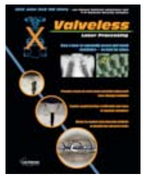
INDEX of SCIENCE HIGHLIGHTS   June 27, 2012

AWARDS AND RECOGNITIONS

LANL receives R&D100 Awards
Polish university recognizes Anna Zurek for materials science contributions
Postdoc Research Day Awards
Margaret Root awarded a Seaborg Research Fellowship



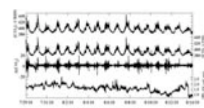


BIOSCIENCE

LANL co-sponsors Sequencing, Finishing, and Analysis in the Future Meeting 2012

EARTH AND ENVIRONMENTAL SCIENCES

Precise and rapid measurements of CO_2 with new-generation laser-based instruments



EXPERIMENTAL FACILITIES

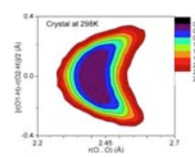
Foam density characterization station is operational
Groundbreaking ceremony for the New Mexico Consortium Biology Laboratory


INTELLIGENCE AND SPACE RESEARCH

Los Alamos Space Weather Summer School and Vela Fellowship Program

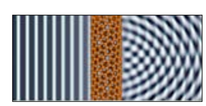
LANSCE

Proton transfer investigated using neutrons



MATERIALS PHYSICS AND APPLICATIONS

Quantum interference detected in carbon nanotubes



MATERIALS SCIENCE AND TECHNOLOGY

Understanding the initial stages of radiation damage

PADSTE HIGHLIGHTS June 27, 2012

AWARDS AND RECOGNITIONS

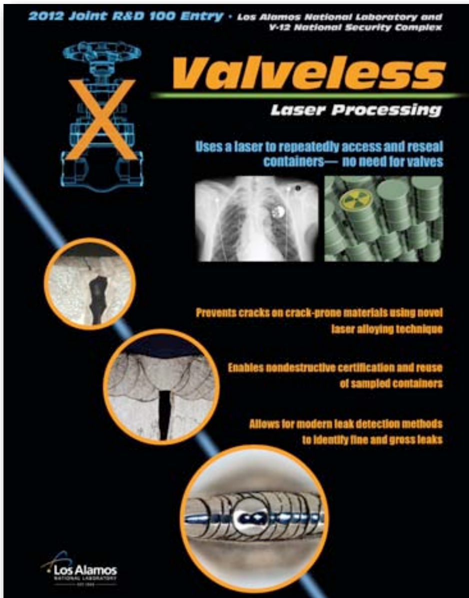
LANL receives R&D 100 Awards

2012 R&D 100 50th ANNIVERSARY

R&D Magazine selected LANL to receive three R&D 100 awards for technology innovations. These awards honor the 100 most technologically significant products introduced into the marketplace over the past year. An independent judging panel and the editors of ***R&D Magazine*** select winners of the awards. Recipients will be recognized at the R&D 100 awards banquet. Technical contact: *Kim Sherwood*

Sequedex speed reads DNA using evolutionary theory. The revolutionary software package can perform one human genome's worth of DNA analysis in 30 minutes on a single core of a laptop computer. A scientist could explore a community of microorganisms by analyzing the DNA from a spoonful of dirt in a few hours. It combines keyword recognition technology from web search engines with evolutionary theory, placing short "reads" of DNA from any organism on the Tree of Life. It is 250,000 times faster than the most commonly used approach (the Basic Local Alignment Search Tool, BLAST) in typical application, and more than 50 times faster than the fastest commercial product. Sequedex has applications in medicine (infectious diseases, tracking drug resistance, and cancer genomics), ecology (profiling microbial communities), chemical manufacturing (discovering industrially useful enzymes and developing sequence-based controls for fermentation processes), and consumer products (measuring the effects of consumer products on microbial communities). Recipients are Joel Berendzen (Applied Modern Physics, P-21), Nicolas Hengartner and Judith Cohn (Information Sciences, CCS-3), and Benjamin McMahon (Theoretical Biology and Biophysics, T-6).

U-Turn (Turning uranium around) synthesizes two new uranium iodide reagents, $UI_3(1,4\text{-dioxane})_{1.5}$ and $UI_4(1,4\text{-dioxane})_2$. U-Turn requires no retooling or specialized equipment, gives reproducible and high-yielding product, can be applied at an industrial scale, and is easy to use. This cost-effective, environmentally green, and safe method provides a nondestructive path forward for more than 5,300 metric tons of stockpiled nuclear waste. The U-Turn process costs 100–140 times less to produce its reagents than it does for competitive processes to produce their reagents. The synthesis could revolutionize the use of depleted uranium in chemistry, catalysis, materials science, and energy. There are applications in future sustainable energy (producing the uranium starting materials needed for research), waste cleanup of depleted uranium metal waste, and catalysts for nitrogen fixation and fertilizer production (converting nitrogen and hydrogen to ammonia as a feedstock for nitrogen-based fertilizers). Award recipients include Jaqueline Kiplinger, Marisa Monreal, Robert Thomson, Thibault Cantat, Nicholas Travia (Materials Chemistry, MPA-MC).



Valveless Laser Processing (VLP) technology eliminates the use of valves in hermetically sealed containers (even those not designed for interrogation) by using a laser to access and reseal the containers. The unique laser-alloying technique prevents cracks on materials that are typically prone to cracking. Researchers can reseal containers by welding them with the alloy material, and then certify these seals to the highest standards. This allows nondestructive certification and reuse of sampled containers. The development eliminates the need for valves and their associated weight, volume, and material costs. It lowers process cost and duration because the technology can access, evacuate, backfill, seal, and leak test in one setup. Applications include environmental remediation (remotely accesses and reseals containers with known or unknown contents), nondestructive analysis (allows sampling, recertification, and reuse of containers typically analyzed by destructive means), and leak testing (enables modern leak detection on pacemakers and other implantable medical devices). Award recipients include Jessie Nichols (Weapons Product Definition, W-11), Pete Pittman (76/W88, W-2), Tom Lienert and Martin Piltch (Metallurgy, MST-6), Marc Robbins and Wynn Christiansen (Applied Engineering Technology, AET-5), and Ken Nicklaus and Chris Hayes (Y-12 National Security Complex).

LANL has won 124 of the prestigious R&D 100 awards since 1978. These technologies include innovative new materials, chemistry breakthroughs, biomedical products, consumer items, testing equipment, and high-energy physics. Since 1995, winning innovations have returned more than $45 million in funding to LANL in Cooperative Research and Development Agreements (CRADAs), Work for Others, User Facility Agreements, and licenses. More than 80 patent awards have been associated with winners, and more patents are pending. More than 25 percent of LANL's commercial licenses and 35 percent of noncommercial licenses can be attributed to R&D 100 winners.

Polish university recognizes Anna Zurek for materials science contributions

Anna Zurek (Group Leader of Materials in Radiation and Dynamic Extremes, MST-8) received a medal of appreciation for contributions to materials science and metallurgy and many years of fruitful international collaboration between the AGH University of Science and Technology and LANL.

Photos. (*Left*): Prof. dr hab. inż. Tadeusz Słomka (Rector of the AGH University, Poland) presents Anna Zurek with a medal of appreciation during a gala ceremony. (*Right*): Close-up of the medal.

Zurek's efforts have led to collaborations between MST-8 staff and students, postdocs, and faculty of the university (especially with Prof. dr hab. inz. Janusz Majta), including two appointments for a long-term visiting scientist. These collaborations have resulted in several PhD theses, a doctoral habilitation thesis, the Maria Sklodowska–Curie International (Polish-American) research Fund II Award (in 1997-2000), and 29 collaborative research papers on the subject of characterization and modeling of materials deformed under extreme, dynamic conditions.

Zurek, who joined Los Alamos in November 1985 in (then) MST-5, earned her master of science degree in the Materials Science and Metallurgy Department from the University of Science and Technology, Krakow, Poland and her doctorate in materials science from the University of Texas at Austin.

The University Rector Prof. dr. hab, inz. Antoni Tajdus and Lakshimi Mittal, CEO of Arcelormittal-Steel of Poland also received medals of appreciation during the ceremony. The event, which featured a choir, chamber orchestra, and faculty parading in the university regalia, commemorated 90 years of the Metals Engineering and Industrial Computer Science Department at the university. Technical contact: *Anna Zurek*

Postdoc Research Day awards

The Postdoc Program Office and the Los Alamos Postdoc Association sponsored the Los Alamos Postdoc Research Day. Postdocs presented summaries of their LANL research and received feedback. The event enhanced collaboration and technical discussions among postdocs and staff. Judges evaluated the 97 posters, representing 17 technical divisions. Senior managers presented the poster awards. John L. Phillips (previous LANL employee and retired NASA astronaut) and John R. Phillips (previous LANL employee and retired CIA Chief Scientist) gave keynote presentations. Technical contact: *Mary Anne With*

Poster Award recipients and their posters include:

Ryan Baumbach (Condensed Matter and Magnet Science, MPA-CMMS), "Search for Quantum Criticality in $CeRu_2M_2X$ (M = Al and Ga, X = B and C)"

Anirban Chaudhuri (Sensors and Electrochemical Devices, MPA-11), "Determination of Sound Speed and Composition in Oil-Water Mixtures using Non-Invasive Ultrasound"

Samrat Choudhury, (Materials Science in Radiation and Dynamic Extremes, MST-8), "Structure and Properties of the Y_2O_3/Fe Interface from First Principles Calculations"

Jonathan Engle, (Inorganic, Isotope and Actinide Chemistry, C-IIAC), "Preliminary Investigation of Parasitic Radioisotope Production using the LANL IPF Secondary Neutron Flux"

David Fredenburg (Shock and Detonation Physics, WX-9), "Consolidation Response of Brittle Particulate Materials at Low- and High-Strain-Rates"

Adam Manzanares (System Integration, HPC-5), "PLFS - A Transformative I/O Middleware Layer"

Xiaoying Pang, (Accelerator and Beam Science, AOT-ABS), "High Performance Beam Dynamics Simulator for the LANSCE Linear Accelerator"

Photo. (*Left to right*): John L. Phillips (guest speaker), David Fredenburg, Adam Manzanares, Ryan Baumbach, Alan Bishop (acting Principal Associate Director for Science, Technology and Engineering, PADSTE), Anirban Chaudhuri, Samrat Choudhury, Jonathan Engle, Xiaoying Pang, John R. Phillips (guest speaker).

Honorable Mention Award recipients include Hussein Aluie (Applied Mathematics and Plasma Physics, T-5), Eric Daub (Geophysics, EES-17 and Center for Nonlinear Studies, T-CNLS), Louise Evans (Safeguards Science and Technology, NEN-1), Ramesh Jha (Advanced Measurement Science, B-9), Satish Karra (Computational Earth Science, EES-16), Graham King (Lujan Center, LANSCE-LC), Sara Kutchesfahani (Systems Design and Analysis, NEN-5), Yan Li (Condensed Matter and Magnet Science, MPA-CMMS and Physics and Condensed Matter and Complex Systems, T-4), Blake Sturtevant (Sensors and Electrochemical Devices, MPA-11), Benjamin Ueland (Condensed Matter and Magnet Science, MPA-CMMS), Marcus Weigand (MPA-CMMS), John Yeager (Shock and Detonation Physics, WX-9), Shixiong Zhang (Center for Integrated Nanotechnologies, MPA-CINT), and Mindy Zimmer (Nuclear and Radiochemistry, C-NR).

Photo. (*Left to right*): Back row: John L. Phillips (guest speaker), John Yeager, Marcus Weigand, Satish Karra, Blake Sturtevant, Graham King, Alan Bishop (acting Principal Associate Director for Science, Technology and Engineering, PADSTE), Benjamin Ueland, Shixiong Zhang, Eric Daub, John R. Phillips (guest speaker). Front row: Hussein Aluie, Sara Kutchesfahani, Louise Evans, Yan Li, Ramesh Jha, Mindy Zimmer.

Margaret Root awarded a Seaborg Research Fellowship

Student researcher Margaret Root (Safeguards Science and Technology, NEN-1) received a prestigious G.T. Seaborg Institute Research Fellowship. She is a graduate research assistant working with Karen Miller (NEN-1) this summer. Root's project is in support of the Next Generation Safeguards Initiative funded instrument, called the Passive Neutron Enrichment Meter (PNEM). The ^{3}He-based nondestructive assay system determines ^{235}U mass and enrichment in uranium hexafluoride (UF_6) cylinders at uranium enrichment plants. It has been field tested at Rokkasho Enrichment Plant in Japan and the Westinghouse Fuel Fabrication Plant in South Carolina. Root uses Monte Carlo modeling to supplement field trial data for more accurate background radiation correction and to understand how UF_6 is distributed inside the cylinders (an important factor in estimating the systematic uncertainty associated with the measurement technique). The Department of Homeland Security funds Root's fellowship. She will present her work at LANL's Student Symposium and at the 2013 American Nuclear Society Student Conference at MIT.

Root has a B.S. in Nuclear Engineering from the University of New Mexico and will begin a dual Master's degree program in Nuclear Engineering and Technology Policy at the Massachusetts Institute of Technology this fall. Technical contact: *Margaret Root*

BIOSCIENCE

LANL co-sponsors Sequencing, Finishing, and Analysis in the Future Meeting

The seventh annual "Sequencing, Finishing and Analysis in the Future" took place in Santa Fe, NM. The DOE Office of Science, the Joint Genome Institute (JGI), and LANL co-sponsored the meeting, with additional support from industry partners. Chris Detter (JGI- LANL, Genomics Center Director) and Patrick Chain (Metagenomics Team Leader, LANL) and other scientists co-organized the meeting. This international gathering for leaders in genome sequencing and their industrial counterparts covered new strategies for combining second and third generation sequencing, finishing, assembly, annotation, and analysis to create "perfect" genome sequence data and applications for their use.

One exciting development was an increased emphasis on the science that is enhanced by sequencing and sequence analysis. Keynote speakers Paul Keim (Northern Arizona University) and Rita Colwell (University of Maryland) gave talks on this topic. Keim discussed how new technology has enabled genomic analysis of *Yersinia pestis* (which causes plague), including the study of trace material from the Middle Ages to understand past and current epidemiology of the disease. Colwell described how zooplankton carry cholera bacteria as a component of their natural flora and that cholera epidemics increase with increased precipitation or sea temperature, likely as a result of zooplankton blooms. Genomics of the cholera bacterium provide a tracking tool to measure the effects of climate change on public health. Many talks discussed the valuable real-time genomic analysis of the *E. coli* outbreak in Germany last year, and there were talks about diagnostic sequencing and single cell sequencing to help develop cellular targeted therapies for cancer patients. The Meeting included with a special half-day session on next generation sequencing for forensics.

Participation in the 2012 Workshop topped all previous ones with over 300 attendees from the major genome research centers, scientists from local labs, program managers, FBI Laboratory researchers, and industry. Speakers from LANL included Matt Scholz (Genome Science/Joint Genome Institute, B-6), who gave a talk on metagenomic assembly; Ben McMahon (Theoretical Biology and Biophysics, T-6), who discussed rapid phylogenetic and functional classification of short genomic fragments; and Michael Fitzsimons (formerly B-6) who described his postdoc work at LANL on gel microdroplet culturing. Patrick Chain and Chris Detter (B-6) chaired some sessions, and Cathy Cleland (Intelligence Defense Counterterrorism, GS-IDC) chaired Forensics Friday. LANL researchers O. Chertkov, A.C. Munk, Bin Hu, Shannon Johnson, Tracy Erkkila, and Armand E K Dichosa (B-6); and Helen Cui (Safeguards Science and Technology, NEN-1) presented posters. B-6 Group Leader Chris Detter has led the organization of the conference since its inception. Technical contact: *Chris Detter*

EARTH AND ENVIRONMENTAL SCIENCES

Precise and rapid measurements of CO_2 with new-generation laser-based instruments

Sensors are important tools for rapid, accurate *in situ* measurements of greenhouse gases for biosphere-atmosphere flux estimates and source attribution applications. Rapid advances in laser-based carbon dioxide (CO_2) sensors enable new, high-resolution observations of the spatio-temporal variations of CO_2. The data are crucial to understand how changes in aerosols, clouds, rain, and climate affect a carbon cycle significantly modified by humankind. Therefore, it is important to conduct instrument inter-comparisons to establish their compatibility under field conditions. Earth System Observations, (EES-14) researchers co-deployed and compared a commercially available cavity ringdown spectrometer (CRDS) and a tunable diode laser (TDL) sensor at LANL's Environmental Research Park and under laboratory conditions. The comparison is valuable for analysis of experiments where multiple high precision fast response instruments measuring greenhouse gases and differences may need to be interpreted and diagnosed. The journal ***Atmospheric Measurement Techniques*** published research.

The scientists characterized the sensors for their accuracy and precision for ambient CO_2 measurements at ground level. The researchers used laboratory and ambient field data to compare the sensors. After the team postprocessed the data to include water vapor correction and calibration to World Meteorological Organization (WMO) reference standards, the mean difference between the CRDS and TDL data for $^{12}CO_2$ was 0.04 ± 1.80 ppm for ambient field data. This result demonstrates that the sensors meet the

WMO /International Atomic Energy Agency compatibility standard of laboratory inter-comparison compatibility of ±0.1 ppm for total CO_2. Over the 19-day period, the ratio of CO_2 measured by CRDS to TDL exhibited a Gaussian distribution centered at 1.003, indicating that it is dominated by random noise rather than bias in sensor output. The CRDS sensor measures $[^{12}C^{16}O_2]$ to a precision of 23 ppb in 1 minute and 6.5 ppb in 58 minutes. At 1 and 58 minutes, the TDL exhibits precisions of 29 ppb and 53 ppb, respectively. The two instruments have operational differences: the CRDS is compact, fast, and stable, and the TDL is larger and requires frequent calibrations.

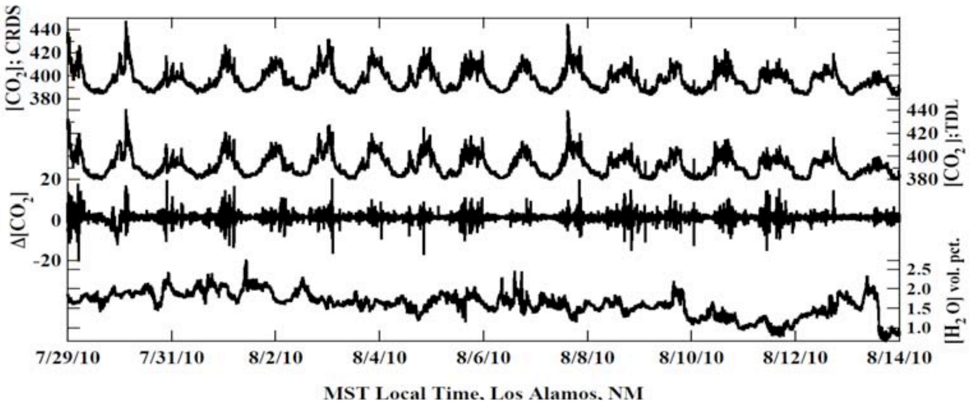


Figure 1. Temporal profile of $[^{12}C^{16}O_2]$ mixing ratio measured near Los Alamos, NM with CRDS and TDL sensors. The CRDS signal has been cross-calibrated. The $\Delta[CO_2]$ trace shows the temporal profile of the $[CO_2]'_{CRDS} - [CO_2]_{TDL}$ difference.

The sensors exhibited consistent hourly averaged diurnal values. This result underscores the interplay of biological, anthropogenic, and transport processes that regulate CO_2 at the site. The CRDS has been deployed during several campaigns: 1) the Carbonaceous Aerosols and Radiative Effects Study, sponsored by Atmospheric System Research/Atmospheric Radiation Measurement, in Sacramento in 2010; and 2) during the Clean Air for London Project campaign in the UK in 2012. The instrument will be deployed on a Gulfstream aircraft (managed by Pacific Northwest National Laboratory) for the GreenOceanAmazon 2014 field campaign in Manaus, Brazil to quantify the tropical carbon cycle.

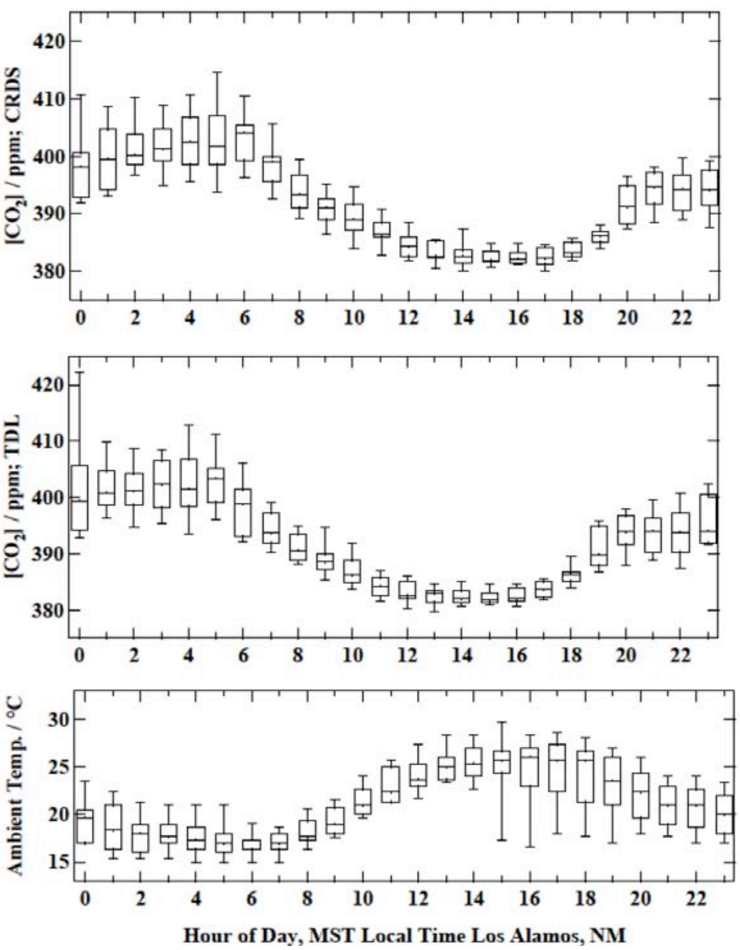


Figure 2. Hourly diurnal median $[CO_2]$ between July 29 -August 16, 2010 at LANL. (*Top*): Scaled CRDS $[^{12}C^{16}O_2]'$; (*middle*): $[^{12}C^{16}O_2]$ TDL; (*bottom*): hourly diurnal median ambient air temperature.

Reference: "Inter-comparison of Two High-accuracy Fast-response Spectroscopic Sensors of Carbon Dioxide: A Case Study," ***Atmospheric Measurement Techniques*** *5*, 991 (2012); doi:10.5194/amt-5-991-2012. www.atmos-meas-tech.net/5/991/2012/ amt-5-991-2012.pdf. Researchers included Brad Flowers, Nate McDowell, and Heath Powers (EES-14), led by instrument mentor Manvendra Dubey (EES-14).

The DOE Office of Science's Climate Change Research Division, LANL's Institute of Geophysics and Planetary Physics (IGPP), and Laboratory Directed Research and Development (LDRD) programs funded different aspects of the research. The DOE's Office of Biological and Environmental Research invested resources from the American Recovery and Reinvestment Act to acquire one of the first cavity ringdown CO_2 sensors manufactured by Picarro. Manvendra Dubey is the climate observations program manager and lead scientist for the study. The work supports the Lab's Energy Security mission area and the Science of Signatures science capability pillar. Technical contact: *Manvendra Dubey*

EXPERIMENTAL FACILITIES AND CAPABILITIES

Foam density characterization station is operational

A foam density characterization station is operational and is assisting in selection of target materials for high energy density physics (HEDP) experiments at the National Ignition Facility (NIF) and the Omega laser. The individual foam components used in the targets are too light to weigh, but small deviations in foam density dramatically impact radiation propagation and complicate assessment of radiation flow models. The foams, with densities ranging from 30-125 mg/cm^3, are silica aerogel or plastic foams used in targets for HEDP experiments. These are the first set of non-ignition related experiments performed at NIF to support development and validation of models used in our codes. Due to the need to characterize the density of these materials, LANL researchers developed imaging station.

J. M. Taccetti, N. Lanier, and R. Aragonez (Plasma Physics, P-24) have designed and, with help from Polymers and Coatings (MST-7) Target Fabrication personnel (D. Schmidt, B. Patterson, K. Obrey, and C. Hamilton), have constructed a dedicated monochromatic X-ray imaging station to determine the density of single component foams. The station includes a Molybdenum La (2.3 keV) and a Chromium Ka (5.4 keV) soft X-ray source. The researchers plan to add a Cu Ka (8.0 keV) source in the future. Depending on the size and density of the part, the density measurement uncertainty can reach the limiting factor of the cold opacity uncertainty of approximately 1%. The instrumentation images the entire target simultaneously to determine the uniformity and density of the whole target component.

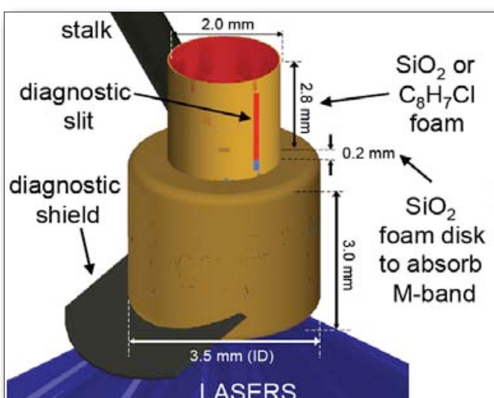


Figure 3. (*Left*): Schematic of a Pleiades NIF target depicts the foam component (red) located at the output of a hohlraum, the radiation cavity used to drive the experiment. (*Right*): Image of a 125 mg/cm^3

C_8H_7Cl foam component obtained on the characterization station. The image shows foam density nonuniformities that motivated researchers to remove this target from the shot cycle.

The Science Campaign 4 Program Office funds the work, which supports the Lab's Nuclear Deterrence mission area and the Materials for the Future Science Pillar. Technical contact: *J. M. Taccetti*

Groundbreaking ceremony for the New Mexico Consortium Biology Laboratory

U.S. Senator Tom Udall and LANL Director Charlie McMillan spoke at the groundbreaking ceremony to mark the start of construction on the New Mexico Consortium's (NMC) biology research facility. Sharon Stover, Chair of the Los Alamos County Council, hosted the event. Local business leaders, state and local political representatives, scientists, Los Alamos residents, and others attended the groundbreaking on May 18 at Entrada Drive in Los Alamos. The 24,000 square foot research facility and greenhouse complements the visions of its partners, including Los Alamos County, LANL, the NMC, and Richard Sayre (Bioenergy and Environmental Science, B-8), who relocated his research team here from the Donald Danforth Plant Science Research Center in St. Louis last October. Sayre holds a joint appointment with the NMC and LANL. When completed in the spring of 2013, the new building will be able to house more than 40 NMC and LANL researchers. The 4,000 square foot greenhouse will be completed first to open in the fall of 2012.

Figure 4. Conceptual rendering of the building. The greenhouse is on the right.

Biofuel research, especially fuels derived from certain plants and algae, will be conducted in the building. Sayre and his team of 12 researchers will be the anchor research program in this facility. The US Air Force, DOE, the National Science Foundation, and the National Institutes of Health have funded them to create alternative, renewable energy sources for the nation. The team is examining cellular processes such as photosynthesis and metabolic regulation in order to optimize biofuel feedstocks. Sayre is also Chief Scientist for the National Alliance for Advanced Biofuels and Bioproducts (NAABB) – a consortium in which LANL is a major partner. With funding from DOE Energy Efficiency and Renewable Energy, the NAABB supports many projects at LANL to address the entire process of developing fuels and products from plants and algae. These include studies on the regulation of plant growth lipid production [Pat Unkefer (Bioscience, B-DO), Min Park (Bioenergy and Environmental Science, B-8), and Scott Twary (Biosecurity and Public Health, B-7)], acoustic harvesting of algae [Babs Marrone and Taraka Dale (Advanced Measurement Science, B-9), and Jim Coons (Chemical Diagnostics and Engineering, C-CDE)], biocatalysis for conversion to usable fuels and bioproducts [Pete Silks (B-8), John Gordon and Susan Hanson (Inorganic, Isotope and Actinide Chemistry, C-IIAC)], and addressing water quality and alternative water source issues [Enid Sullivan (C-CDE)].

The Biological Research Laboratory and Greenhouse is a $12 million project in total, with $8 million for construction. The Los Alamos County Council unanimously agreed to provide $2 million in county funds for the new building, as well as the two-acre parcel of land on which it will be built. The remaining construction costs are being financed with a loan from Los Alamos National Bank. The New Mexico Consortium is a non-profit partnership of the three New Mexico Universities. The NMC promotes scientific research and education collaborations with LANL, which support the Lab's Energy Security mission area and the Materials for the Future science pillar. Technical contacts: *Shannan Yeager* (NMC) and *José Olivares* (LANL Biofuels Program Manager)

INTELLIGENCE AND SPACE RESEARCH

Los Alamos Space Weather Summer School and Vela Fellowship Program

The Space Science and Applications Group (ISR-1) organized the Los Alamos Space Weather Summer School, which takes place from June 4 to July 27. An independent evaluation committee selected seven top-ranked graduate students from a countrywide search to participate in the program and to receive a prestigious Vela Fellowship. The Institute of Geophysics and Planetary Physics (IGPP), Laboratory Directed Research and Development (LDRD), and the Center for Information Science and Technology (IS&T) sponsor the students, who work with internationally recognized researchers in Los Alamos.

LANL traces its space science heritage back to the Vela project, which used space-based nuclear detonation sensors to verify the 1963 Limited Test Ban Treaty. That mission continues today after having successfully launched more than 70 instruments into space in support of this program. Vela was the first constellation of satellites to measure the space environment thoroughly, discovering gamma-ray bursts, heavy ions in the solar wind, and opening many scientific questions regarding geomagnetic storms. In honor of the multiple science contributions of the Vela program, LANL organizes and hosts the Annual Space Weather Summer School.

The summer school students have the opportunity to attend science lectures given by distinguished researchers at LANL. Topics are related to space weather research including plasma physics, radiation belts, numerical modeling, solar wind physics, satellite debris, and space instrumentation. In addition, the students work on an exciting research topic with access to Los Alamos GPS and geosynchronous data. At the end of the summer school, students will present their work in a technical forum. Josef Koller (ISR-1) is the Director of the School. Lecturers include Greg Cunningham, Reiner Friedel, Peter Gary, Mike Henderson, Vania Jordanova, Brian Larsen, Eberhart Moebius, Steve Morley, Geoff Reeves, Mike Shoemaker, John Sullivan, Weichao Tu, Sorin Zaharia, (ISR-1); Jon Niehof (ISR-3); Herb Funsten (ISR-DO); and Humberto Godinez (T-5). More information: http://SpaceWeatherSchool.org. Technical contact: *Joseph Koller*

LANSCE

Proton transfer investigated using neutrons

Lujan Neutron Scattering Center (LANSCE-LC) researchers and collaborators performed an experimental and theoretical study on short, strong hydrogen bonding in tetraacetylethane (TAE), a model system for proton transfer. Proton transfer is one of the most important reactions in biology and biochemistry. Proton-driven machines populate cell membranes and are necessary for biological processes. Proton transfer reactions are of central importance in redox systems, ionic reactions, and chemical catalysis. Numerous proton transfer mechanisms are possible and are still poorly understood in spite of years of study. Modeling the structures and dynamics of protons and of proton transfer with *ab initio* techniques requires difficult and costly quantum chemical calculations, few of which have been validated experimentally in detail. The team's research, which appears in the ***Journal of Physical Chemistry A***, highlights a novel mechanism for facilitating proton transfer or stabilization of hydrogen bond geometry mediated by the dynamics of adjacent functional groups in a very short, strong hydrogen bond. These are possible intermediates in enzyme catalysis, where such a process would have enormous complexity. This complexity would be difficult to unravel with anything like the detail possible with the team's model system.

Hydrogen bonding occurs when hydrogen is shared between electronegative atoms located on different parts of the same molecule (intramolecular) or on different molecules (intermolecular). A hydrogen atom bound to an electronegative atom can interact strongly with another electronegative atom or even be transferred between atoms. Hydrogen bonding plays an important role in biochemistry because it is occurs in proteins and nucleic acids. Between single strands of DNA, it stabilizes the double helix. Hydrogen bonding strongly influences the structure and dynamics of materials. Therefore, model systems with short strong hydrogen bonds are of great interest to scientists in various fields.

Tetraacetylethane $(CH_3CO)_2CH{=}CH(COCH_3)_2$ is a highly symmetric molecule with short, strong intramolecular hydrogen bonds. The researchers performed periodic density functional theory (DFT) calculations of the structure and the dynamics of crystalline TAE as well as molecular dynamics simulations. They validated the results against experimental neutron scattering data. The team derived potential energy surfaces for the hydrogen bond to determine the factors that govern proton transfer. The methyl groups (CH_3 groups) on each "side" of the TAE molecule form weak intermolecular hydrogen bonds in the solid to the oxygen atom (of the intramolecular H-bond) of a neighboring molecule. The researchers showed experimentally that the movement of the methyl groups (mainly rotation) strongly correlates with the position of the proton between the oxygen atoms and vice versa. This phenomenon supports or hinders the proton transfer process. A mechanism that interferes with proton transfer had not been recognized previously.

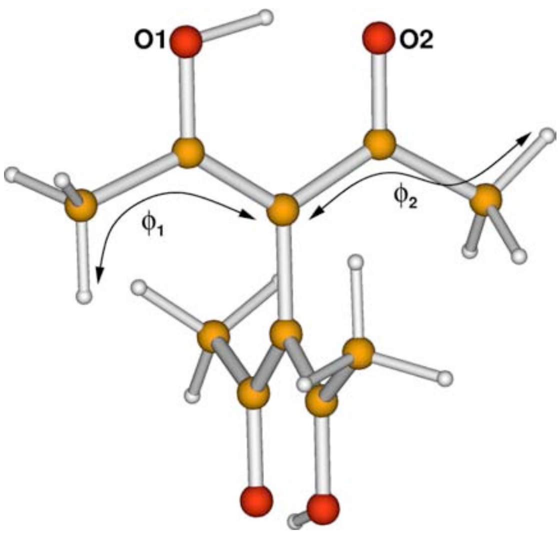


Figure 5. Ball-stick-representation of an isolated molecule of tetraacetylethane in the lowest energy conformation.

The scientists could study the proton in the hydrogen bonds and the methyl group dynamics easily because incoherent inelastic neutron scattering (IINS) is particularly sensitive to H-atom motion. Although the computational determination of the electronic structure of hydrogen-bonded systems is difficult, the neutron vibrational spectrum can readily be obtained from such computational studies. The simplicity of the neutron-nucleus interaction permits calculation of the position and intensity of the vibrational modes for direct comparison with the experimental neutron vibrational spectrum. This is a powerful tool for the validation of *ab initio* calculations, which have become an indispensable part of spectroscopic studies.

The researchers used experimental and computations to determine the correlations between the movement of the various parts of the system with that of the bridging H-atom on its potential energy surface. Calculations on a fully periodic system representing the crystal reveal the important effect of the intermolecular interactions on the potential energy surface of the hydrogen bond, as compared with the result for an isolated molecule (Figure 6).

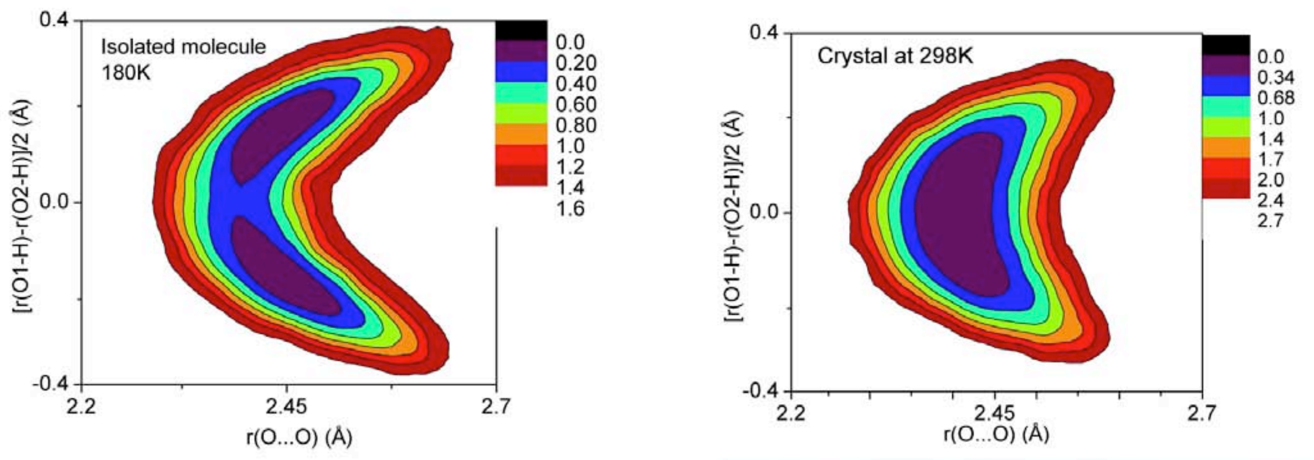


Figure 6. Potential energy surface of the hydrogen bond in an isolated molecule (*left*) and in a crystal (*right*). The well in the crystal is 0.1 Å wide in the O…O coordinate (energy < 0.34 Kcal/mol) and 0.4 Å along the approximate O…H coordinate. At low temperature, the reorientation of the methyl groups leads to a preferred O-atom for the bridging proton. The amplitude of methyl torsions becomes larger with increasing temperature, so that free energy minimum for the proton becomes flat, in contrast with the isolated molecule case.

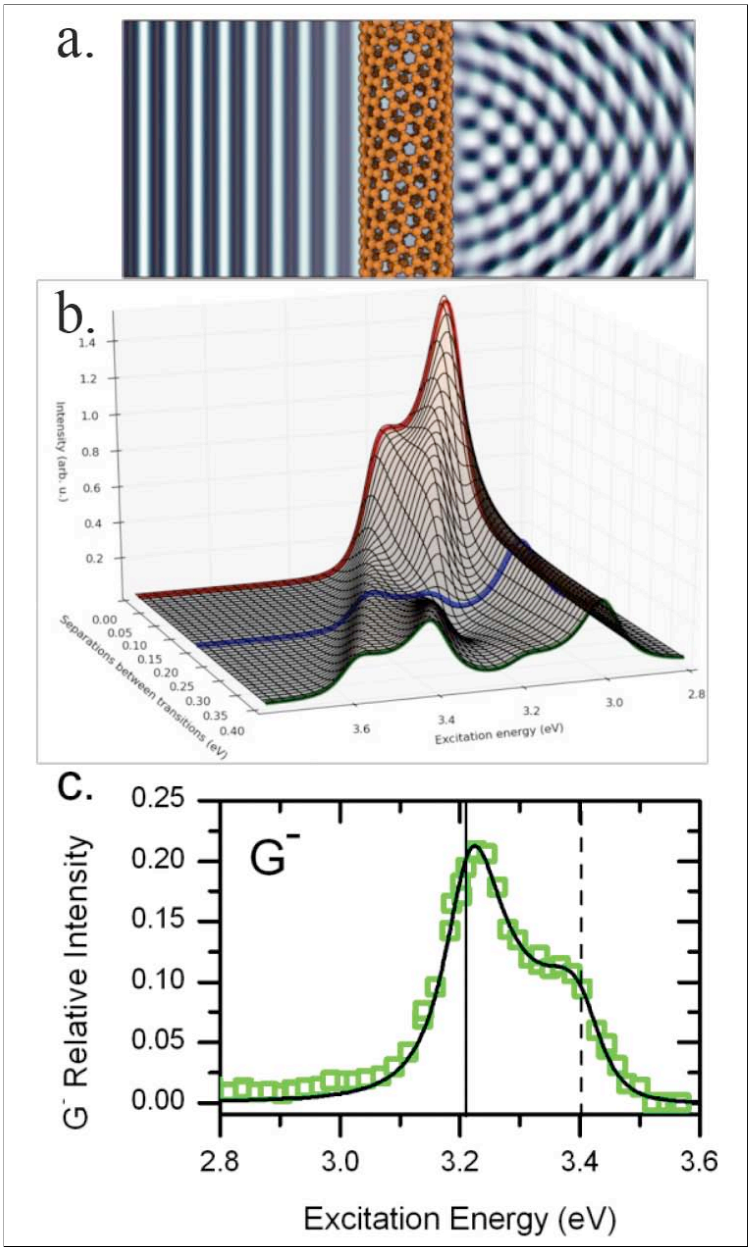
The team collected incoherent inelastic neutron scattering data on the Filter Difference Spectrometer at the Lujan Center. Reference: "Methyl Dynamics Flattens Barrier to Proton Transfer in Crystalline Tetraacetylene," ***Journal of Physical Chemistry A*** *116*, 2283 (2012); doi:org/10.1021/jp210212q. Researchers include Gordon Kearley (Australian Nuclear Science and Technology Organization), Jernej Stare (National Institute of Chemistry, Slovenia), Ramzi Kutteh (University of Sydney), Luke Daemen and Monika Hartl (LANSCE-LC), and Juergen Eckert (University of South Florida). DOE Basic Energy Sciences funded the LANL research, which supports the Lab's Energy Security mission area and the Materials for the Future and Science of Signatures science pillars. Technical contact: *L. Daemen*

MATERIALS PHYSICS AND APPLICATIONS

Quantum interference detected in carbon nanotubes

Quantum interference in the resonance Raman response from carbon nanotubes is expected when certain conditions are met, but it has been a long-standing challenge in nanotube spectroscopy to demonstrate the effect. In research published in ***Physical Review Letters***, Steve Doorn and Hagen Telg (Center for Integrated Nanotechnologies, MPA-CINT), Juan Duque (Physical Chemistry and Applied Spectroscopy, C-PCS), and collaborators provide the first clear evidence of the phenomenon in carbon nanotubes.

Quantum interference is a general wave concept for any coherent interaction. The double slit experiment, which demonstrates that matter and energy can display characteristics of both waves and particles, is the most prominent example. Although this example has its classical analog in interfering electromagnetic or particle waves, other cases of quantum interference usually lack a classical equivalent. Thus, the phenomenon can only be understood more generally as the interference of probability waves resulting from the mathematical construct behind quantum mechanics. In resonance Raman spectroscopy, the observed signal can be strongly affected by interference. Typically, responses are not easily interpreted because the interference arises from broad, poorly-resolved optical transitions. However, the unique signatures of interference can be a powerful tool for revealing fundamental underlying behaviors, including demonstrating changes in electron-phonon interactions and mixing of electronic states that may determine optical relaxation pathways critical to photonics and energy harvesting applications of carbon nanotubes.



In the publication, the researchers have demonstrated that the Raman equivalent of the double slit experiment (depicted conceptually in Figure 7a) can be observed in semiconducting carbon nanotubes. The ability to investigate samples highly enriched in specific nanotube structures (provided by the National Institute of Standards and Technology, NIST), paired with LANL's unique tunable ultraviolet Raman capability, enabled the experiments. To examine the effect, the scientists chose nanotube structures with two closely spaced optical transitions that have Raman interference between them. The researchers observed nearly textbook quantum interference behavior due to the narrow, well-defined transitions found in carbon nanotubes. The result enabled the team to extract the sign-behaviors of the related electron-phonon coupling, which can only be observed in the presence of interference. Structural tuning of the transition energy spacings allowed the researchers to access behaviors ranging from strong constructive interference to nearly complete destructive interference (Figures 7b and 7c).

Figure 7. (a) Conceptualization of Raman interference effect in carbon nanotubes. (b) Simulation of Raman response for G^- phonon mode at varying energy separation of the two interfering electronic states and reflecting response for non-interacting states (green trace), destructive interference at moderate

energy separations (blue) and strong constructive interference at near-zero energy separation (red). (c) Experimental G^- phonon Raman intensity response as a function of excitation energy displaying nearly exactly the strong constructive interference case of the model. Note the reversal of the energy axis in (b) and (c).

Reference: “Quantum Interference Between the Third and Fourth Exciton States in Semiconducting Carbon Nanotubes Using Resonance Raman Spectroscopy”, ***Physical Review Letters*** *108*, 117404 (2012); doi: 10.1103/PhysRevLett.108.117404. Researchers include Juan Duque (C-PCS), Hagen Telg (MPA-CINT), Hang Chen and Anna Swan (Boston University), Andrew P. Shreve (MPA-CINT and University of New Mexico), Xiaomin Tu and Ming Zheng (NIST), and Stephen K. Doorn (MPA-CINT).

The research was performed in part at the Center for Integrated Nanotechnologies (CINT), a DOE Office of Basic Energy Sciences User Facility. The LANL Laboratory Directed Research and Development (LDRD) program funded the research. The work supports the Lab’s Energy Security and Global Security mission areas and the Materials for the Future and Science of Signatures science pillars.
Technical contact: *Stephen Doorn*

MATERIALS SCIENCE AND TECHNOLOGY

Understanding the initial stages of radiation damage

Nuclear reactions produce highly energetic ions that can travel long distances in matter. When one of these fast ions traverses a material, it loses energy due to atomic and electronic collisions, producing damage. At high projectile energies, the main dissipation mechanism is friction with the electrons, which follows the rules of quantum mechanics. Like a speedboat in a calm lake, the passage of the fast ions creates a disturbance of the electron density in the shape of a wake. Alfredo Caro (Materials Science in Radiation and Dynamic Extremes, MST-8) and collaborators simulated this quantum friction of the electrons. This is the first calculation of the connection between the nuclear and electronic stopping cross section. This is possible because the simulation takes into account the individual dynamics of the electrons in an approach known as Ehrenfest dynamics. The journal ***Physical Review Letters*** published the research and featured it on the journal’s cover.

Figure 8. Model of the electronic wake (blue surfaces) generated by an energetic proton (red sphere) traveling in an aluminum crystal. The resulting change in electronic density is responsible for modification of chemical bonds between the atoms and consequently for a change in their interactions.

The team simulated the passage of a proton in crystalline aluminum. By accounting for how much energy is absorbed by the electrons and how much impulse is given to the rest of the atoms, the researchers predicted how the inter-atomic interactions are altered by the excitation of the electrons. This is a precise measure of how much damage energy is deposited into the material. The momentum transfer is radial outwards. It is related to the loss of the ability of electrons to provide chemical bonding as they become excited.

These are the first steps towards the development of a unified first-principles simulation framework of the electron-nuclear radiation damage problem, showing that it is feasible to include both the nuclear and electronic aspects of the problem. The new method allows prediction of the behavior of complex materials under the effect of radiation. A full understanding of these early stages of radiation damage provides knowledge and tools to manipulate them. This understanding not only applies to materials for nuclear applications, but also for materials related to the space industry, novel processing techniques using lasers and ions, and for assessing the effects of radiation on living tissues, both for understanding damage and for therapeutic use such as cancer-therapy conducted by charged particles.

Reference: "Nonadiabatic Forces in Ion-solid Interactions: The Initial Stages of Radiation Damage," ***Physical Review Letters*** *108*, 213201 (2012); doi: 10.1103/PhysRevLett.108.213201. Researchers include Alfredo A. Correa (Lawrence Livermore National Laboratory), Jorge Kohanoff (Queen's University, Belfast, UK), Emilio Artacho (University of Cambridge, UK), Daniel Sanchez-Portal (San Sebastian, Spain); and Alfredo Caro, MST-8).

The Center for Materials at Irradiation and Mechanical Extremes, a DOE Energy Frontier Research Center, and the LANL Laboratory Directed Research and Development (LDRD) Program funded different aspects of the research at Los Alamos. The work supports the Lab's Energy Security and Global Security mission areas and the Materials for the Future and Information Science and Technology science pillars. Technical contact: *Alfredo Caro*