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MPA Materials Matter

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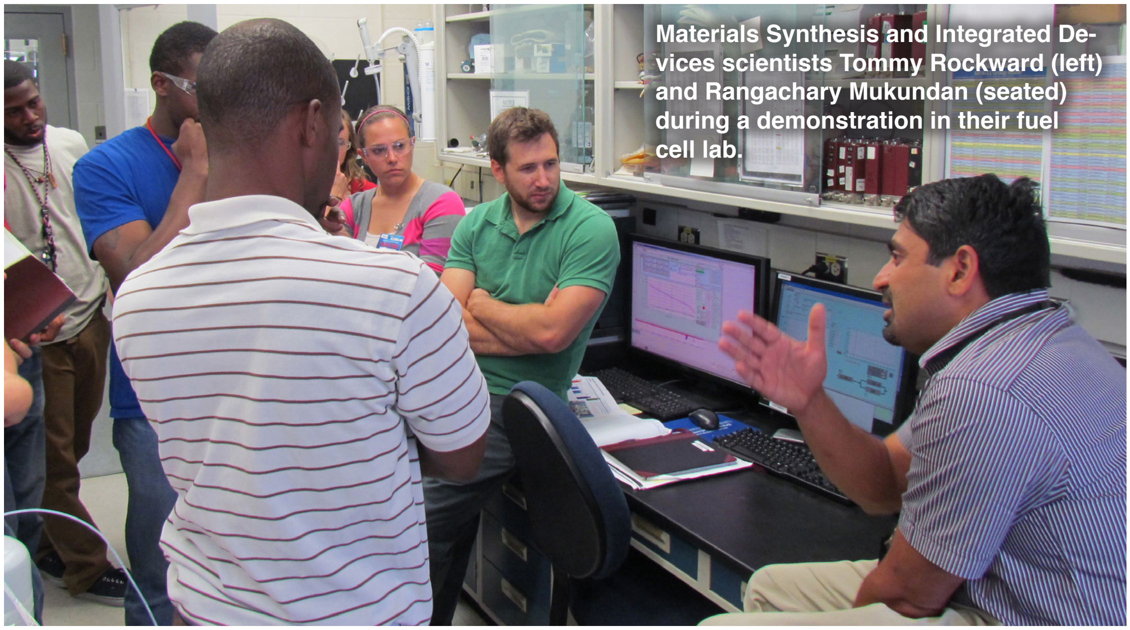


Materials Synthesis and Integrated Devices scientists Tommy Rockward (left) and Rangachary Mukundan (seated) during a demonstration in their fuel cell lab.

Sharing fuel cell expertise

Three-day hands-on course broadens awareness of Laboratory's energy security research, capabilities

For three days at Los Alamos National Laboratory, members of industry and academia explored the science and technology of fuel cells, taking notes as Laboratory researchers shared their expertise and showcased the capabilities they use to design fuel cell prototypes and analyze fuel cell performance.

In support of the U.S. Department of Energy's (DOE) Technology-to-Market activities in the Office of Energy Efficiency and Renewable Energy, Fuel Cell Technology Office, Los Alamos researchers hosted the hands-on short course on fuel cells. The DOE's Technology-to-Market activities efforts place emphasis on national laboratories increasing their industrial contacts, engaging more companies, and developing technology skills.

Fourteen participants from industry, universities, and colleges attended, including from Giner, Inc.; Pajarito Powders, LLC; University of Delaware; Pittsburg State University; University of New Mexico; New Mexico State University; Southern University; Tuskegee University; and Benedict College.

During the workshop, participants gained valuable insight by interacting and working alongside the Los Alamos fuel cell team, including taking part in laboratory demonstrations analyzing fuel cell performance, cyclic voltammetry, and impedance spectroscopy. The participants also learned about hydrogen and lab safety, the Laboratory's membrane-and-electrode process, and fuel cell materials characterization, modeling, durability, and testing.

Los Alamos remains at the forefront of fuel cell research and development, and its leadership and commitment have been instrumental in supporting DOE R&D efforts. The DOE funded this effort under the Office of Energy Efficiency and Renewable Energy's Technology-to-Market initiative. The work supports the Laboratory's Energy Security mission area and the Materials for the Future science pillar through development of fuel cells for clean transportation.

From Rick's desk . . .

Thank you to all who have attended Mary's purpose statement meetings, and thank you for engaging in dialog and providing suggestions regarding areas for improvement. Please be sure to read Kristin's article regarding our purpose and "bumps" along the way.

In this issue, I will focus on the financial outlook for fiscal year 2016 (FY16) and programmatic areas where we have opportunities to enhance our portfolio. We completed another fiscal year just before the release of this issue of *MPA Materials Matter*. It was a strong year for MPA with numerous accomplishments and publications.

Our BES projects remain strong, with the recent completion of our CINT users meeting in September. In FY16 we will continue to look for opportunities to broaden our portfolio, particularly in the area of soft and related biological materials. The current funding profile for BES appears relatively flat for both CINT and our BES material science and engineering portfolio.

Work for others and NSF-supported capabilities such as the NHMFL remain strong, although our funding is relatively flat. In FY15 it was announced that the Magnet Laboratory would not need to re-compete its contract, but instead submit a contract renewal by June 2016. The External Advisory Board for the NHMFL provided strong support for the pulsed field facility at LANL, with suggestions for enhanced growth. While this is great news, it is also important for us to identify areas for recapitalization and opportunities to enhance our science basis and supporting publications.

In FY15, LDRD was reduced by about approximately 20% across the Laboratory to a funding level of $121M. In FY16, the overall program will experience a further decrease to approximately $112M due in part to the creation of the Office of Environment Management. We start off FY16 with several new ERs and a DR to pursue the design of new topological states of matter that arise from strong electronic correlations. LDRD will continue to be a strong focus area for MPA although overall funding has gone down and it remains highly competitive.

Overall the weapons program will experience growth in FY16 for the life extension programs and enhanced surety, both of which provide opportunities for MPA. In addition, there is a strong push to increase our fundamental understanding of high explosive initiation and hostile environments and to provide new options for safety and surety. MPA's funding to support the science basis of the stockpile appears to be stronger in FY16 and we anticipate modest growth over the next several years.

Energy related programs are currently the area with the largest potential for growth. MPA-11 was recently identified as one of the leads for the Fuel Cell Consortium for Performance and Durability. There is currently a call underway for lightweight materials for sustainable transportation. In addition, support for advanced manufacturing remains strong, which may provide new opportunities for nanotechnologies, functional materials, and scale-up.

FY16 is shaping up to be another great year for MPA. Funding for science is strong with growth in areas of energy and directed stockpile work. I look forward to the opportunities ahead and our continued contributions to physics and material science. Your work changes the world, and I hope like me, you are proud to be associated with Los Alamos National Laboratory.

MPA Deputy Division Leader Rick Martineau

"FY16 is shaping up to be another great year for MPA. Funding for science is strong with growth in areas of energy and directed stockpile work. I look forward to the opportunities ahead and our continued contributions to physics and material science."

From Kristin's desk . . .

By now, most of us have attended at least one meeting on Los Alamos's new purpose statement. I have been fortunate to attend three: the Director's initial rollout and two meetings within our AD. As a group-level manager, the ADEPS meetings provide a useful window into the frustration many of us feel with our current circumstances. From facilities problems, to indirect costs, to the lack of a clear path for career development, the list of issues we face in our workplace every day can seem insurmountable. The good news is, we have a clear mandate to discuss these issues with our AD, and we have an AD who is genuinely interested in improvement. The bad news is, by making lists of problems with no clear solutions, we risk losing sight of the positive aspects of working at the Laboratory.

Over the years, I've seen many of my colleagues leave Los Alamos for greener pastures. One went to EPA—right before EPA began using Concur. He tells me their implementation of Concur is much harder to navigate than ours. One went to DHS, which lost her clearance, then required her to complete a six-month background check to handle OUO information. She says she misses our clearance processing folks and the classification office. One went to a lab run by a nonprofit organization where his supervisor micromanaged his work and discouraged him from talking with his colleagues because it would be too "distracting." He misses the relatively hands-off style of our management and the many opportunities he had to collaborate. We can all agree that Los Alamos is not perfect, but over the years, I've concluded that few places *are*.

Mary Hockaday has asked us to identify areas in which we, *personally*, can improve processes, remove impediments, and make the Lab a better place to work. That's a tough challenge, because it's much easier (though less productive) to point out how *other* parts of the Lab need to change. The first paragraph of A.A. Milne's *Winnie-the-Pooh* describes the difficulties I'm having with Mary's charge:

> *"Here is Edward Bear, coming downstairs now, bump, bump, bump, on the back of his head, behind Christopher Robin. It is, as far as he knows, the only way of coming downstairs, but sometimes he feels that there really is another way, if only he could stop bumping for a moment and think of it. And then he feels that perhaps there isn't."*

As a manager, I often suspect I could be doing things better, if only the incessant bumping would stop so I could think about it. I've been here 16 years, and many of our processes are so ingrained that I find it hard to imagine doing things differently. However, if I think back, over time, there are processes that have improved notably. For example, classification review: with designated unclassified subject areas (DUSAs) and RASSTI, approving a poster or presentation for unlimited release—a process that used to take days—takes only a few minutes now. With the VOIP phone system, moving a phone line—which also used to take days—is as easy as plugging the phone in at its new location. Admittedly, other processes have gotten more difficult, and it's not always clear why; but sometimes we can mitigate this. For example, in CINT, we've brought in more support for procurement to remove some of the burden on staff.

It's hard to see a clear line from improvements in everyday processes to the "greatest imaginable challenge" (GIC) of 10-20% growth per year. That's something I see us struggling with during the purpose meetings. But I believe we have the best talent, that we can perform at the highest levels, and that we provide people with opportunities to do things they could never imagine. And I believe if we can stop the bumping for long enough, we can figure out how to bring the GIC within reach. So if you have ideas for improvement—especially if they involve something within the Division's span of control—I encourage you to talk to me or another member of the Division management team. And I promise I'll try to take a break from the bumping to listen.

"Mary Hockaday has asked us to identify areas in which we, personally, can improve processes, remove impediments, and make the Lab a better place to work."

MPA-CINT Deputy Group Leader Kristin Omberg

Successful search for novel topological states

Madhab Neupane, a 2015 Director's Postdoctoral Fellow with Condensed Matter and Magnet Science (MPA-CMMS), is searching for bulk-insulating material with metallic surface properties that could revolutionize the electronics industry. His study of various materials at Los Alamos National Laboratory has already resulted in several significant papers.

The new concept of topological states in condensed matter and material science predicts the existence of surface states that are insensitive to environmental conditions, like contamination, due to protection by fundamental symmetries. Neupane's work is focused on strongly correlated topological insulators—unusual materials that host both strong correlations in the bulk material and topologically protected metallic surface states. He wants to find topological surface states in *f*-electron systems that could be used in spintronics and quantum computing. Tomasz Durakiewicz (MPA-CMMS) is his mentor.

The rare-earth-hexaboride YbB_6 was predicted to be a topological insulator, where hybridization of localized *f* electrons with conduction electrons leads to opening of the gap and inhibits the metal's ability to carry an electric current. However, according to his report in *Physical Review Letters*, Neupane's angle-resolved photoemission studies (ARPES) showed instead that YbB_6 exhibits a novel topological insulator state in the absence of a Kondo mechanism (see figure). Through experiment and theory, Neupane and collaborators provide a new approach for realizing a topological insulator in rare-earth materials—a significant breakthrough because this mechanism was not known before.

Neupane has also investigated other possible topological insulators, including the superconductor BiPd and the rare-earth hexaboride CeB_6.

He received a PhD in physics from Boston College in 2010 for angle-resolved photoemission work on ruthenates and iron-based superconductors. He spent four years at Princeton University, performing frontier work on topological insulators. He has coauthored more than 40 peer-reviewed publications, with more than 1,400 citations.

The U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences, and the Los Alamos Laboratory Directed Research and Development program funded his research. The work supports the Lab's Energy Security mission area and Materials for the Future science pillar by establishing the scientific foundations to design the functionality of strongly correlated materials with non-trivial topology.

Technical contact: Madhab Neupane

References:

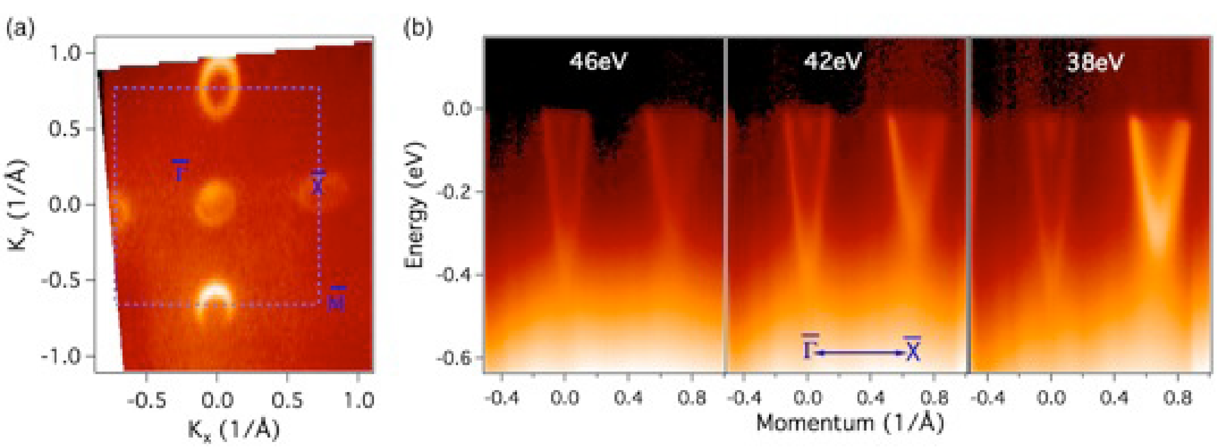
1.) "Non-Kondo-like electronic structure in the correlated rare-earth hexaboride YbB_6," *Physical Review Letters* **114**, 016403 (2015).

Madhab Neupane (Princeton University) and Tomasz Durakiewicz (MPA-CMMS) with collaborators from University of California at Irvine, National Tsing Hua University (Taiwan), Academia Sinica (Taiwan), National University of Singapore, and Northeastern University.

2.) "Gigantic surface life-time of an intrinsic topological insulator," (2015) accepted, *Physical Review Letters*, Neupane, Durakiewicz, and collaborators.

3.) "Discovery of the topological surface state in a noncentrosymmetric superconductor BiPd," arXiv preprint arXiv:1505.03466 (May 14, 2015), by Neupane and Durakiewicz with co-authors from Princeton University, National Tsing Hua University (Taiwan), Academia Sinica (Taiwan), National University of Singapore, Northeastern University, Polish Academy of Sciences

4.) "Fermi surface topology and hotspots distribution in Kondo lattice system CeB_6," arXiv preprint arXiv:1411.0302. Madhab Neupane, Durakiewicz, and collaborators.



Fermi surface and dispersion map. (a) ARPES measured Fermi surface of YbB_6. Circular-shaped pockets are observed at $\bar{\Gamma}$–$\bar{X}$ points. The Fermi surface is measured with a photon energy of 50 eV at a temperature of 15 K. (b) ARPES dispersion maps measured with different photon energy. The measured photon energies are noted on the plots. These data were collected at the Advanced Light Source, Lawrence Berkeley National Laboratory.

A hybrid ultrasmall gold nanocluster for enzymatic fuel cells

New technique removes barrier to development of fuel cells with efficient performance

With fossil fuel sources dwindling, an urgent demand exists for alternate sources of energy using natural resources such as air, water, and sunlight.

Enzymatic fuel cells and nanomaterials show great promise in this regard—and as they can operate under environmentally benign neutral pH conditions—are a greener alternative to existing alkaline or acidic fuel cells, making them the subject of worldwide research endeavors.

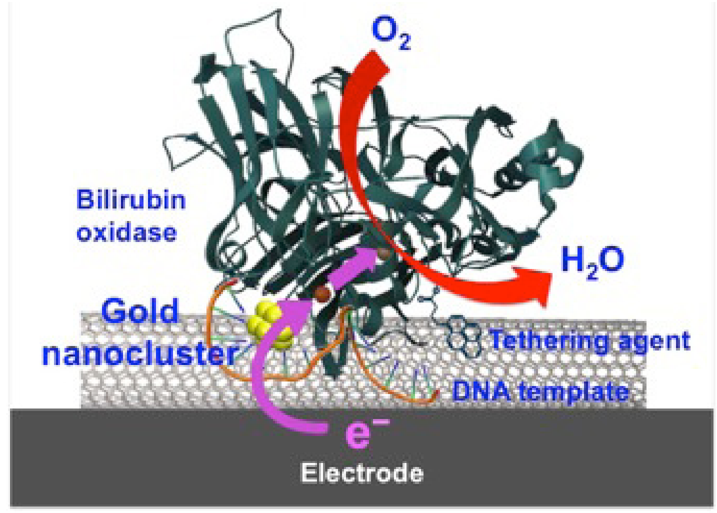
In enzymatic fuel cells, fuel is oxidized on the anode, while oxygen reduction reactions (ORR) take place on the cathode, often using multi copper oxidases. Enzymatic fuel cell performance depends critically on how effectively the enzyme active sites can accept and donate electrons from the electrode by direct electron transfer (ET). However, the lack of effective ET between the enzyme active sites, which are usually buried ~10Å from their surface, and the electrode is a major barrier to their development. Therefore, effective mediators of ET are needed.

In research published in the *Journal of the American Chemical Society*, Los Alamos researchers and external collaborators synthesized and characterized a new DNA-templated gold nanocluster (AuNc) that enhanced ET. This novel role of the AuNC as enhancer of ET at the enzyme-electrode interface makes it a potential candidate for the development of cathodes in enzymatic fuel cells, thus removing a critical methodological barrier for efficient biofuel cell design.

Possessing many unique properties due to their discrete electron state distributions, metal nanoclusters (<1.5 nm diameter; ~2-144 atoms of gold, silver, platinum, or copper) show application in many fields.

Ligands are necessary to form stable nanoclusters. For this study, the researchers chose single-stranded DNA as the ligand, as DNA is a natural nanoscale material having high affinity for metal cations and can be used to assembly the cluster to other nanoscale material (e.g. carbon nanotubes).

Hypothesizing that due to the ultra-small size (the clusters are ~7 atoms, ~0.9 nm in diameter), and unique electrochemical properties, the AuNC can facilitate ET to an ORR enzyme active site and therefore, lower the overpotential of ORR. When self assembled with bilirubin oxidase and carbon nanotubes the AuNC acts as enhancer of ET and lowers the overpotential of ORR by a significant ~15 mV (as opposed to ~1-2 mV observed using other types of mediators) compared to the enzyme alone. The AuNC also causes significant enhancement of electrocatalytic current densities.



Schematic showing the integration of the AuNC with bilirubin oxidase, and carbon nanotubes deposited as composite materials on electrode surface. The role of the AuNC to enhance enzymatic ORR by facilitating efficient electron transfer (thus lower overpotential and improved kinetics) from the electrode to the enzyme active site is shown as purple arrows.

Finally, the presence of AuNC does not perturb the mechanism of enzymatic O_2 reduction as a clean $4e^-$ reduction of O_2 was observed with minimal (~3%) production of $2e^-$ reduction product (H_2O_2). Such unique application of AuNC as facilitator of ET by improving thermodynamics and kinetics of O_2 reduction is unprecedented.

Reference: "A hybrid DNA-templated gold nanocluster for enhanced enzymatic reduction of oxygen," *JACS* DOI: 10.1021/jacs.5b05338.

Researcher affiliations: Saumen Chakraborty, Reginaldo C. Rocha, Anil Desireddy, Amy E. Boncella , and Jennifer S. Martinez (all Center for Integrated Nanotechnologies, MPA-CINT); Sofia Babanova, Kateryna Artyushkova, Plamen Atanassov (Center for Micro-Engineered Materials, CMEM, and Department of Chemical & Biological Engineering, The University of New Mexico)

The study was a CINT user project with additional funding from Los Alamos's Laboratory Directed Research and Development program (TEM/EDX), DOE's Basic Energy Sciences Biomolecular Materials Program (assembly), and the Air Force Office of Scientific Research and the ARO-Multi-University Research Initiative grant (for electrode testing, UNM).

This work supports the Materials for the Future Science Pillar in developing materials with emergent phenomena that supports U.S. energy security.

Technical contacts: Saumen Chakraborty, Jennifer S. Martinez

Los Alamos researchers develop high-speed fiber-optic-based strain and pressure interrogation system for dynamic conditions of materials in extremes

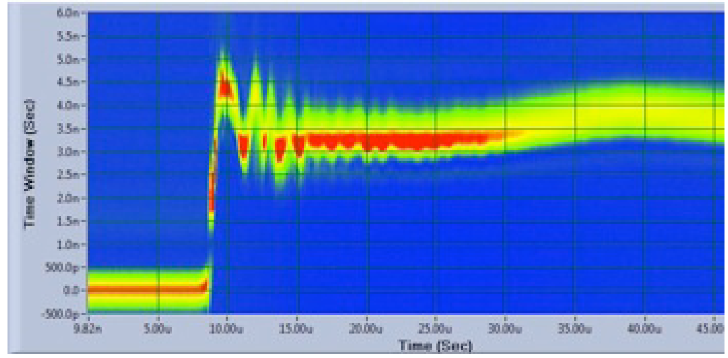
Los Alamos researchers recently developed and demonstrated the use of a novel fiber Bragg grating (FGB) sensing interrogation system in dynamical extreme conditions not possible using traditional FBG interrogation approaches deemed too slow to capture such events.

The Los Alamos breakthrough research is described in a July *Optical Society of America* "Spotlight on Optic" article as "an important step towards real-time measurement and analysis of process dynamics" for understanding material behavior in extremes.

Fiber optic sensors for measurements in difficult environments have been intensively studied for many years. Some of their most important advantages are high sensitivity, immunity to electromagnetic interference, and high speed. Among others, sensor setups to measure temperature, strain and pressure have gained significant importance, and FBG sensors in particular have been widely investigated and used for these applications.

In the article, Rodriguez and co-workers concentrate on very fast sensors for difficult environments, namely time-resolved ultrahigh magnetic field measurements and pressure dynamics analysis in thermal ignition of explosives. Although the general response of an FBG to temperature, strain, and pressure has been well known for years, the key advance was the development of high speed (100 MHz) interrogation rate methods surpassing by several orders of magnitude the previously existing interrogation speed techniques, thus enabling real-time diagnosis of dynamical events. The system developed measures the Bragg wavelength shift with a high repetition femtosecond laser, a stretching fiber performing a spectral-domain-to-time-domain conversion of the sensing signal, a high-speed (35 GHz) detector, and a high-speed sampling oscilloscope (50 GS/s). It relies on chromatic dispersion of the FBG interrogating optical pulse to transform a time pulsed repetitive signal to be transformed into the spectral domain via group velocity dispersion introduced by the dispersion in the fiber that temporally disperses the pulses. The high-speed detector samples the spectral content of each pulse every 20 ps as provided by the sampling speed of the oscilloscope.

Two impressive examples are given to demonstrate this interrogation technology. The first deals with the measurement of magnetic-field-driven magnetostrictive effects. The dynamics of the strain in a magnetostrictive material are at extremely high magnetic fields in the order of 150 T. The system's high resolution in the time domain allows the observation of, e.g., acoustic effects and phase transitions in the material. In addition to these results, some new questions arise that will stimulate future research. The second example is in the field of pressure measurement in thermal ignition of high explosives. In the presented measurements,



An example plot of processed coherent time domain FBG waveform data from a pulsed magnetic field (150 T) driven magnetostriction strain experiment on the 2-mm long magnetic perovskite $LaCoO_3$ system followed by launch an acoustic wave after elongation of the sample. The researchers show a time-time plot of the 1555 nm 1-mm FBG sensor versus for 50.036 km of dispersion. The left ordinate axis is a window of 6.5 ns within one laser clock period time slice (10 ns), and the abscissa axis is the event time beginning from the trigger of the NHMFL single-turn capacitor bank and has not been time corrected for the various delays in the signal and trigger paths. Conversion of the left ordinate time axis of into FBG wavelength shift yields a λ-shift ($\Delta\lambda$ vs. t) time plot as shown in the right ordinate axis labels. A positive shift to longer wavelength indicates that the strain resulted in elongation of the sensor/sample combination. A mean FBG wavelength shift of over $\overline{\Delta\lambda} \geq +4$ nm is observed.

effects such as material phase changes become visible. Different process phases like heating and pressurization can be observed and analyzed in detail.

Reference: "Coherent pulse interrogation system for fiber Bragg grating sensing of strain and pressure in dynamic extremes of materials," *Optics Express* **18** (11**)** (2015); Optical Society of America "Spotlight on Optics" www.osapublishing.org/spotlight/summary.cfm?id=318940.

The Los Alamos research team includes George Rodriguez and Abul Azad (Center for Integrated Nanotechnologies LUMOS Team, MPA-CINT), Laura Smilowitz and Bryan Henson (Physical Chemistry and Applied Spectroscopy, C-PCS) for the thermally driven explosives work, and Marcelo Jaime, Fedor Balakirev, and Chuck H. Mielke (National High Magnetic Field Laboratory, Condensed Matter and Magnet Science, MPA-CMMS) for the strain measurement in an ultrahigh magnetic field. Early concept development for the approach was in collaboration with Brandon La Lone and Bruce Marshall from the Special Technologies Laboratory in Santa Barbara, Calif., of National Security Technologies, LLC. The research supports the Laboratory's mission and Materials for the Future science pillar by enhancing materials dynamics diagnostic capability for complex materials

continued on next page

HeadsUP!

Improving our work control systems

Call for micro-experiment solutions

Todd Conklin worked at Los Alamos National Laboratory for 26 years, leaving in 2012 to work as a safety consultant to help organizations better understand and improve their human performance. After the arc flash event here this summer, he returned to the Laboratory as a consultant. He reviewed the event and others and presented a talk to senior managers. He told the managers that the Laboratory needed to change its definition of success. There are two key quotes from his slides as related to work control:

- "We have conflicting missions: my success is based upon world-class science. Their success is based upon ZERO risk."
- The second was a challenge to managers: "You have a duty to produce a different outcome: perfection cannot be the expectation; you must design your systems with the capacity to recover. This is a deliberate management strategy."

Todd recommended that we look at our systems and then try what he called micro-experiment solutions. In other words, we develop and try new ideas before we build huge systems.

To deliver world-class science, ADEPS is proposing to look at R&D skill-based activities, work that can be done without written instructions. The goal of the micro-experiment would be to identify in each group one skill-based work activity and to then convert the integrated work document for this class of activities to a one-pager.

A call for volunteers was made and the first activity of the group, the ADEPS team, was a video conference with Lawrence Livermore National Laboratory staff on their new work control initiative. After the conference, the team compiled a list of positive and negative attributes of the system relative to the needs at Los Alamos. The concept of a skilled worker was well received to reduce the need for work documents and to address the idea of "skill of craft" for worker qualifications.

Another well-received idea, although it goes against the idea of huge systems, was that Livermore has an online system tracking all requirements: work control, training requirements, worker qualification, RLM approvals, etc.

Since the video teleconference, Los Alamos has initiated an institutional effort to look at the integrated work management system. Mary Hockaday is leading that effort. In a note to the volunteer group, she wrote, "If we are going to live up to our dream and accomplish our greatest imaginable challenge, we need to change the systems that are limiting our ability to perform efficiently."

During the month of October, concurrent with the institutional effort, Mary has asked the team to brainstorm the biggest payoff activity we can do with our micro-experiment. If you have ideas or would like to join the team, please e-mail Howard Nekimken at hnek@lanl.gov.

Celebrating service

Congratulations to the following MPA Division employees celebrating service anniversaries recently:

John Joyce, MPA-CMMS	25 years
Andrew Dattelbaum, MPA-11	15 years
Troy Semelsberger, MPA-11	15 years
Steve Gilbertson, MPA-CINT	5 years

Extremes cont.

and energetic materials under conditions of extremes. It is also applicable to Laboratory weapons physics experimental diagnostic capability.

This Los Alamos work was funded by Laboratory Directed Research and Development and the National Science Foundation NHMFL programs.

Technical contact: George Rodriguez

MPA Materials Matter

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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822 or kkippen@lanl.gov.
To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml.

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