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Tommy Rockward (left) watches as University of New Mexico graduate student Andre Spears (right) attaches fuel cell hardware to a test bench. Spears is funded as a graduate research assistant through the African American Partnership Program.

Photo by Michael Pierce (XIT-TSS)

Tommy Rockward

Fueling a new generation of materials scientists

By H. Kris Fronzak, ADEPS Communications

“
One of the most exciting things for me is when students come away from my classes with an understanding of both the lectures and the 'career talk.' I like providing them with certainty in their career paths
”

When not at Los Alamos developing more efficient fuel cells in his lab, Tommy Rockward moonlights as another kind of experimentalist: a breeder of African cichlids. In his Rio Rancho home, he raises thousands of these colorful, freshwater fish—what he estimates to be the largest variety in New Mexico. One of his most recent creations is a hybrid that flashes purple and yellow hues “like the [Los Angeles] Lakers” when it wants to show off.

Rockward applies that same sense of innovation to his work as a researcher in Materials Synthesis and Integrated Devices (MPA-11). For example, as part of a DOE-funded project he spent 10 years developing an international standard for the purity of hydrogen fuel for vehicles. By probing different fuel impurities and their concentrations, Rockward

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The materials capability, guided by our strategy, is the joint platform that connects all our work to the rest of the Lab—people, facilities, instrumentation—and the Lab’s missions of nuclear, global, and energy security.

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Tanja

From Tanja’s desk . . .

It’s already March! Hard to believe . . . Our Materials Capability Review is only a few weeks away, at the time of writing. First of all, I want to thank everyone who is contributing—speakers, poster presenters, and all our professional staff who actually make it happen. This year it’s been a particular challenge due to the large number of posters. We are reviewing all seven areas of leadership! On the bright side, the review should provide an excellent opportunity for everyone to get a full overview of our materials capability in a short amount of time. Why would that matter to you? The materials capability, guided by our strategy, is the joint platform that connects all our work to the rest of the Lab—people, facilities, instrumentation—and the Lab’s missions of nuclear, global, and energy security. It’s a great opportunity to make connections with folks from outside MPA and learn about materials research going in other parts of the Lab. It might inspire new ideas or forge new collaborations, so come and join us!

As a reminder, the Materials Capability Review will take place in April: the technical sessions are Monday and Tuesday, April 9 and 10, and the outbrief will be on Wednesday, April 11. Contact MPA-DO for the current version of the agenda. Once we have the final version, we will distribute it via email.

The entire MPA-DO has been extremely busy with lay downs and dry runs of the review material, and that will continue for a few more weeks. This also means that we have less time to be out in the field, and both Rick and I look forward to having more time to see you all once the review is done. Nevertheless, don’t ever hesitate to contact us with any questions or concerns that you may have.

MPA Division Leader Tanja Pietraß



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According to a 2007 study published in *Circulation Research: Journal of the American Heart Association*, most women younger than 55 that experienced a heart attack did not recognize the symptoms.

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George

From George's desk ...

February was Heart Health Month, and this is a topic that hits close to home for me. According to the American Heart Association (AHA), heart disease is the number 1 killer in the United States for both men and women and accounts for nearly 1/3 of all female deaths. One reason heart disease is so deadly for women is that the symptoms of a heart attack exhibited by women are often atypical and subtler when compared to the chest or radiating arm pain more commonly experienced by men. In my family I have first-hand experience with this. My mother has had two episodes that landed her in the hospital, and she did not exhibit classic heart attack symptoms either time. One time she said she was feeling pressure “like an elephant sitting on my chest” and the other time she was feeling extremely fatigued and a stabbing back pain. The first time my mother went to the emergency room she ended up with a couple of stents, but the second time she ended up with a month-long stay to recover from quadruple bypass surgery.

Despite being the leading cause of death for women in the country, only 1 in 5 women believe heart disease is her greatest health threat. In fact, many women do not recognize the symptoms of a heart attack and they are more likely to write off the symptoms as something less severe, such as acid reflux, the flu, or aging. According to a 2007 study published in *Circulation Research: Journal of the American Heart Association*, most women younger than 55 that experienced a heart attack did not recognize the symptoms. While 90% of the women in the study reported some degree of chest pain, only 42% of these patients suspected the chest pain was related to heart problems and most of the women believed they were suffering from indigestion or heartburn. Other symptoms commonly experienced by women during a heart attack include pain in the jaw or shoulder, sweating, nausea, shortness of breath, indigestion or heartburn, and fatigue. Because these symptoms are so common, they are not often associated with heart health and are misdiagnosed even within the medical community. In that same 2007 study, 38% of the women did seek treatment for their symptoms from a primary care physician, yet only 56% of these women said their doctors told them their symptoms could be heart-related.

My family has been very fortunate so far... My mother survived both of her episodes because her family recognized something was wrong and got her to the hospital before she had a heart attack. The Laboratory is going through a period of significant transition with the upcoming contract change. While this doesn't change our need to execute our missions safely and securely, it surely adds additional stress to our lives. We all know the detrimental effects stress can have on our health, including an increased risk for heart attack. So, in honor of all of the important women in your life, I encourage you to take a few minutes to learn about the AHA sponsored Go Red for Women Initiative (www.goredforwomen.org). In the meantime, stay safe and take care of yourselves and your colleagues!

MPA-11 Deputy Group Leader George Goff

Rockward cont.

and his colleagues in industry, academia, and other national labs established the effects on fuel cell performance, durability, and cost. The resulting specification is still in use today.

With nine older siblings, Rockward said he “was tutored every step of the way” in life and in his studies. He carved a unique space for himself in the family at an early age, making do-it-yourself baking soda and vinegar volcanoes. Rockward attended a rigorous college preparatory high school before attending Southern University A&M, where he joined the school’s ongoing fuel cell research program. He quickly determined that fuel cells were “an exploding field in science with a lot of promise,” he said—a field where he could make an impact.

Rockward graduated with a master’s degree in applied physics, a taste for teaching gained through a semester as a teacher’s assistant, and a keen interest in fuel cells. An internship at Los Alamos further cemented his interest in clean energy for transportation, and he formally began his career at the Laboratory in 1997 as a graduate student.

Rockward has accumulated several awards and patents over his career, including a DOE Hydrogen and Fuel Cells Program R&D award and the patents “Non-aqueous liquid composition of ion exchange” and “Hydrogen fuel quality analyzer with self-humidifying electrochemical cell and methods of testing fuel quality.” He was also the chair of an ASTM International committee formed to lead inter-laboratory studies on detection of contaminants in fuel cells.

To ensure that a new generation has similar opportunities, Rockward created CMaES, the Consortium for Materials and Energy Security. The program aims to diversify the pipeline of researchers at national labs by introducing minority students to the scientific lab environment via positions at Los Alamos and Lawrence Livermore National Laboratory. Rockward first proposed the program to the National Nuclear Security Administration in 2012 and now serves as an informal mentor for many of CMaES’s participants. The program, funded by the NNSA, Los Alamos’s Director’s Office, and the DOE’s Fuel Cell Technology Office, has helped many young researchers attend graduate school and accept full-time lab positions.

“Tommy is an amazing mentor. I can always go to him with problems or questions and know that he will help as much as he can,” said Shaylynn Crum, a CMaES participant in Chemical Diagnostics and Engineering (C-CDE) who is developing an additively manufactured polymer. “Deciding to come to Los Alamos was one of the greatest decisions I could have made.”

Rockward’s passion for helping students extends to his after-work hours. He is an associate professor at Northern New Mexico College where he teaches math to undergraduate students. He was named Northern’s Teacher of the Year in 2010.

“One of the most exciting things for me is when students come away from my classes with an understanding of both the lectures and the ‘career talk.’ I like providing them with certainty in their career paths,” he said. “Teaching is my way of giving back to the community.”

Tommy Rockward’s favorite experiment

What: Investigating the impact of both hydrogen sulfide (H_2S) and carbon monoxide (CO) in an operating PEM fuel cell.

Why: The current ISO14687-2/SAE J2718 Hydrogen Fuel Specification allows both species to be present at low levels. Understanding their simultaneous interaction in fuel cells could help determine the appropriate impurity levels in fuel specifications and develop appropriate mitigating strategies.

When: 2008-2009

Who: Tommy Rockward, Idoia Urdampilleta, Francisco Uribe, and Fernando Garzon (all at Los Alamos at the time).

How: Using pre-mixed gases and calibrated mass flow controllers, we introduced the contaminants H_2S and CO into the anode stream of an operating fuel cell.

The “a-ha” moment: Our initial fuel quality experiments fixed the H_2S and CO concentration ratios and exposure time while varying fuel cell operating conditions. The information obtained from these experiments proved useful, but it was challenging to decouple which species was responsible for fuel cell performance decay (since both species can adsorb on electrochemically active platinum sites and block hydrogen dissociation). So, instead of performing the experiments in fuel cell mode we used cyclic voltammetry, a technique used to probe the surface of electrochemically active materials such as platinum. We were able to experimentally show that CO adsorbs much faster than H_2S on the surface of platinum but becomes displaced as exposure time is increased.

CINT researchers develop a new, contact-free neuroimaging microscope

Instrument can also image electric fields in inorganic materials

Decades of research have been dedicated to improving contact-free neuroimaging techniques that allow users to image neurons in the brain. Recently, Center for Integrated Nanotechnologies (CINT) scientists developed an advanced microscopy system that visualizes materials' internal and surface structures through nonlinear-optical interaction induced by external lasers. The system is unique in that it provides for multiple image contrast mechanisms, including sensitivity to vibrational resonances and quasi-static electric fields in the sample. This capability, combined with the expertise of CINT scientists, could offer novel modalities for sample imaging and diagnostics for CINT users.

The optical microscopy system was created by Anatoly Efimov and Evan Perillo (Center for Integrated Nanotechnologies, MPA-CINT). It could prove an important avenue for studying biological, organic, and inorganic materials, and Efimov anticipates the instrument being used by Los Alamos and external researchers in biology, chemistry, and materials sciences via the CINT user program.

Efimov and Perillo designed the microscope to send femto-second laser pulses to a sample in the mid-infrared frequency range and to allow users to probe both transparent and opaque materials. The tool can use both laser scanning and sample scanning to obtain the image. Because the excitation path of the microscope is all-reflective, there are no issues with attenuation, dispersion, and chromatic aberrations typical for standard refractive microscopes. Photon counting detectors are used for extremely low light levels typically encountered in nonlinear imaging modalities. Provisions are made to accommodate electrical and electrophysiology probes for sample connectivity. Available image contrasts include multiple-photon fluorescence, vibrationally resonant harmonic and sum-frequency generation, and coherent and stimulated Raman processes. The lasers' wavelengths can be tuned continuously in the 1-5 μm range, letting the user

target vibrational resonances in molecules and enhance specific nonlinear interactions. Excitation lasers can be temporally synchronized and variably delayed to enable pump-probe interrogation of the sample and allow for time-based image contrast, such as lifetime and delayed response.

The instrument was designed and built with funding from the Laboratory Directed Research and Development program exploratory project "Sensitive optical super-resolution neuroimaging," which aims to image the quasi-DC electric field of the neuronal action potential. Such chemical imaging of live neurons yields an intrinsic high-contrast signal that lets users study high-speed firing events in large groups of neurons.

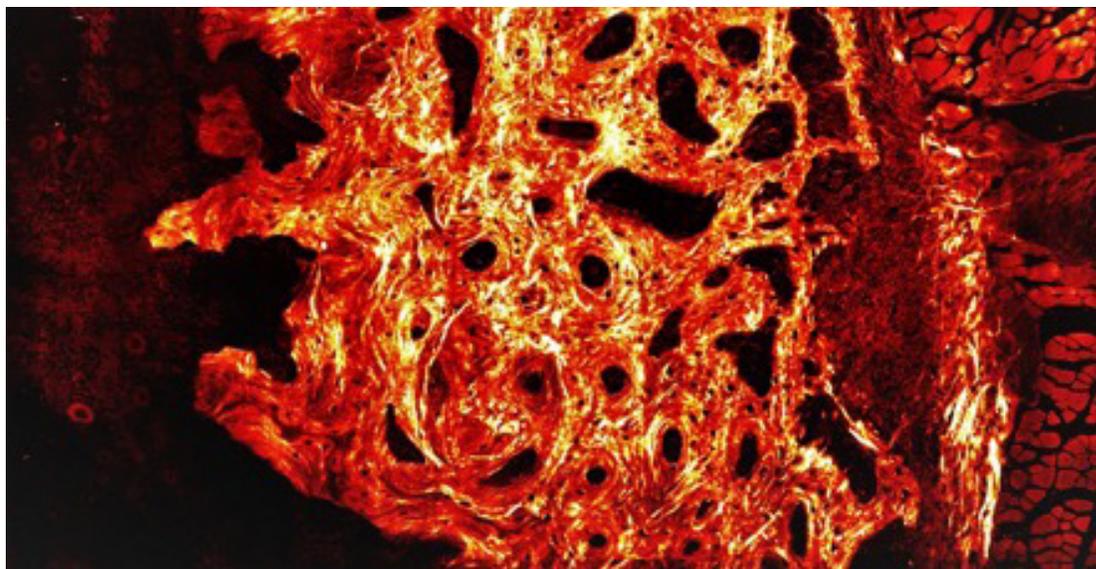
In a broader scope, the system can be used to image electric fields in materials and samples relevant to the Laboratory's Science of Signatures and Materials for the Future missions. The work supports the Laboratory's Global Security mission area.

Efimov and Perillo are preparing the instrument for use in the lab. They plan to continue testing the microscope's sensitivity limits to the DC-electric field using lithography-manufactured non-biological samples and to explore lateral resolution limits, field of view extents, and imaging speeds. The pair is also running baseline experiments with simple biological samples to reproduce past results from literature.

CINT is a DOE Office of Basic Energy Sciences user facility operated by Sandia National Laboratories and Los Alamos National Laboratory. It offers access to a unique combination of expertise and equipment in a world-class nanoscale science research center.

Technical contact: Anatoly Efimov

An image of mammalian compact bone taken by the new neuroimaging microscope. The signal originates from second harmonic generation of collagen within the osteons of the bone. Image size is 0.75 mm by 1 mm.



Prasankumar elected secretary-treasurer of American Physical Society's Division of Laser Science

Rohit Prasankumar (Center for Integrated Nanotechnologies, MPA-CINT) was elected secretary-treasurer of the American Physical Society's (APS) Division of Laser Science.

The division promotes laser science interests within the APS and other societies and sponsors numerous awards, conferences, and educational programs.



As secretary-treasurer, Prasankumar will serve through October 2020 and be responsible for maintaining the records and funds in the division.

Prasankumar earned his PhD in electrical engineering from the Massachusetts Institute of Technology in 2003. His thesis focused on developing and applying saturable absorbers to femtosecond solid-state laser mode-locking. He joined Los Alamos National Laboratory as a postdoctoral researcher with CINT's Laboratory for Ultrafast Materials and Optical Science team and became a staff member in

2006. He oversees two optical laboratories at CINT, where he pursues new research at the intersection of ultrafast laser science, condensed matter physics, and nanotechnology. In particular, his research focuses on ultrafast dynamics and phenomena in complex quantum materials from terahertz to x-ray frequencies. Prasankumar has published more than 50 peer-reviewed articles and has more than 1,500 citations.

CINT is a DOE Office of Basic Energy Sciences national user facility jointly operated by Sandia National Laboratories and Los Alamos National Laboratory. Prasankumar's research supports the Lab's Materials for the Future strategy by advancing research vital to the Lab's quest for controlled functionality and by examining the properties of quantum materials.

The American Physical Society is a non-profit membership organization working to advance and disseminate the knowledge of physics through its outstanding research journals; scientific meetings; and education, outreach, advocacy, and international activities. APS represents more than 53,000 members, including physicists in academia, national laboratories, and industry around the world.

Technical contact: Rohit Prasankumar

First experimental measurement identifies exciton mass in new class of 2D semiconductors

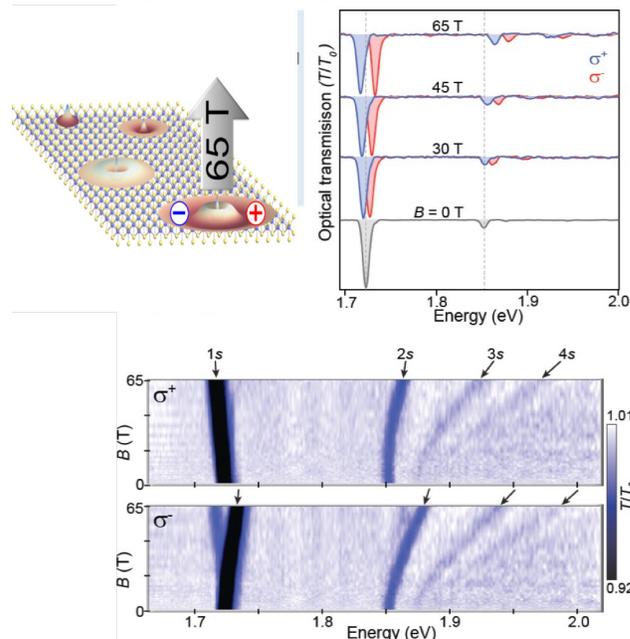
Understanding this fundamental material parameter could be key to developing new technologies

In work published in *Physical Review Letters*, Los Alamos National Laboratory researchers and their colleagues report the first direct measurement of the mass of the fundamental particles in an atomically thin semiconductor by using high magnetic fields.

The results are important not only as a guide to theoretical models but also to the widely anticipated rational design and engineering of future ultrathin, lightweight, and efficient optoelectronic devices based on this new class of two-dimensional semiconductors. The research appears as an "Editor's Suggestion" in the journal.

Using the high magnetic fields at the National High Magnetic Field Laboratory-Pulsed Field Facility at Los Alamos, the researchers measured the optical spectrum of a single monolayer of tungsten diselenide (WSe_2), an archetypal member of the recently discovered class of atomically thin semiconductors known as the transition-metal dichalcogenides. In doing so, they were able to directly measure the mass of the material's fundamental optical excitation—an electron-hole pair, or "exciton." In all semiconductors, excitons play an essential role in technological applications such as solar cells or light-emitting diodes. An exciton has a certain weight, or mass, that influences most aspects of device

Continued on next page



Using WSe_2 monolayers placed over the core of single-mode fibers, researchers measured circularly-polarized optical spectra from 0-65 T in a pulsed magnet. The field-dependent diamagnetic shifts of the 1s, 2s, 3s, and 4s excited (Rydberg) states of the neutral exciton are clearly observed, providing a robust measurement of the exciton's mass for the first time in this new class of two-dimensional semiconductors.

First cont.

performance, so understanding its specific mass is critical to modeling and developing devices.

The team used the mag lab's 65-T capacitor-driven pulsed magnet to perform these measurements. Together with colleagues at the University of Washington, they carefully positioned single monolayers of high-quality WSe_2 over the tips of single-mode optical fibers, thereby ensuring a rigid alignment between the optical path and the small monolayer crystals that is immune to the vibrations that are otherwise inherent in pulsed-magnet measurements.

The Los Alamos portion of the work was funded by the National Science Foundation, the Department of Energy, and the State of Florida. The study supports the Laboratory's Energy Security mission area and its Materials for the Future science pillar and its Emergent Phenomena science theme by providing experimental measurements of fundamental material parameters. Such measurements aid efforts to develop materials with predictable performance and controlled functionality, a core vision of the Laboratory's materials strategy.

Researchers: Andreas V. Stier (formerly National High Magnetic Field Laboratory Pulsed Field Facility [NHMFL-PFF], now Plasma Physics, P-24), Kirill A. Velizhanin (Physics and Chemistry of Materials, T-1), Nathan P. Wilson and Xiaodong Xu (University of Washington), Junichiro Kono (Rice University), and Scott A. Crooker (NHMFL-PFF).

Reference: "Magneto-Optics of Exciton Rydberg States in a Monolayer Semiconductor," *Physical Review Letters* **120**, 057405 (2018).

Technical contact: Scott Crooker

Celebrating service

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

Dipen Sinha, MPA-11	35 years
Rick Martineau, MPA-DO	30 years
Yu Seung Kim, MPA-11	15 years
Boris Maiorov, NHMFL-PFF	15 years
Cristian Pantea, MPA-11	15 years
Chris Sheehan, MPA-CINT	15 years
Hoon Chung, MPA-11	10 years
Millicent Firestone, MPA-CINT	5 years
Wanyi Nie, MPA-11	5 years

HeadsUP!

VPP recertification celebration

The Laboratory recently celebrated its re-certification as a DOE Voluntary Protection Program (VPP) Star Site.

Since 2014, Los Alamos National Laboratory has held the title of the largest Department of Energy VPP Star site. Every Laboratory worker's visible contribution and demonstration of ownership and leadership in safety and security made this three-year recertification possible. Only DOE contractors with outstanding safety and health programs are awarded Star recognition, the highest achievement level.



As part of celebrations held across the Lab recognizing LANL's recertification as a DOE Voluntary Protection Program Star Site, employees at the Los Alamos Neutron Science Center enjoyed light refreshments and the opportunity to receive a commemorative keepsake.

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



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