DOE/NA-0114

National Nuclear Security Administration

Stewardship Science Today

Office of Research, Development, Test, and Evaluation (RDT&E)

VOLUME 3 | NUMBER 1 | MARCH 2021

Stewardship Science Today (SST) highlights the stewardship science and academic programs supported by the Department of Energy/National Nuclear Security Administration (DOE/NNSA). SST is published quarterly by the NNSA Office of Research, Development, Test, and Evaluation. Questions and comments regarding this publication should be directed to Terri Stone via email at terri.stone@nnsa.doe.gov.

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CALENDAR

4/27-30/2021
Omega Laser Users Group (OLUG) 2021 Workshop University of Rochester Laboratory for Laser Energetics, Zoom

6/24-7/2/2021
ISC High Performance 2021 Digital, early registration from mid April - 5/6/2021

7/19-22/2021
Computational Science Graduate Fellowship Virtual Program Review, Zoom

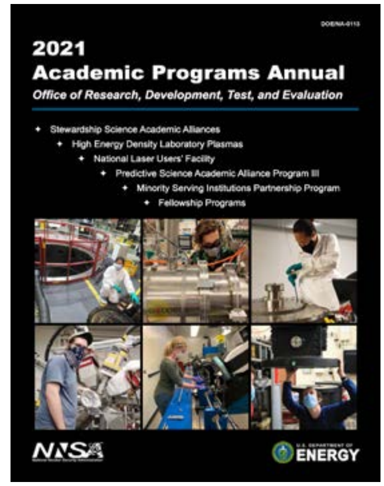
8/10-11/2021
Stewardship Science Graduate Fellowship/ Laboratory Residency Graduate Fellowship Annual Meeting Virtual Program Review

INSIDE

*Contractor Support **National Laboratory Detailee

Amidst the continued isolation brought about by the global COVID-19 pandemic, the Stewardship Science Academic Programs (SSAP) Annual Symposium went virtual this year and achieved record participation. The poster competition set even more records showing the enthusiasm of both the students and the judges. The SSAP Symposium was an excellent opportunity for us all to gather together in cyberspace and exchange ideas and fellowship, and we extend our sincere thanks to the staff and the community who worked so hard to make the Symposium a reality this year. It was another successful year. You can read more about the Symposium in this issue.

Even in these trying times our work continues to break new ground. The first-ever experiment with high explosives was conducted at the National Ignition Facility (NIF). Understanding the performance of high explosives is essential to our mission, and the data from these NIF experiments will add to our knowledge-base and advance our modeling of nuclear weapon performance. Another recent advancement featured in this issue is work at Sandia National Laboratories to develop composite materials whose mechanical and thermal properties are tuned to create new options for thermal protection system materials which are vital to the evolving stockpile.



The 2021 Academic Programs Annual is available for download by clicking here.

Stay safe. Stay well. Protect yourself and those around you. We'll get through this pandemic together.

Dr. Mark C. Anderson
Assistant Deputy Administrator for Research, Development, Test, and Evaluation

2021 Annual Stewardship Science Academic Programs Symposium

by Dr. Michael Kreisler, Advisor to the National Nuclear Security Administration

The Department of Energy/National Nuclear Security Administration (DOE/NNSA) celebrated another successful Stewardship Science Academic Programs (SSAP) Symposium. The 2021 SSAP Symposium, held virtually February 16-18, 2021, hosted a record 500 registered participants from across the United States and from other countries.

After the opening announcements, Brian Kanagaki, the Lead for Academic Programs in the NNSA Office of Research, Development, Test, and Evaluation (RDT&E), spoke about the recent change of Academic Programs now reporting directly to the Assistant Deputy Administrator of the Office of RDT&E, and he named the subprograms of Academic Programs: Stewardship Science Academic Alliances (SSAA), Joint Program in High Energy Density Laboratory Plasmas (HEDLP), Predictive Science Academic Alliance Program (PSAAP), Minority Serving Institutions Partnership Program (MSIPP), Tribal Education Partnership Program, and the following three fellowship programs: the Stewardship Science Graduate Fellowship, Laboratory Residency Graduate Fellowship, and Computational Science Graduate Fellowship.

In addition, he presented the goals of Academic Programs:

- **Workforce Pipeline**: providing diverse, skilled, technical stockpile stewards of the future;
- **External Expertise**: assuring quality through external review, critique, challenge; and

(continued on page 4)

The National Ignition Facility Conducts First-Ever Shot with Explosives

by Michael Padilla (Lawrence Livermore National Laboratory)

The first-ever shot to study a high explosive sample was recently conducted at the National Ignition Facility (NIF), the world's most energetic laser. The results from the shot included novel data that will help researchers unlock the mysteries of high-explosive (HE) chemistry and position Lawrence Livermore National Laboratory (LLNL) to continue its legacy as a leader in HE science and diagnostic innovation.

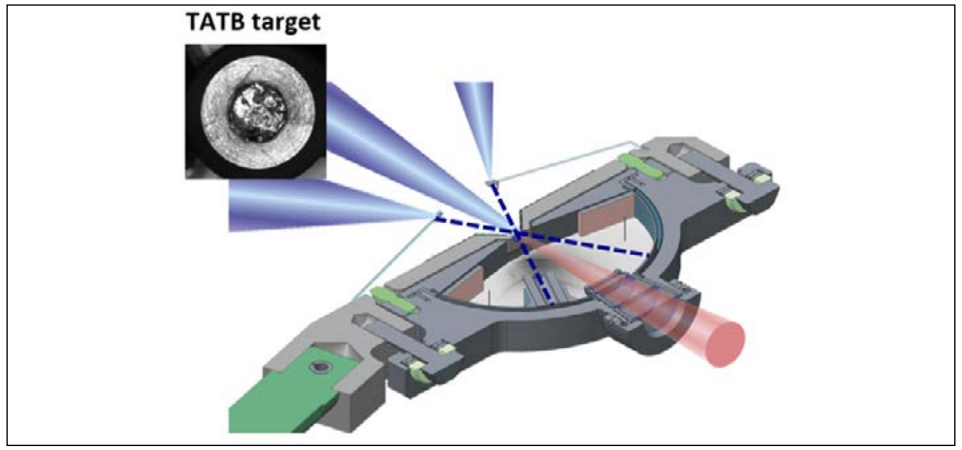


Figure 1. A schematic of the TARDIS platform showing the drive beam and the two X-ray sources. The top left portion of the schematic shows a greyscale optical image of the TATB target as it was mounted on the diagnostic.

"This shot is the first in a series that will transform the Lab's understanding of high explosives by producing never-before-captured experimental data quantifying the response of laser-driven high explosives during reaction," said Lara Leininger, director of LLNL's Energetic Materials Center (EMC) and lead for this Laboratory Directed Research and Development (LDRD) project.

"The results also allow LLNL to critically evaluate predictive computational capabilities and the lab's world-class thermochemical code, Cheetah, and greatly expand experimental capabilities being applied in high explosives," Leininger said.

Prior to the November 4 NIF shot, solid carbon products (or condensates) from this type of chemical reaction could be calculated by LLNL's physics and thermochemistry codes, but their atomic structure had never been directly measured *in situ*, with two X-ray probe beams on the same target, in <50 nanoseconds. "It is gratifying to see the TARDIS (TARget Diffraction In Situ) platform that we developed for very different scientific and programmatic applications to be useful, especially its dual-probe and large spot-size options, to new areas of research important to the laboratory mission," said Jon Eggert.

The shot used a non-detonable quantity of less than 7 milligrams of single-crystal triaminotrinitrobenzene (TATB). TATB is an insensitive high explosive and unusual in its low sensitivity (relative to conventional high explosives) to stimuli such as friction, pressure, temperature, impact or spark. The relative safety of this material renders it important for the National Nuclear Security Administration's (NNSA) Defense Programs and the Department of Defense. The shot captured a time evolution of products under shock compression exceeding 150 GPa (1.5 million times Earth's atmosphere).

An entire series of shots is planned to greatly enhance the lab's understanding of HE science by evaluating the range from low-pressure ignition to overdriven initiation and points in-between.

"Utilizing the unique capabilities of NIF, specifically the long laser drive (60 nanoseconds) coupled with the two X-ray probes per shot, we can begin to understand reaction product formation as a function of shock pressure," said Samantha Clarke, the lead scientist for the shot. "We obtained excellent data from all diagnostics and see clear evidence for the formation of products within 50 ns."

The results of the shot are directly relevant to the lab's ongoing work of science-based stockpile stewardship activities in LLNL's Weapons and Complex Integration (WCI) directorate.

Tom Arsenlis, head of Physics & Engineering Models, said these experiments allow LLNL to investigate the structure of HE detonation products during the detonation and help validate models of HE performance.

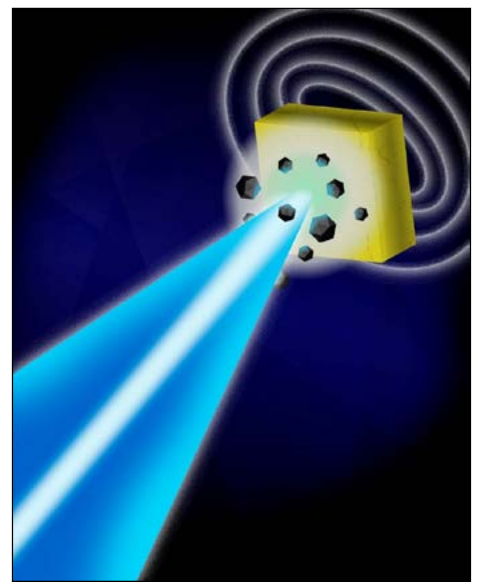


Figure 2. Artist's representation of the NIF drive lasers hitting the TATB target creating reaction products.

"With the exquisite diagnostics at NIF, we are able to work with small samples and greatly reduce the risks of working with high explosives while getting programmatically relevant data," he said.

In LLNL's Global Security directorate, these experiments will inform detection technologies for nonproliferation and interdiction technologies for nuclear counter-terrorism. In addition, the shot showcases LLNL's commitment as a NNSA Center of Excellence in High Explosives.

Understanding the Explosive Shot

Because of its relative insensitivity to external stimuli, TATB is important

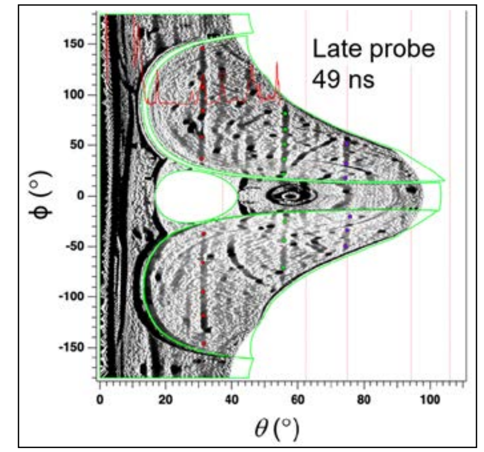


Figure 3. A schematic of the TARDIS platform showing the drive beam and the two X-ray sources. The top left portion of the schematic shows a greyscale optical image of the TATB target as it was mounted on the diagnostic.

to LLNL's WCI and to NNSA and is used as the main charges in weapons systems.

"We know that TATB detonations end in solid carbon, but the temporal evolution, morphology, and allotrope is still unknown for all conditions," Leininger said. "NIF is a unique experimental facility that may enable the quantification of the kinetics of solid carbon production in TATB reactions under detonation conditions."

Just like a wood fire produces soot, detonation of CHNO (carbon, hydrogen, nitrogen, and oxygen-based) explosives like TATB can produce solid carbon. Leininger explains that every explosive is different and predicting the amount, phase (i.e., diamond or graphite), and time evolution of this carbon condensate production is important for the development of predictive modeling.

Project Conducted in Three Phases

The work funded by the LDRD Program, started in 2017, focused on multi-disciplinary strategic initiative leveraging two core competencies at LLNL: high explosives science and high energy density photon science.

The first phase of the project was the development of diagnostic technologies. The project team developed and innovated, then applied novel diagnostic techniques for measuring *in-situ*, dynamic, laser-driven high-explosive reactions. The focus of this phase was the rapid development and shrewd termination of non-viable concepts. The first experiment took place at LLNL's Jupiter facility under the leadership of Joseph Zaug.

In the second phase, concepts were evaluated on a series of shots at the Omega Laser Facility at the University of Rochester Laboratory for Laser Energetics (UR/LLE). Significant diagnostic developments have been made by the NIF Materials Integrated Experimental Team (IET) over many years, and this enabled the team, led by Michelle Marshall, to prove the feasibility of measuring solid products *in-situ* using X-ray diffraction with laser-backlighter X-ray probe beams and to investigate target preparation, configuration and diagnostic set-ups. Marshall is part of an ongoing collaboration for additional Omega experiments to investigate solid product formation in TATB that are complementary to NIF experiments and to measure the equation of state of other insensitive explosive materials.

The capstone phase of the project was performed at NIF and combined the developments into a comprehensive characterization of the detonation reaction zone. Successful transition from Omega to NIF over a short time scale was enabled by the NIF Materials IET. The November 4 shot integrated the techniques developed in the first two phases and provided data on the evolving chemistry of this reacting insensitive high explosive. Clarke noted that the final target at NIF was 6.92 milligrams. With a detonation energy of ~4 kilojoule per gram, the energy output of this target was ~30 Joules of energy. By comparison, the NIF laser can deliver more than ~2,000,000 Joules of energy on target.

Teamwork

The team relied on LLNL's Jupiter Laser Facility and the Omega Laser Facility at the UR/LLE to conduct work prior to conducting the shot at NIF. Using HE material at NIF, a radiological facility, required careful analysis and preparation. As with other hazardous or radioactive materials, NIF had to develop and implement rigid, formal operational protocols to ensure that the high explosive experiments would be conducted safely and within NIF's authorized limits of operation, according to Ken Kasper, who leads the NIF Safety Program.

"NIF's advanced diagnostic systems are able to extract the required experimental data from the tiniest TATB samples," Kasper said. "This small sample size makes managing the hazard much more straightforward."

Of special note, Leininger said, were the attention and diligence from the LLNL Explosives Safety Committee Chair, Kevin Vandersall, and the LLNL Controlled Materials Group, including Don Schneider, who traveled on an overnight flight to Rochester, New York to ensure that explosives targets were properly packaged for a return shipment to LLNL.

Key team members include Samantha Clarke, Michelle Marshall (University of Rochester), Joseph Zaug, Paulius Grivickas, Suzanne Ali, Bruce Baer, Matt Nelms, Ray Smith, Martin Gorman, Damian Swift, Amalia Fernandez-Pañella, Larry Fried, Thomas Myers, Ben Yancey, Carol Davis, Franco Gagliardi, Korbie Le Galloudec, Lisa Lauderbach, Trevor Willey, James McNaney, Jon Eggert, and Lara Leininger.

LLNL-MI-820373. This work was performed under the auspices of the U.S. Department of Energy/National Nuclear Security Administration by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. We gratefully acknowledge the LLNL LDRD program for funding support of this project under tracking #18-SI-004. ◆

Ideas for Articles

Do you have ideas for future *Stewardship Science Today* articles? Would you like to submit an article? If so, please contact Terri Stone at terri.stone@nnsa.doe.gov.

Thermo-tolerant and Impact Resistant Materials Development for Thermal Protection Applications

by LaRico Treadwell, James Nicholas, Bryan Kaehr, Timothy J. Boyle, Khalid M. Hattar, Bernadette A. Hernandez-Sanchez (Sandia National Laboratories)

Thermal protection system (TPS) materials, used in energy and aerospace applications, can withstand high temperature environments reaching well above 900°C. To further advance future applications requires new TPS materials with enhanced thermal and mechanical resiliency. Sandia National Laboratories is developing composites with tuned microstructures and refractory materials for high-throughput testing of the mechanical and thermal properties to test and optimize performance. The materials will advance both the flexibility and performance options for TPS within the stockpile.

The team is currently working on two approaches: the development of refractory constituent materials (particles, fibers, precursors, coatings) for TPS and their implementation into conformable, multilayered materials with nacre-like micro-architectures.[1] Guided by previous research and computation (see Figure 1), the constituent materials are being incorporated as "knobs" to "dial-in" to cultivate the optimum thermal and mechanical resiliency. The addition of the novel constituents introduces unknowns into the processing and performance of the new composite materials. These unknowns materialize as voids, cracks, interface disbonds, and delaminations. To address the defect science of the new materials, advanced processing techniques are being developed to have precise control

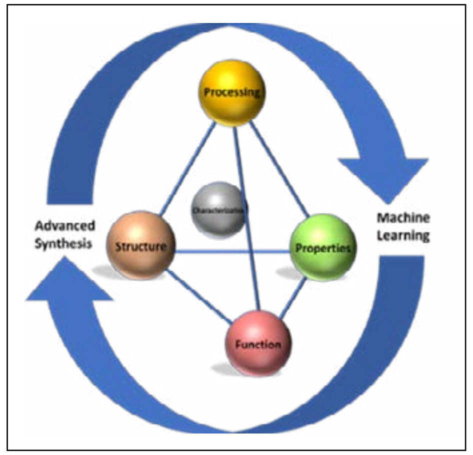


Figure 1. Interactive Synthesis-Computational structure to develop next generation thermal protection materials.

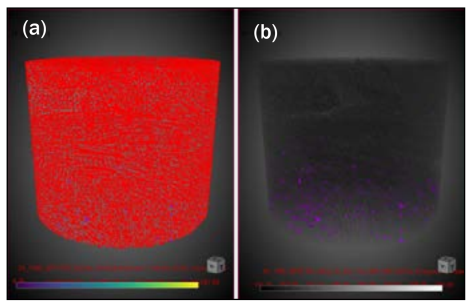


Figure 2. Micro X-ray computed topography scan of composite material (a) Image post processing to contrast reinforcement phase and matrix phase of material (b) Image post processing to identify void and crack defects.

and *in situ* monitoring of pressure, temperature, and atmosphere. Micro X-ray topography (µCT) is used to evaluate the microstructure developed during the processing. Figure 2 shows the image post processing of the µCT scan. The post processing in Figure 2a allows clear identification of the reinforcement phase (red) and the matrix phase (gray), and Figure 2b clearly identifies the defects. Additional evaluation of the unique nano to microstructures obtained for the composites include *in situ* heating and laser annealing conducted during transmission electron microscopy experiments to understand stability

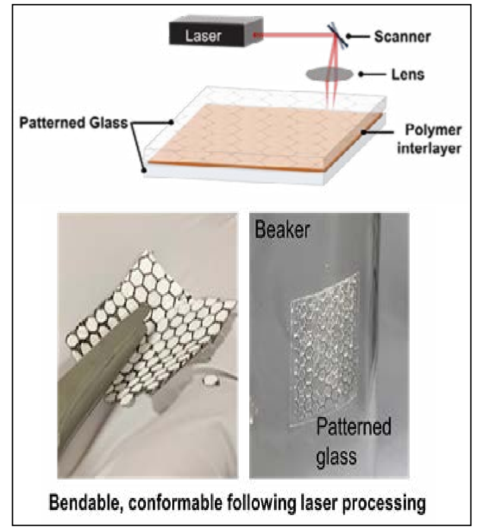


Figure 3. Advanced manufacturing for high-throughput testing of layered materials using a micropattern to increase toughness.

for performance and processing. In parallel, an advanced manufacturing approach for high-throughput testing of layered TPS materials is being developed with a focus on micropatterned, conformable composites for increased toughness (see Figure 3). Finally, material performance characterizations are performed in a high temperature and high flux atmospheric-controlled chambers at Sandia's National Solar Testing Facility and shock testing at the Shock Thermodynamics Applied Research (STAR) Facility. Holistically, this project provides performances evaluations in simulated environments that will lead to expedited qualifications of advanced TPS.

Reference

[1]Z. Yin, Florent Hannard, and F. Barthelat, "Impact-resistant Nacre-like Transparent Materials." Science 364.6447, 1260-1263 (2019).

This work was performed under the auspices of the Department of Energy/National Nuclear Security Administration by Sandia National Laboratories under contract DE-NA-0003525. ◆

2021 SSAP Symposium *(continued from page 1)*

- **Creative Input**: leveraging expertise in areas thinking outside the mission.

As in past years, the Symposium featured presentations on recent accomplishments given by representatives of the SSAA Centers of Excellence and grants supported by the SSAP. This includes the SSAA, HEDLP, and National Laser Users' Facility programs. Five of the nine SSAA Centers of Excellence presented this year. The remaining Centers will present their research next year.

Principal Investigators and government staff were invited to a special session by Jim Mowry, an NNSA Counterintelligence Officer on Case Studies in Academic Risk Management: What Happens When Academic Risk and National Security Risk Collide. This session discussed several issues of concern regarding the involvement of foreign countries in DOE-sponsored research and generated a great deal of interaction with the speaker.

Talks were also given by staff from the NNSA national laboratories and sites discussing opportunities available at their locations. Following these talks, there was the opportunity to meet with representatives from the labs, sites, NNSA, Krell Institute (who manages the fellowships for NNSA), and user facilities' staff.

The keynote address was given by Dr. Mark C. Anderson, the Assistant Deputy Administrator for RDT&E. His talk was entitled "The Role of Science in the National Security Enterprise (NSE)." After reviewing the impact of science on the NNSA mission, he stressed the importance of the young scientists currently supported as future leaders of the NNSA and its national laboratories and sites. He encouraged all to consider careers in the NSE.

David Etim with the Office of Advanced Simulation and Computing and Institutional Research & Development is the Federal Program Manager for the PSAAP. He gave an overview of the program that awards funding for projects that utilize high performance computing (HPC) to address challenging research projects while advancing developments in and personnel who are adept at taking advantage of HPC.

David Canty, Federal Program Manager for the MSIPP described the program that is focused on increasing the exposure to science, technology, engineering, and mathematics (STEM) projects in minority serving institutions of higher learning. This talk inspired a great deal of discussion about the opportunities being made available. It was followed by an interesting presentation by Charles Weatherford of Florida A&M University who is the Principal Investigator of a MSIPP award, the Consortium for High Energy Density Science.

The Symposium featured guest speakers from NNSA, the NNSA national laboratories, and academia.

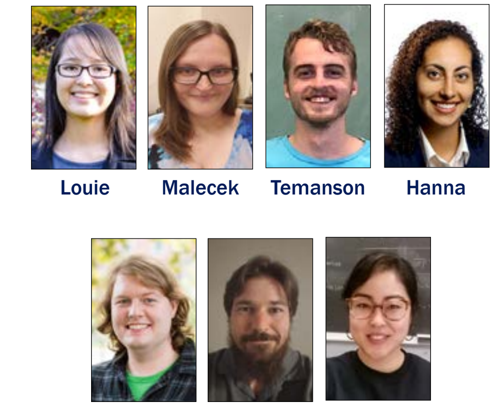
- Yogendra Gupta and Paulo Rigg, Washington State University, Dynamic Compression of Materials—Continuum to Atomic Scale Understanding
- Hye Young Lee, Los Alamos National Laboratory, Direct Measurement of Neutron-Induced Reactions with a Radioactive NI-56 at LANSCE
- Jamie Messman, Kansas City National Security Campus, Materials in Extreme Environments: Enabling Manufacturing for the Future
- Kristee Hall, NNSA, Conversation with a Grants Officer
- Alison Saunders, Lawrence Livermore National Laboratory; Saryu Fensin, Los Alamos National Laboratory; and Benjamin Galloway, Sandia National Laboratories participated in the Early Career Perspective Panel. They discussed what it is like to work at a nation laboratory, providing invaluable information and resources to the audience.

The poster session and awards ceremony remained a highlight of the Symposium. The poster session was a bit different this year, as only graduate students were eligible to submit posters. Because of the restrictions of the on-line platform and the 170 posters submitted, live chats with presenters were not possible. Instead, the students recorded a five-minute presentation of their research which was available on the Symposium website. Those who wished to discuss the posters further with the students could reach out to them via email. Although this procedure allowed posters to be viewed and presented, the live interaction with poster presenters was missed greatly.

The poster competition set records this year, even though the entire process was done remotely. The number of posters submitted by graduate students (174) was a major increase over the number submitted in 2020 (113), and the number of judges who submitted grades (124) represented an even larger increase over the number from 2020 (45). The winners of the 2021 SSAP Symposium Poster Session follow.

Outstanding Poster Award Winners

2021 SSAP Symposium



Christina Louie, Washington State University, *Probing Interfacial Molecules at Air-Aqueous Interfaces Using Vibrational Sum Frequency Generation Spectroscopy*

Rachel Malecek, Louisiana State University, *Studying Low-Lying States of 9B with the Super-Enge Split-Pole Spectrograph*

Eli Temanson, Florida State University, *Development of Planacon MCP-PMT's Coupled to Para-Terphenyl for Low Energy Neutron Measurements*

Sylvia Hanna, Northwestern University, *Discovery of Spontaneous De-Interpenetration Through Charged Point-Point Repulsions*

Nathan Dasenbrock-Gammon, University of Rochester, *Superconducting Yttrium Hydride at 262 K through Catalyzed Hydrogenation*

Daniel Mayes, University Nevada, Reno, *Observation and Characterization of Trends in the Ionization of the Warm Absorber Photoionized Plasma Experiment at Z*

Patricia Cho, University of Texas at Austin, *Spectral Line Identification in Photoionized Silicon Plasma Emission*

Congratulations to all! ◆