the Sanford Underground Research Facility. A key component on the ultrasensitive detector is the copper photomultiplier tube mounting structure (shown in the photo), which was designed and built by LLNL. Livermore researchers have been involved in the LUX experiment since 2008. "We at LLNL initially got involved in LUX because of the natural technological overlap with our own nonproliferation detector development programs," said Adam Bernstein, who leads Livermore's Advanced Detectors Group.

Groundbreaking work that set the stage for LUX was supported by LDRD, including an early project (07-ERD-056) and a later strategic initiative (10-SI-015) that Adam led as principal investigator.



LAB'S PATHOGEN-DETECTION TECHNOLOGY AMONG FASTEST IN INTERNATIONAL EXERCISE

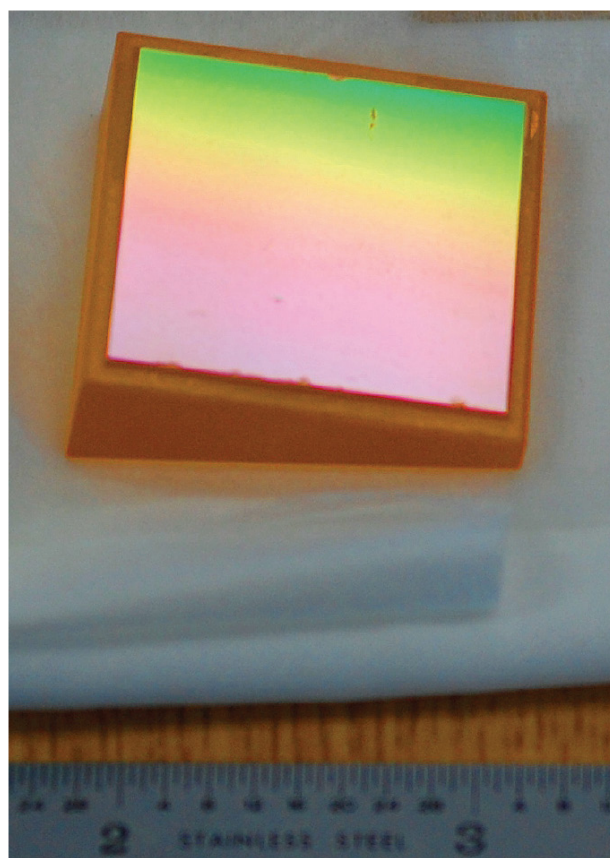
An LLNL team used the Lawrence Livermore Microbial Detection Array (LLMDA) to successfully identify unknown pathogens during an international exercise this fall. In the exercise, which was hosted by Canada and the U.K., participants from the U.S., France, Germany, Italy, and Mexico were sent unidentified tissue samples spiked with nucleic acids from harmless vaccine strains of several viral pathogens. The purpose was to allow countries to exercise their techniques, compare results, and establish connections that could prove useful the next time a new pandemic appears. The LLMDA, containing more than 720,000 DNA probes capable of identifying all sequenced viruses and bacteria, successfully detected Rift Valley fever virus in the bovine and human blood samples. The LLMDA was among the first techniques to produce correct results, taking only 72 hours to do so, in contrast with the 8 to 13 days required by other techniques. Said Computation's Tom Slezak, "It was an excellent forum for discussing how to deal with unknown pathogens and for promoting international collaboration among expert labs." Since September, the Centers for Disease Control's Bioterrorism Rapid Response and Advanced Technology Laboratory and the U.S. Army Medical Research Institute of Infectious Diseases have begun a two-year evaluation of LLMDA, working closely with the LLNL developers. "This should allow LLMDA to be used on a variety of real-life unknown samples available to these groups, as well as for a large set of controlled testing to validate performance," Tom said.

TWO AAAS FELLOWS NAMED

Chris Keane and Jane Long have been named fellows of the American Association for the Advancement of Science (AAAS). Election as a fellow is an honor bestowed upon AAAS members by their peers to recognize distinguished efforts to advance science or its applications. Chris is recognized for "distinguished technical and scientific leadership in developing inertial confinement fusion and high-energy-density science, and leading a robust global science community in this area." He serves as director of the NIF User Office. Jane Long has been recognized by AAAS for "distinguished contributions to assessing the societal implications of technology development, including in areas of climate change, geoengineering, nuclear waste and energy technology." Recently retired from LLNL, Jane is a senior contributing scientist for the Environmental Defense Fund, visiting researcher at UC Berkeley, consultant for geoengineering at the Bipartisan Policy Center, and chair of the California Council on Science and Technology's California's Energy Future committee. The awards will be presented in February 2013 at the AAAS 2013 Annual Meeting, to be held February 14–18 in Boston.

LLNL-MACHINED OPTIC TO FLY ON JAMES WEBB SPACE TELESCOPE

Using unique in-house capabilities, LLNL engineers have produced a zinc selenide grism (optical dispersing element) for a Canadian infrared imager and spectrograph to be integrated onto NASA's James Webb Space Telescope, an infrared-optimized space **telescope** that will look for the first galaxies that formed in the early Universe. The grism was fabricated on the Precision Engineering Research Lathe (**PERL**), an LLNL-built diamond turning machine. Although built in the 1980s, this R&D 100 Award-winning system still represents the state of the art in machining accuracy. The Canadian Space Agency came to LLNL after unsuccessful attempts by commercial vendors to fabricate this optical component. The spectrograph will have the capability of determining the atmospheric composition of Earth-like exoplanets. Detection of oxygen and water vapor in those atmospheres would provide a strong indication of the presence of life.

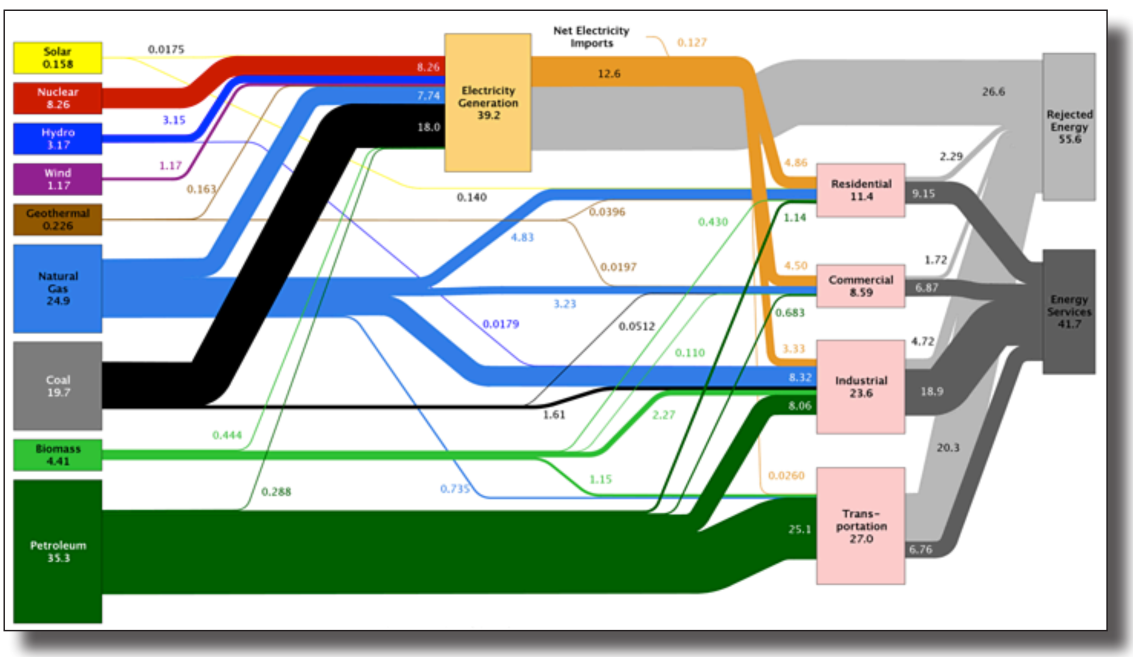


NUCLEIC ACID DETECTOR TECHNOLOGY LICENSED

Corporos, Inc. has optioned LLNL technology for the point-of-care detection of nucleic acid in samples. The option applies to the field of pathogen detection. Corporos, Inc. is a startup located in Berwyn, Pennsylvania, that develops and tests point-of-care detectors for use in food safety and biosecurity.

LATEST VERSION OF "FAMOUS" ENERGY FLOWCHARTS RELEASED

LLNL released the latest versions of the energy-use **flowcharts** that have gained worldwide attention for their visually simple presentation of American energy use. According to the new figures, wind power saw the biggest jump between 2010 and 2011—from 0.92 quadrillion BTU (quad) to 1.17 quads. "Wind energy jumped significantly because, as in previous years, many new wind farms came online," said A. J. Simon, an LLNL energy systems analyst who develops the flowcharts using data provided by DOE's Energy Information Administration. "This is the result of sustained investment in wind power."



R&D 100 AWARD-WINNING TOOL DEBUGS MILLION-PROCESS PROGRAM ON SEQUOIA

LLNL researchers have used the Stack Trace Analysis Tool (**STAT**)—a highly scalable, lightweight tool—to debug a program running more than one million processes on the IBM Blue Gene/Q-based Sequoia supercomputer. The debugging tool is a significant milestone in LLNL's multiyear collaboration with the University of Wisconsin, Madison, and the University of New Mexico to ensure supercomputers run more efficiently. STAT, a 2011 R&D 100 Award **winner**, has helped both early access users and system integrators quickly isolate a wide range of errors, including particularly perplexing issues that only manifested at extremely large scales of up to 1,179,648 cores. Sequoia delivers 20 petaflops of peak power and was ranked No. 1 on the TOP500 list in June of this year. It is currently ranked No. 2, behind Oak Ridge National Laboratory's Titan.

As LLNL takes delivery of the Sequoia system and works to move it into production, computer scientists will migrate applications that have been running on earlier systems to this newer architecture. Said Kim Cupps, leader of the High-Performance Computing Division: "Having a highly effective debugging tool that scales to the full system is vital to the installation and acceptance process for Sequoia. It is critical that our development teams have a comprehensive parallel debugging tool set as they iron out the inevitable issues that come up with running on a new system like Sequoia."

NEUTRON-DETECTING PLASTIC WINS AWARD

The world's first-ever plastic capable of efficiently distinguishing neutron radiation from gamma rays—developed by LLNL researchers—was awarded first place in the nuclear and radiation detection category of *Government Security News* **magazine**'s fourth annual Homeland Security Awards competition. The award was presented at a November 29 dinner in Washington, D.C., attended by more than 200 government officials and business leaders. The material was developed by a team led by Steve Payne and Natalia Zaitseva. With its low cost, the material could be fashioned into huge plastic sheets for dramatically larger surface areas than is possible with any other neutron detector currently available. The technology has already been licensed to **Eljen Technology**, a Texas-based scintillator company.

$2.75M FROM NASA–OFFICE OF SCIENCE HED PROGRAM

NNSA and the Office of Science have **awarded** more than $14 million in research awards as part of their Joint Program in High-Energy-Density (HED) Laboratory Plasmas, of which six LLNL researchers have received nearly $2.75 million for their projects. A total of 147 project proposals were received in response to the call. After an evaluation process that included a rigorous peer review by outside experts, 37 projects were selected for funding, with the awards ranging from one to three years. The LLNL principal investigators chosen are Brian Wilson (to study the electronic structure of warm, dense matter), Prav Patel (fast ignition HED science), Scott Wilks (isochoric heating of reduced-mass targets), Hye-Sook Park (measuring magnetic fields in collisionless shocks), Jave Kane (scaled Eagle Nebula experiments on NIF), and Yuan Ping (x-ray absorption fine structure study of electron–ion equilibration in warm dense matter).

ACADEMY OF SCIENCES EARTHQUAKE SHOW SELECTED AS FINALIST FOR NSF AWARD

The full-dome show "Earthquake: Evidence of a Restless Planet" at the California Academy of Sciences in Golden Gate Park uses 3-D earthquake simulations and earth-structure visualizations that were developed by Arthur Rodgers and a team of LLNL seismologists and computer scientists (Christina Morency, Nathan Simmons, Anders Petersson, Bjorn Sjogreen, Michael Loomis, and Rich Cook), working with Cheryl Vanderbilt at the California Academy of Sciences. Now this show has been selected as a finalist in the National Science Foundation's 2012 International Science and Engineering Visualization Challenge. There are ten finalists in the "video" category, and the winner will be determined by public votes.

RESEARCHERS ELECTED TO PLASMA EDGE COMMITTEE

During the October 29–November 2 meeting of the American Physical Society's Division of Plasma Physics (APS-DPP), the DOE Office of Fusion Energy Sciences Edge Coordinating Committee (**ECC**) elected Ilon Joseph to a two-year term as vice chair, to be followed by a two-year term as chair beginning in 2014. In addition, Maxim Umansky was elected to a three-year term as a member of the ECC. The Office of Fusion Energy Sciences created the ECC in 2004 to identify and prioritize key edge-plasma issues for magnetic fusion energy devices and to facilitate collaborations between national experimental groups and international fusion programs. The ECC, which consists of 14 members from the U.S. magnetic fusion energy community, plus an ex officio Office of Fusion Energy Sciences representative, holds two business meetings yearly and also holds a one-day, special-topic workshop.

LLNL CO-SPONSORS 12TH INTERNATIONAL WORKSHOP ON FAST IGNITION

Pravesh Patel (PLS) co-chaired the 12th International Workshop on Fast Ignition of Fusion Targets in Napa Valley, November 4–8. The **workshop** is held every two years, rotating between the U.S., Europe, and Asia. This year's workshop was co-hosted by LLNL and UC San Diego and attended by 85 scientists, postdocs, and students working on the fast-ignition scheme for inertial confinement fusion. The workshop's main topics were integrated, sub-scale, fast-ignition coupling experiments; progress towards developing an ignition point design based on fast electron or ion heating; and experimental validation of the simulations and underlying physics of relativistic-intensity laser–plasma interaction. Overview talks reported on progress of integrated experiments at the Laboratory of Laser Energetics, the Gekko XII facility in Japan, and the Shenguang II facility in China. Livermore's L. J. Perkins gave a plenary talk on advanced ignition concepts for NIF.

LIVERMORE HPC REPRESENTED AT COMPUTING-IN-SEISMOLOGY CONFERENCE

Steve Bohlen, Deputy Director of the Laboratory's Energy and Environmental Security Program, represented LLNL at a meeting of the National Academy of Sciences Committee on Seismology and Geodynamics on the use of high-performance computing (HPC) in the field of computational seismology and geodynamics. The meeting was held November 19 in Washington, D.C., and focused on creating awareness of the needs of the community in using HPC to advance seismology and geodynamics and the potential for the community to partner with Livermore and other DOE labs to achieve that goal.

RAPID PCR TECHNOLOGY OPTIONED

Livermore executed an option agreement with Velocity Diagnostics, LLC, for an LLNL polymerase chain reaction (PCR) **technology** titled "PCR Amplification under Three Minutes." The option agreement gives the company the right to negotiate an exclusive, time-limited license in the fields of human diagnostic testing, veterinary diagnostics, agriculture product testing, and food testing. Velocity Diagnostics is a startup located in Morristown, New Jersey, and will be commercializing the PCR amplification technology for use in diagnostics and product testing.

LLNL LEADS NEW INITIATIVE TO IMPROVE LITHIUM-ION BATTERIES

A multi-institution team led by LLNL has won a five-year, $3.7 million award from DOE's Office of Basic Energy Sciences and Office of Advanced Scientific Computing Research to develop a new methodology for performing first-principles quantum mechanical simulations on an unprecedented scale, and to use that methodology to understand key aspects of the chemistry and dynamics of lithium-ion batteries. A successful outcome will pave the way for substantial advances in battery performance and lifetime. The team, led by LLNL physicist John Pask, brings together physicists, chemists, applied mathematicians, and computer scientists from LLNL and Lawrence Berkeley National Laboratory, including two postdocs. Lithium-ion batteries have revolutionized electrical storage, but progress beyond the current state of the art has been hindered by an incomplete understanding of the basic chemistry and dynamics. Today, however, the combination of state-of-the-art quantum mechanical methods, such as LLNL's Qbox code at LLNL; the new "discontinuous Galerkin" electronic structure methodology being developed jointly at LLNL and LBNL; and the two laboratories' leadership-class computing facilities permits a fully quantum mechanical treatment of the length and time scales required to capture essential aspects of a lithium-ion battery, without recourse to empirical schemes.

SCIENTIST TO SERVE ON AMS RENEWABLE ENERGY SUBCOMMITTEE

Atmospheric scientist Sonia Wharton has been selected as one of seven new members of the American Meteorological Society's Renewable Energy Subcommittee. The primary goal of the subcommittee is to bring together the weather, climate, and energy communities to facilitate dialog about the respective needs and responsibilities of the public, private, and academic sectors in providing the environmental sciences data required for the increased use of renewable energy in the nation. A secondary goal is to encourage the education and development of the future pool of workers to support the renewable energy community. Sonia will serve a 3-year term on the subcommittee.

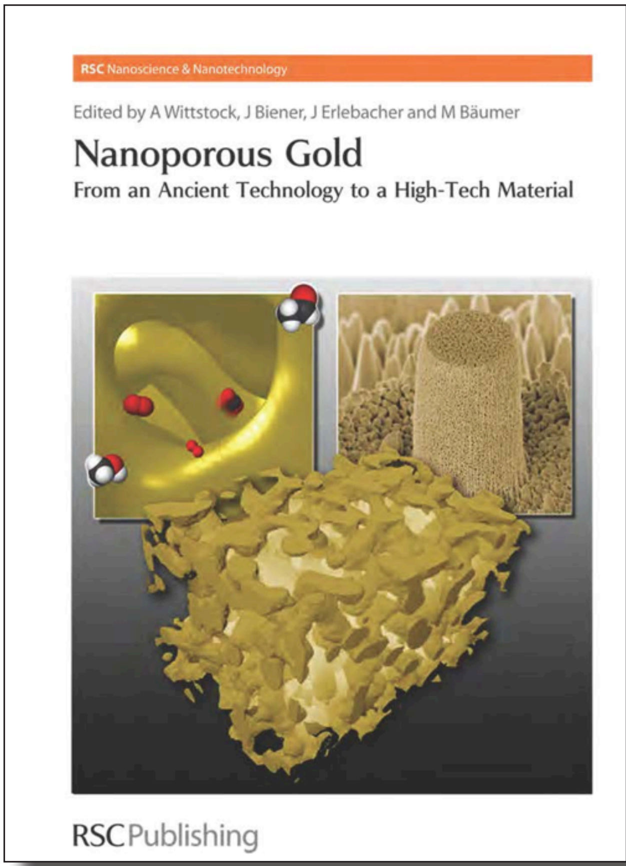
LLNL AUTHORS DELIVER "BEST PRESENTATION" AT GEOTHERMAL MEETING

At the Geothermal Resources Council's 36th Annual Meeting, held in Reno, Nevada, September 30–October 3, an LLNL–Princeton University presentation titled *Integrated Geothermal–CO_2 Storage Reservoirs: Adaptable, Multi-Stage, Sustainable, Energy-Recovery Strategies That Reduce Carbon Intensity and Environmental Risk* was chosen as one of the 15 best presentations (out of 214) at the meeting. The authors of the work were Thomas A. Buscheck, Thomas R. Elliot (Princeton), Michael A. Celia (Princeton), Mingjie Chen, Yue Hao, Chuanhe Lu, and Yunwei Sun.

LICENSEE EXHIBITS AT CONFERENCE ON ANTI-IED TECHNOLOGY

LLNL licensee Field Forensics was an invited exhibitor at a three-day conference in September in Mumbai, India, focused on state-of-the-art solutions for countering improvised explosive devices (IEDs). High-level speakers at the conference represented the Indian government, U.S. Pacific Command, and military staff from the New Zealand Defense Force, the European Union, and the Association of Southeast Asian Nations, among others. Field Forensics demonstrated its explosive trace detector products based on Livermore's **ELITE** technology, which the company exclusively licensed in 2007.

BOOK ON NANOPOROUS GOLD

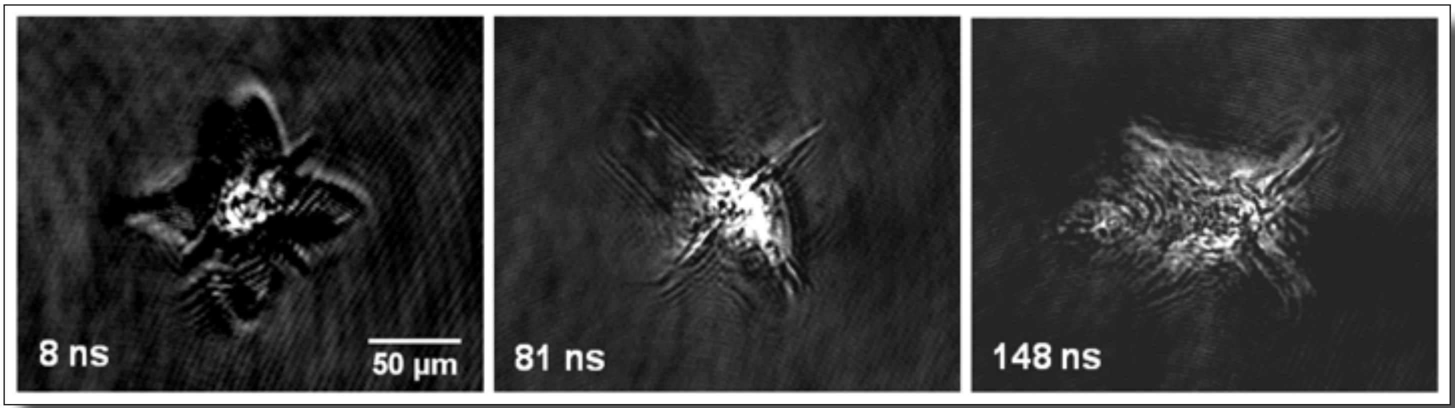


Jüergen Biener and Arne Wittstock, together with colleagues from Johns Hopkins University and Germany's Institute of Applied and Physical Chemistry, are editors of a **new book** titled *Nanoporous Gold: From an Ancient Technology to High-Tech Material*. Nanoporous gold has been intensively investigated in recent years because of its promise for numerous applications. This book provides an up-to-date, multidisciplinary exposition of the synthesis and properties of nanoporous gold and covers both experiment and theory. In addition to serving as co-editors, Jüergen and Arne co-authored the introductory chapter and a chapter on surface chemistry and catalytic properties.

NEW INSIGHT INTO LASER-INDUCED CRYSTAL DAMAGE

Deuterated potassium dihydrogen phosphate (DKDP) crystals are used for frequency conversion and beam control in high-power, large-aperture laser systems such as NIF. Exposure to high laser energies increases the materials' localized temperature and pressure, which can lead to irreversible material damage. In an **article** published in *Optics Express*, Raluca Negres and other LLNL researcher report on studies that have provided new insights into the dynamics of transient changes in the optical properties of bulk DKDP material.

Understanding the electronic and optical properties of these transient phases is important for the fundamental understanding of material response under extreme conditions as well as for the optimization of current or near-future laser applications. The research provides the basis for future studies to better understand and control the energy deposition of laser power in materials and the behavior of optical materials for high-power laser systems. The figure gives typical ratio images of intrinsic bulk damage in DKDP, indicating how damage varies depending on the delay time between pump and probe.

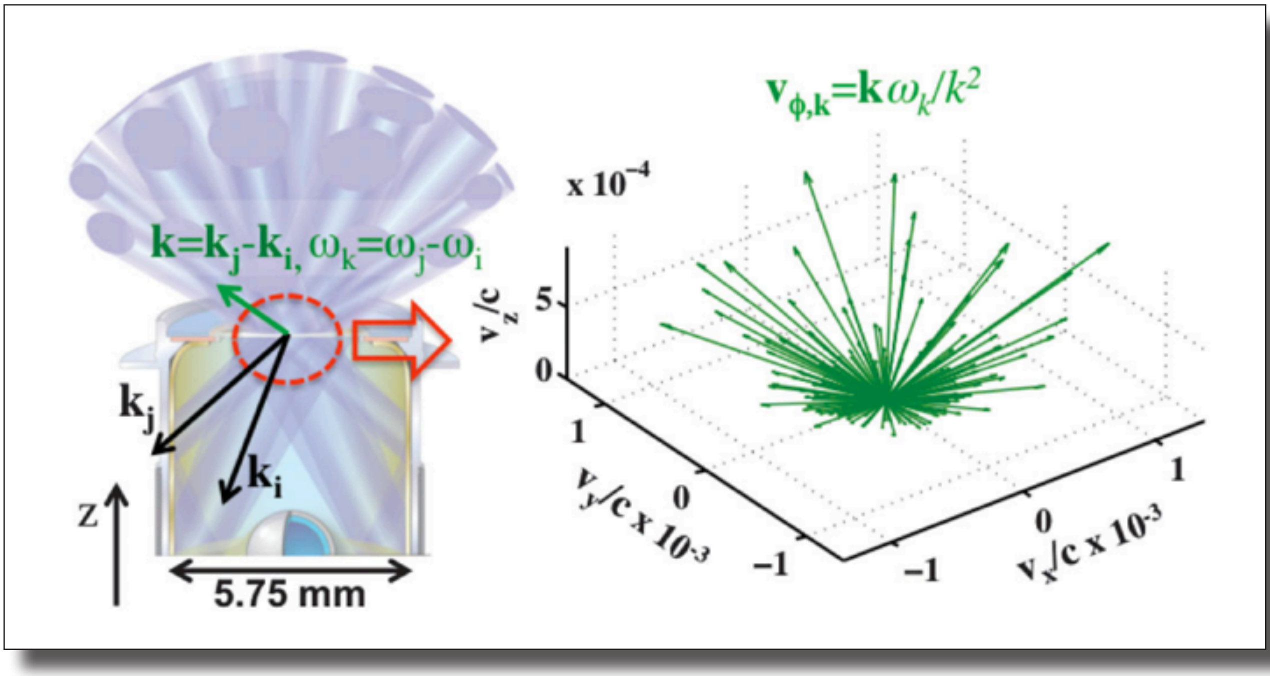


ION-HEATING PAPER IN *PRL* IS HIGHLIGHTED ON APS SYNOPSIS

An LLNL-authored **paper** published in the November 11 edition of *Physical Review Letters* was chosen by the editors of the American Physical Society (APS) journals to be **featured** on the APS Synopsis website. In the paper, Livermore's Pierre Michel and colleagues show that the interference of different laser frequencies can mitigate some of the problems of cross-beam transfer and strongly heat plasma ions. In their simulations—modeled after experiments done at NIF—beat waves adjusted in groups create electrostatic potentials that push the ions around and heat the plasma. The authors calculated the time evolution of the ion-velocity distribution and its effect on cross-beam transfer. They find that the energy is redistributed very quickly and that saturation effects cause the cross-beam transfer to stabilize within nanoseconds. The analysis suggests that with proper control of the beat waves, input-laser energy losses could be reduced and the plasma more efficiently heated to temperatures up to 45 million kelvin. The figure shows (left) the upper half of a NIF hohlraum, where 96 of the 192 NIF laser beams, grouped in 24 quadruplets, overlap to produce 276 possible individual pairs. Each pair of quads drives a beat wave, represented on the right (green arrows).

NEW FRAMEWORK TO INTERPRET FORCE SPECTROSCOPY

In a **paper** published in *Proceedings of the National Academy of Sciences*, Alex Noy, former LLNL researcher Jim De Yoreo (now at LBNL), and a Sandia colleague show that a model involving only a single energy barrier can explain the observed force-spectroscopy systematics of dynamic force spectroscopy, which allows researchers to characterize the microscopic basis of inter- and intra-molecular bonding in a simple experiment. Their new model considers two fundamental regimes of bond rupture: a near-equilibrium regime, produced either by bond reforming in the case of a single bond or by asynchronous rupture of multiple individual bonds, and a kinetic regime produced by fast, non-equilibrium bond rupture. Data from 10 different molecular systems show that the new interpretation provides a comprehensive description of force spectra for a diverse suite of bonds over experimentally relevant loading rates and eliminates the inconsistencies present in previous explanations. Furthermore, the approach allows determination of the equilibrium free energy of a bond, which means that the single-molecule binding free energies for a vast number of bonds, as already measured by previous force-spectroscopy measurements, can now be utilized.

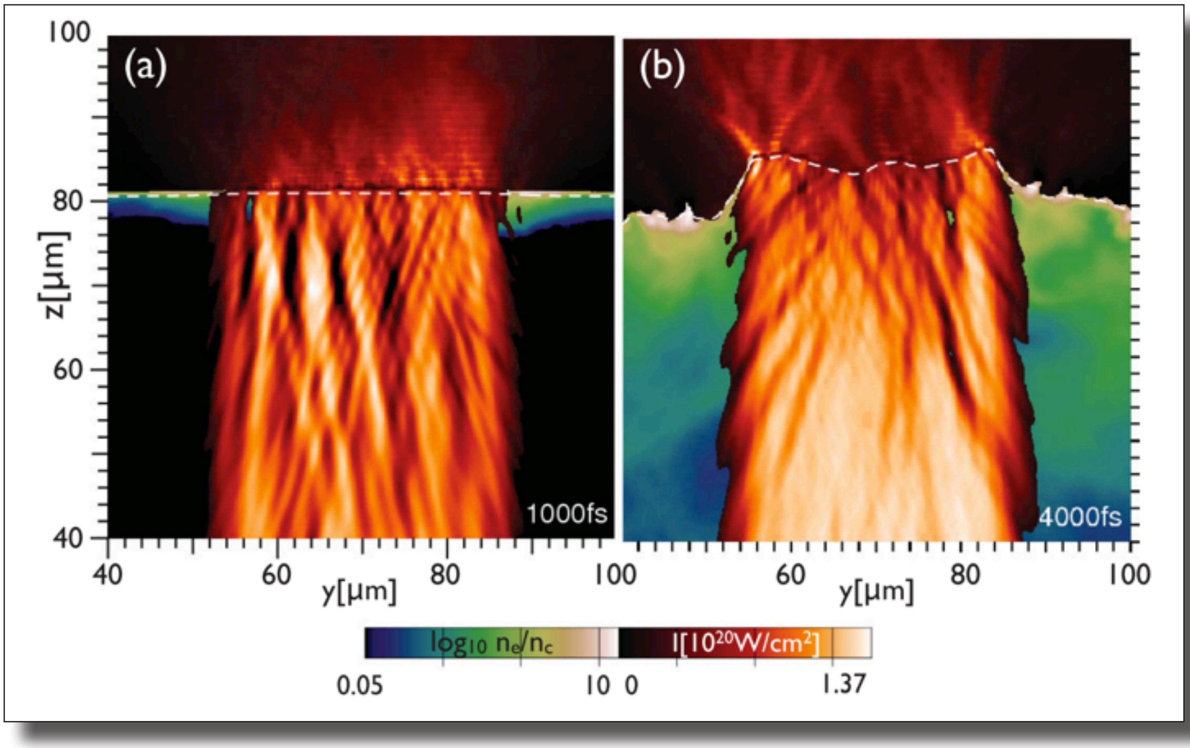


PAPER IN *PRL* ON ENERGY DISTRIBUTION OF FAST ELECTRONS FOR FAST IGNITION

In the November 8 edition of *Physical Review Letters*, physicists Andreas Kemp and Laurent Divol **report** on the physics of the interactions between petawatt laser pulses of a few picoseconds duration with overdense plasma. Using the results of two- and three-dimensional kinetic particle simulations, the authors show how nonlinear saturation of laser-driven density perturbations at the target surface causes recurrent emissions of plasma, which stabilize the surface and cause absorption of the laser energy to remain high. These dynamics lead to the acceleration of three distinct groups of electrons up to energies many times the laser's ponderomotive potential. The resulting energy distribution and divergence of the laser-generated electron beam has important implications for applications such as the fast-ignition approach to inertial confinement fusion. The figure shows a relativistic petawatt laser pulse interacting with overdense plasma at 1 ps (a) and 4 ps (b), with energy flux density along *z* (in red) showing continuously high conversion from the laser into a relativistic electron beam.

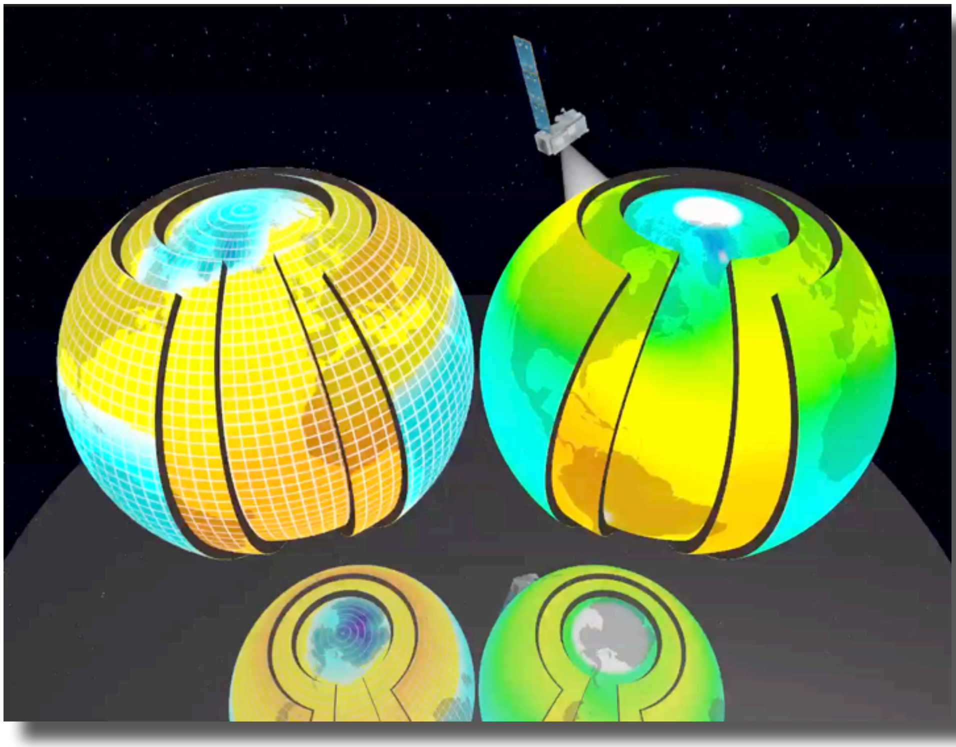
POSSIBLE PATH TO TABLETOP EXPERIMENTS ON DYNAMIC COMPRESSION

A Lab team including Michael Armstrong and Jonathan Crowhurst, along with a collaborator at the Carnegie Institution of Washington's Geophysical Laboratory, recently published a **conceptual article** on the prospects for achieving high dynamic compression with low energy in *Applied Physics Letters*. The study establishes a lower bound to the reduction of length, time, and energy scales in dynamic compression experiments, and shows that in materials with picosecond equilibration times, some types of experiments may be possible with orders-of-magnitude less drive energy than currently used. Simulations performed by the team under an LDRD-funded project show that the compression energy for geometrically similar experiments varies as the third power of the time scale of compression. In many cases, dynamic compression experiments require large-scale laser systems to obtain extreme conditions in materials, and so reducing the energy required to a scale achievable by tabletop laser systems would enable substantially higher throughput, as well as more extreme conditions for a given drive energy.



Signal of Human-Caused Climate Change Detected in the Noise

Atmospheric scientist Benjamin Santer is lead author of a **paper** published in *Proceedings of the National Academy of Sciences* describing a 17-organization team's comparison of 20 different computer models to satellite observations, which concludes that tropospheric and stratospheric temperature changes are clearly related to human activities. The new climate model simulations analyzed by the team will form the scientific backbone of the upcoming 5th assessment of the Intergovernmental Panel on Climate Change, due in 2014. Both satellite observations and simulations show the lower stratosphere cooled markedly over the past 33 years, primarily as a response to the human-caused depletion of stratospheric ozone. The observations and model simulations also show a common pattern of large-scale warming of the lower troposphere, with the greatest warming over the Arctic and muted warming over Antarctica. Tropospheric warming is mainly driven by human-caused increases in well-mixed greenhouse gases. "It's very unlikely that purely natural causes can explain these distinctive patterns of temperature change," said Ben. The figure is a screen capture of an **animation** depicting atmospheric temperature change in different atmospheric layers over a 32-year period (1979–2011) as simulated with a model (left) and based on satellite observations (right).

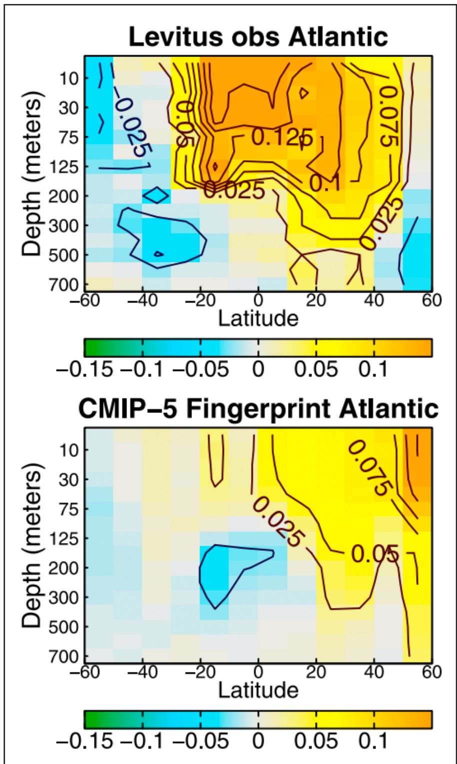


Evaluation of Historical Beryllium Abundance Published

Lab researchers Mark Sutton, Richard Bibby, Gary Eppich, Steven Lee, Rachel Lindvall, Kent Wilson, and Brad Esser have published, in *Science of the Total Environment*, an **evaluation** of historical beryllium abundance in soils, airborne particulates, and LLNL facilities. LLNL soils and airborne particulates have been collected and analyzed for hazardous and radioactive contamination for more than 30 years. This new study compared historical data with multi-element analyses of archived samples and recently collected facility carpet dust. Using the ratio of beryllium to correlated elements allows the discrimination of natural versus process-induced beryllium in the workplace. Beryllium in soils at the main LLNL site is typical both with respect to its concentration and its correlation to other metals relative to local and US soils. Soil at the Lab's Site 300 contains a higher level of beryllium, likely due to the difference in soil type. Analysis of historical air filters shows that LLNL's beryllium work has had negligible impact on the beryllium content of airborne particulates at both the main site and at Site 300. The study's authors recommend that other beryllium-handling facilities use multi-element analysis and multiple elemental marker ratios to supplement current beryllium surveillance activities.

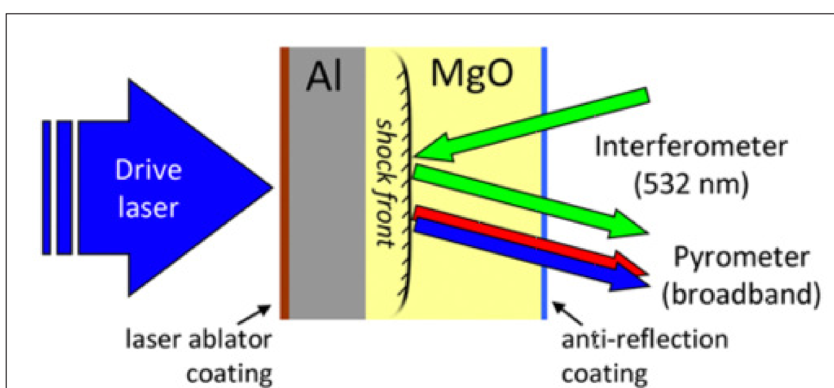
IN OCEAN SALINITY, HUMAN FINGERPRINT IN CLIMATE CHANGE

According to a **new study** by researchers at LLNL and Scripps Institution of Oceanography, changes in ocean salinity over the second half of the 20th century are consistent with changes driven by human activities and are inconsistent with natural climate variations. Observed salinity changes agree with what computer models have suggested would happen to salinity patterns in a warming world. Salinity observations over the second half of the 20th century show an intensification of existing patterns. These suggest that salty ocean regions have experienced even more evaporation, becoming saltier, and relatively fresh regions have becoming even more diluted with precipitation because of global changes in precipitation and evaporation. This study, say its authors, provides an independent check of the effects of climate change on the global water cycle using completely different instruments and techniques than with land-based rainfall measurements. Studies of rainfall changes over land are harder to place in context of climate change because of the episodic nature of storms, which bring rainfall to land areas, and changes to the observing network over the years. “Salinity in the ocean averages out all that variability,” said lead author David Pierce, of Scripts.



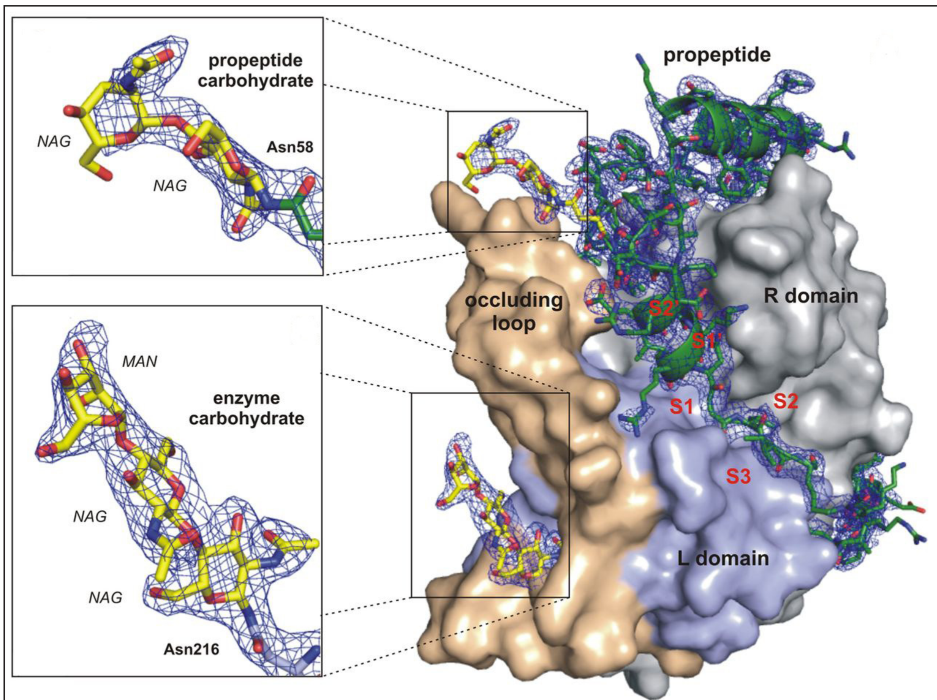
SCIENCE PAPER CONFIRMS METALLIC LIQUID STATE OF MAGNESIUM OXIDE

Until now, researchers have struggled to reach the pressures and temperatures needed to validate predictions of how magnesium oxide (MgO) behaves in planetary interiors. In a **paper** published in *Science*, a team of researchers from LLNL, the Carnegie Institution of Washington, and UC Berkeley report on laser-driven shock-compression experiments on MgO in which they used the Lab’s Jupiter Laser Facility and the Omega Laser Facility at the University of Rochester to generate pressures exceeding 1.4 TPa and temperatures of about 50,000 K. They confirmed that MgO transforms into a metallic liquid at 0.65 TPa and 14,000 K. This finding has major ramifications for understanding how planetary magnetic fields are generated, such as whether a large rocky planet lacking molten iron inside it might still have enough metallic molten MgO to generate a magnetic field, which protects against harmful radiation and helps retain an atmosphere, both of which make a planet more conducive to life. Lead author and Carnegie Institution researcher Stewart McWilliams, who did his Ph.D. thesis research at LLNL, says, “Our findings blur the line between traditional definitions of mantle and core material and provide a path for understanding how young or hot planets can generate and sustain magnetic fields.” The figure is a schematic of the laser-shock experiments, showing the drive laser impinging on an aluminum (Al) buffer plate to which the MgO sample is attached.



FIRST-EVER DETERMINATION OF PROTEIN STRUCTURE WITH X-RAY LASER

An international team of researchers, including LLNL physicist Matthias Frank and postdoc Mark Hunter, have for the first time used an ultra-intense x-ray laser to determine the previously unknown atomic-scale structure of a protein. The work was **reported** in the online edition of *Science*, which also **featured** the story as a News Flash. The team determined the structure of an enzyme key to the survival of the single-celled parasite, *Trypanosoma brucei*, responsible for African sleeping sickness, a disease that kills 30,000 people each year. This new structural information should help guide the search for drugs that act like the propeptide, tying up the enzyme and killing the parasite. To determine the structure of the precursor form of the protein—which does not form crystals large enough for traditional x-ray diffraction—submicron nanocrystals produced by the parasite were analyzed by the "diffraction before destruction" technique, in which individual nanocrystals are passed, one by one, through the x-ray beam at the Linac Coherent Light Source, followed by "stacking" of the resultant diffraction data—in this case, from 178,875 individual nanocrystals. The achievement also demonstrates that the approach can provide otherwise unobtainable biomolecular information, potentially ushering in a new era of protein crystallography. Livermore researchers—whose participation in the research is supported by the LDRD Program—include the development of the nanoparticle injectors, setting up laser pump probe experiments, sample preparation, damage modeling, and data acquisition at the LCLS. The figure shows the quality of the electron density (blue) in the calculated structure.



NEW TECHNIQUE YIELDS POWERFUL—AND STABLE—EXPLOSIVE

Philip Pagoria and colleagues from LLNL and the University of Michigan **describe**, in *Crystal Growth & Design*, how a technique for engineering medicines and other materials—cocrystallization—has yielded an improved explosive. Cocrystallization involves combining two materials into a new crystal architecture with the goal of producing an improved material. The team has cocrystallized a standard military explosive, HMX, with a powerful explosive called CL-20, which by itself is too prone to accidental detonation for military use. Mixing the two, however, produced a new explosive with a blast wave that would travel almost 225 miles per hour faster than that of the purest form of HMX, meaning a much more powerful blast. Moreover, the new explosive was as stable and resistant to accidental detonation as HMX. The authors suggest that it has the potential to replace HMX as the new state of the art in military explosives.

RECENT PUBLICATIONS BY LLNL AUTHORS

Adare, A., et al., 2012, "Evolution of π^0 suppression in Au+Au Collisions from $\sqrt{s_{NN}}$ = 39 to 200 GeV": *Physical Review Letters*, v. 109, no. 15.

Adare, A., et al., 2012, "Direct photon production in p+p collisions at $\sqrt{s}$ = 200 GeV at midrapidity": *Physical Review D*, v. 86, no. 7.

Afanasiev, S., et al., 2012, "Measurement of direct photons in Au+Au collisions at $\sqrt{s_{NN}}$ = 200 GeV": *Physical Review Letters*, v. 109, no. 15.

Alamo-Martinez, K. A. et al., 2012, "Globular cluster systems in fossil groups: NGC 6482, NGC 1132, and ESO 306-017": *Astronomy & Astrophysics*, v. 546.

Angus, J. R., Krasheninnikov, S. I., and Umansky, M. V., 2012, "Effects of parallel electron dynamics on plasma blob transport": *Physics of Plasmas*, v. 19, no. 8.

Bailie, C., McFarland, J. A., Greenough, J. A., and Ranjan, D., 2012, "Effect of incident shock wave strength on the decay of Richtmyer-Meshkov instability-introduced perturbations in the refracted shock wave": *Shock Waves*, v. 22, no. 6, p. 511.

Balakrishnan, K., Kuhl, A. L., Bell, J. B., and Beckner, V. E., 2012, "An empirical model for the ignition of explosively dispersed aluminum particle clouds": *Shock Waves*, v. 22, no. 6, p. 591.

Beane, S. R. et al., 2012, "Hyperon–nucleon interactions from quantum chromodynamics and the composition of dense nuclear matter": *Physical Review Letters*, v. 109, no. 17.

Benedict, L. X. et al., 2012, "Molecular dynamics simulations and generalized Lenard-Balescu calculations of electron-ion temperature equilibration in plasmas": *Physical Review E*, v. 86, no. 4.

Bhattacharia, S. K., Maiti, A., Gee, R. H., and Weeks, B. L., 2012, "Sublimation properties of pentaerythritol tetranitrate single crystals doped with its homologs": *Propellants Explosives Pyrotechnics*, v. 37, no. 5, p. 563.

Boates, B., Teweldeberhan, A. M., and Bonev, S. A., 2012, "Stability of dense liquid carbon dioxide": *Proceedings of the National Academy of Sciences*, v. 109, no. 37, p. 14808.

Bolton, O., Simke, L. R., Pagoria, P. F., and Matzger, A. J., 2012, "High-power explosive with good sensitivity: a 2:1 cocrystal of CL-20:HMX": Crystal Growth & Design, v. 12, no. 9, p. 4311.

Borja, R. I., Liu, X. Y., and White, J. A., 2012, "Multiphysics hillslope processes triggering landslides": *Acta Geotechnica*, v. 7, no. 4, p. 261.

Bromley, K. M. et al., 2012, "Amelogenin processing by MMP-20 prevents protein occlusion inside calcite crystals": *Crystal Growth & Design*, v. 12, no. 10, p. 4897.

Casner, A. et al., 2012, "Designs for highly nonlinear ablative Rayleigh-Taylor experiments on the National Ignition Facility": *Physics of Plasmas*, v. 19, no. 8.

Chang, J., Paulson, C., and Welsh, P., 2012, "Development of micropower ultrawideband impulse radar medical diagnostic systems for continuous monitoring applications and austere environments": *Proc. 2012 IEEE Radar Conference*.

Chatrchyan, S. et al., 2012, "Search for new physics in the multijet and missing transverse momentum final state in proton–proton collisions at $\sqrt{s}$ = 7 TeV": *Physical Review Letters*, v. 109, no. 17.

Chatrchyan, S. et al., 2012, "Search for supersymmetry in events with b-quark jets and missing transverse energy in *pp* collisions at 7 TeV": *Physical Review D*, v. 86, no. 7.

Chatrchyan, S. et al., 2012, "Measurement of the pseudorapidity and centrality dependence of the transverse energy density in Pb–Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV": *Physical Review Letters*, v. 109, no. 15.

Chatrchyan, S., et al., 2012, "Measurement of the Λb cross section and the Λb-to-Λb ratio with *J*/ψΛ decays in *pp* collisions at √s = 7 TeV CMS Collaboration": *Physics Letters B*, v. 714, no. 2-5, p. 136.

Chatrchyan, S., et al., 2012, "Search for narrow resonances in dilepton mass spectra in *pp* collisions at √s = 7 TeV": *Physics Letters B*, v. 714, no. 2-5, p. 158.

Choi, W. I., Kim, K., and Narumanchi, S., 2012, "Thermal conductance at atomically clean and disordered silicon/aluminum interfaces: A molecular dynamics simulation study": *Journal of Applied Physics*, v. 112, no. 5.

Chrzan, D. C. et al., 2012, "Embedded binary eutectic alloy nanostructures": *JOM*, v. 64, no. 10, p. 1158.

Connors, J. M., Howell, J. S., and Layton, W. J., 2012, "Decoupled time stepping methods for fluid–fluid interaction": *SIAM Journal on Numerical Analysis*, v. 50, no. 3, p. 1297.

Dougherty, M. J. et al., 2012, "Glycoside hydrolases from a targeted compost metagenome, activity-screening and functional characterization": *BMC Biotechnology*, v. 12.

Farooq, A. et al., 2012, "Shock tube studies of methyl butanoate pyrolysis with relevance to biodiesel": *Combustion and Flame*, v. 159, no. 11, p. 3235.

Fernandez-Perea, M. et al., 2012, "Triple-wavelength, narrowband Mg/SiC multilayers with corrosion barriers and high peak reflectance in the 25–80 nm wavelength region": *Optics Express*, v. 20, no. 21, p. 24018.

Fotiades, N. et al., 2012, "States built on the 9/2+ isomers in 91,93Y": *European Physical Journal A*, v. 48, no. 9.

Gao, T. J. et al., 2012, "Characterization of de novo synthesized GPCRs supported in nanolipoprotein discs": *PLoS One*, v. 7, no. 9.

Gettings, D. P. et al., 2012, "The massive distant clusters of Wise Survey: the first distant galaxy cluster discovered by Wise": *Astrophysical Journal Letters*, v. 759, no. 1.

Grote, D. P., Friedman, A., and Lee, E. P., 2012, "Nonparaxial pulse broadening in a solenoid focusing element": *Physical Review Special Topics-Accelerators and Beams*, v. 15, no. 10.

Guttormsen, M. et al., 2012, "Observation of large scissors resonance strength in actinides": *Physical Review Letters*, v. 109, no. 16.

Hadjadj, A., Yee, H. C., and Sjogreen, B., 2012, "LES of temporally evolving mixing layers by an eighth-order filter scheme": *International Journal for Numerical Methods in Fluids*, v. 70, no. 11, p. 1405.

Hamel, S. et al., 2012, "Equation of state of CH1.36: First-principles molecular dynamics simulations and shock-and-release wave speed measurements": *Physical Review B*, v. 86, no. 9.

He, X. L. et al., 2012, "Synthesis and transformation of Zn-doped PbS quantum dots": *Journal of Physical Chemistry C*, v. 116, no. 41, p. 22001.

Hu, Q. et al., 2012, "The thermodynamics of calcite nucleation at organic interfaces: classical vs. non-classical pathways": *Faraday Discussions*, v. 159, p. 509.

Hunt, R. M. et al., 2012, "Diffusion bonding beryllium to reduced activation ferritic martensitic steel: development of processes and techniques":

Fusion Engineering and Design, v. 87, no. 9, p. 1550.

Hupin, G. et al., 2012, "Ab initio calculations of light-ion fusion reactions": *AIP Conference Proceedings*, v. 1491, p. 387.

Hurricane, O. A. et al., 2012, "Validation of a turbulent Kelvin-Helmholtz shear layer model using a high-energy-density OMEGA laser experiment": *Physical Review Letters*, v. 109, no. 15.

Ileri, N. et al., 2012, "Mesoscale simulations of biomolecular transport through nanofilters with tapered and cylindrical geometries": *Physical Chemistry Chemical Physics*, v. 14, no. 43, p. 15066.

Kajstura, J. et al., 2012, "Cardiomyogenesis in the aging and failing human heart": *Circulation*, v. 126, no. 15, p. 1869.

Karimi, S., Cosman, P., Wald, C., and Martz, H., 2012, "Segmentation of artifacts and anatomy in CT metal artifact reduction": *Medical Physics*, v. 39, no. 10, p. 5857.

Keiluweit, M. et al., 2012, "Nanoscale investigation of the association of microbial nitrogen residues with iron (hydr)oxides in a forest soil O-horizon": *Geochimica et Cosmochimica Acta*, v. 95, p. 213.

Kreiss, H. O., and Petersson, N. A., 2012, "Boundary estimates for the elastic wave equation in almost incompressible materials": *SIAM Journal on Numerical Analysis*, v. 50, no. 3, p. 1556.

Kuhl, A. L., and Balakrishnan, K., 2012, "Gasdynamic model of dilute two-phase combustion fields": *Combustion, Explosion and Shock Waves*, v. 48, no. 5, p. 544.

Landa, A. et al., 2012, "Ab initio study of advanced metallic nuclear fuels for fast breeder reactors": *Actinides and Nuclear Energy Materials*, v. 1444, p. 67.

Le Beon, M. et al., 2012, "Quaternary morphotectonic mapping of the Wadi Araba and implications for the tectonic activity of the southern Dead Sea fault": *Tectonics*, v. 31.

Loubeyre, P. et al., 2012, "Extended data set for the equation of state of warm dense hydrogen isotopes": *Physical Review B*, v. 86, no. 14.

Louie, R. F. et al., 2012, "Effects of dynamic temperature and humidity stresses on point-of-care glucose testing for disaster care": *Disaster Medicine and Public Health Preparedness*, v. 6, no. 3, p. 232.

Manley, M. E. et al., 2012, "Measurement of the phonon density of states of PuO_2(+2%Ga)": *Actinides and Nuclear Energy Materials*, vol. 1444, p. 141.

Marian, J., and Hoang, T. L., 2012, "Modeling fast neutron irradiation damage accumulation in tungsten": *Journal of Nuclear Materials*, v. 429, no. 1-3, p. 293.

Marsh, R. A. et al. 2012, "Modeling and design of an X-band RF photoinjector": *Physical Review Special Topics—Accelerators and Beams*, v. 15, no. 10.

Martin, T. et al., 2012, "New high-stopping-power thin scintillators based on Lu_2O_3 and $Lu_3Ga_{2-x}In_xO_{12}$ for high-resolution x-ray imaging": *IEEE Transactions on Nuclear Science*, v. 59, no. 5, p. 2269.

Mattoon, C. M., Brown, D., and Elliott, J. B., 2012, "Covariance applications with Kiwi": *EPJ Web of Conferences*, vol. 27.

McLaughlin, K., Cioce, C. R., Belof, J. L., and Space, B., 2012, "A molecular H_2 potential for heterogeneous simulations, including polarization and many-body van der Waals interactions": *Journal of Chemical Physics*, v. 137, no. 12.

Meier, E. T., and Shumlak, U., 2012, "A general nonlinear fluid model for reacting plasma-neutral mixtures": *Physics of Plasmas*, v. 19, no. 8.

Moresco, M., et al., 2012, "Improved constraints on the expansion rate of the Universe up to *z* similar to 1.1 from the spectroscopic evolution of cosmic chronometers": *Journal of Cosmology and Astroparticle Physics*, no. 8.

Moses, W. W. et al., 2012, "The origins of scintillator nonproportionality": *IEEE Transactions on Nuclear Science*, v. 59, no. 5, p. 2038.

Myers, M. T. et al., 2012, "Defect microstructure in heavy-ion-bombarded (0001) ZnO": *Acta Materialia*, v. 60, no. 17, p. 6086.

Myers, M. T. et al., 2012, "Phase transition, segregation and nanopore formation in high-energy heavy-ion-irradiated metallic glass": *Scripta Materialia*, v. 67, no. 11, p. 887.

Nagayama, T. et al., 2012, "Investigation of a polychromatic tomography method for the extraction of the three-dimensional spatial structure of implosion core plasmas": *Physics of Plasmas*, v. 19, no. 8.

Nelson, A. J. et al., 2012, "Adsorption of atmospheric gases on Pu surfaces": *Actinides and Nuclear Energy Materials*, vol. 1444, p. 79.

Nielsen, M. H. et al., 2012, "Structural evolution, formation pathways and energetic controls during template-directed nucleation of $CaCO_3$": *Faraday Discussions*, v. 159, p. 105.

Oganessian, Y. T. et al., 2012, "Production and decay of the heaviest nuclei ^{293,294}117 and ^{294}118": *Physical Review Letters*, v. 109, no. 15.

Orce, J. N. et al., 2012, "Reorientation-effect measurement of the $<2_1^+ \| \hat{E}2 \| 2_1^+>$ matrix element in ^{10}Be": *Physical Review C*, v. 86, no. 4.

Perez, F., Gremillet, L., Decoster, A., Drouin, M., and Lefebvre, E., 2012, "Improved modeling of relativistic collisions and collisional ionization in particle-in-cell codes": *Physics of Plasmas*, v. 19, no. 8.

Perez, F. et al., 2012, "Efficient laser-induced 6–8 keV x-ray production from iron oxide aerogel and foil-lined cavity targets": *Physics of Plasmas*, v. 19, no. 8.

Petri, M. et al., 2012, "Structure of ^{16}C: testing shell model and ab initio approaches": *Physical Review C*, v. 86, no. 4.

Ping, Y. et al., 2012, "Dynamics of relativistic laser–plasma interaction on solid targets": *Physical Review Letters*, v. 109, no. 14.

Prasad, M. K., and Snyderman, N. J., 2012, "Statistical theory of fission chains and generalized Poisson neutron counting distributions": *Nuclear Science and Engineering*, v. 172, no. 3, p. 300.

Rau, G. H., McLeod, E. L., and Hoegh-Guldberg, O., 2012, "The need for new ocean conservation strategies in a high-carbon-dioxide world": *Nature Climate Change*, v. 2, no. 10, p. 720.

Reyes, C. et al., 2012, "Characterization of axial and proximal histidine mutations of the decaheme cytochrome MtrA from *Shewanella* sp strain ANA-3 and implications for the electron transport system": *Journal of Bacteriology*, v. 194, no. 21, p. 5840.

Robey, H. F., et al., 2012, "Shock timing experiments on the National Ignition Facility: initial results and comparison with simulation": *Physics of Plasmas*, v. 19, no. 4.

Roecker, C. et al., 2012, "Reconstruction algorithms for directional neutron detection using a time projection chamber": *Nuclear Technology*, v. 180, no. 2, p. 231.

Rountree, B. et al., 2012, "Beyond DVFS: a first look at performance under a hardware-enforced power bound," *Proceedings of 2012 IEEE 26th International Parallel and Distributed Processing Symposium Workshops and Ph.d. Forum*, p. 947.

Sadigh, B., and Erhart, P., 2012, "Calculation of excess free energies of precipitates via direct thermodynamic integration across phase boundaries": *Physical Review B*, v. 86, no. 13.

Safronova, U. I., Safronova, A. S., and Beiersdorfer, P., 2012, "Relativistic atomic data for Cu-like tungsten": *Physical Review A*, v. 86, no. 4.

Santala, M. K. et al., 2012, "Nanosecond-scale time-resolved electron imaging during laser crystallization of GeTe": *Physica Status Solidi B*, v. 249, no. 10, p. 1907.

Satcher, J. H. et al., 2012, "Portable thin layer chromatography for field detection of explosives and propellants": *Chemical, Biological, Radiological, Nuclear, and Explosives*, vol. 8358.

Saw, C. K. et al., 2012, "Hydrogen corrosion of plutonium: Evidence for fast grain-boundary reaction and slower intragrain reaction": *Journal of Nuclear Materials*, v. 429, no. 1-3, p. 128.

Scheichl, R., Vassilevski, P. S., and Zikatanov, L. T., 2012, "Multilevel methods for elliptic problems with highly varying coefficients on nonaligned coarse grids": *SIAM Journal on Numerical Analysis*, v. 50, no. 3, p. 1675.

Schmid, T. E. et al., 2012, "Micronutrients intake is associated with improved sperm DNA quality in older men": *Fertility and Sterility*, v. 98, no. 5, p. 1130.

Scullard, C. R., 2012, "Percolation critical polynomial as a graph invariant": *Physical Review E*, v. 86, no. 4.

Seeley, Z. M. et al., 2012, "Phase stabilization in transparent Lu_2O_3:Eu ceramics by lattice expansion": *Optical Materials*, v. 35, no. 1, p. 74.

Shao, Q. et al., 2012, "Gamma discrimination in pillar structured thermal neutron detectors, in fountain": *Chemical, Biological, Radiological, Nuclear, and Explosives*, vol. 8358.

Sharifzadeh, S. et al., 2012, "Quantitative molecular orbital energies within a G_0W_0 approximation": *European Physical Journal B*, v. 85, no. 9.

Simmons, N. A. et al., 2012, "LLNL-G3Dv3: Global P wave tomography model for improved regional and teleseismic travel time prediction": *Journal of Geophysical Research—Solid Earth*, v. 117.

Sinenian, N. et al., 2012, "Total energy loss to fast ablator-ions and target capacitance of direct-drive implosions on OMEGA": *Applied Physics Letters*, v. 101, no. 11.

Sorensen, P., 2012, "Importance of upgraded energy reconstruction for direct dark matter searches with liquid xenon detectors": *Physical Review D*, v. 86, no. 10.

Soukhanovskii, V. A. et al., 2012, "Snowflake divertor configuration studies in National Spherical Torus Experiment": *Physics of Plasmas*, v. 19, no. 8.

Suratwala, T. I. et al., 2012, "Polishing and local planarization of plastic spherical capsules using tumble finishing": *Applied Surface Science*, v. 261, p. 679.

Suss, M. E. et al., 2012, "Capacitive desalination with flow-through electrodes": *Energy & Environmental Science*, v. 5, no. 11, p. 9511.

Thompson, L. H., 2012, "Recognition, signaling, and repair of DNA double-strand breaks produced by ionizing radiation in mammalian cells: the molecular choreography": *Mutation Research—Reviews in Mutation Research*, v. 751, no. 2, p. 158.

Tobin, J. G. et al., 2012, "Pre-eminence of the indirect channel in the resonant inverse photoelectron spectroscopy of cerium oxide": *Actinides and Nuclear Energy Materials*, vol. 1444, p. 289.

Toupadakis, C. A. et al., 2012, "Long-term administration of AMD3100, an antagonist of SDF-1/CXCR4 signaling, alters fracture repair": *Journal of Orthopaedic Research*, v. 30, no. 11, p. 1853.

Trabert, E. et al., 2012, "Isoelectronic trends of the E1-forbidden decay rates of Al-, Si-, P-, and S-like ions of Cl, Ti, Mn, Cu, and Ge": *Journal of Physics B*, v. 45, no. 21.

Van Cleve, E., Charnvanichborikarn, S., and Kucheyev, S. O., 2012, "Controlling surface hydroxylation of nanoporous silica by ion bombardment": *Journal of Physics D*, v. 45, no. 44.

Van Essen, B. et al., 2012, "On the role of NVRAM in data-intensive architectures: an evaluation": *Proceedings of IEEE 26th International Parallel and Distributed Processing Symposium*, p. 703.

Wang, E. et al., 2012, "Linear gyrokinetic analysis of a DIII-D H-mode pedestal near the ideal ballooning threshold": *Nuclear Fusion*, v. 52, no. 10.

Weilhammer, D. R. et al., 2012, "Host metabolism regulates growth and differentiation of *Toxoplasma gondii"*: *International Journal for Parasitology*, v. 42, no. 10, p. 947.

Wittstock, A., Wichmann, A., and Baumert, M., 2012, "Nanoporous gold as a platform for a building block catalyst": *ACS Catalysis*, v. 2, no. 10, p. 2199.

Wood, B. C. et al., 2012, "Methane and carbon dioxide adsorption on edge-functionalized graphene: a comparative DFT study": *Journal of Chemical Physics*, v. 137, no. 5.

Yang, X. et al., 2012, "Nanopillar array on a fiber facet for highly sensitive surface-enhanced Raman scattering": *Optics Express*, v. 20, no. 22, p. 24819.

Zylstra, A. B. et al., 2012, "Measurements of hohlraum-produced fast ions": *Physics of Plasmas*, v. 19, no. 4.

Questions? Comments?

Please contact Paul Kotta at **kotta1@llnl.gov** or (925) 424-4018.