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

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CALENDAR

10/8-9/2020
Massachusetts Institute of Technology Center of Excellence Review, virtual

11/9-13/2020
62nd American Physical Society Division of Plasma Physics Meeting, virtual

12/2-4/2020
FY 2020 Office of Experimental Science Program Review, virtual

12/6-10/2020
47th IEEE International Conference on Plasma Science (ICOPS), virtual

12/13-17/2020
23rd Topical Conference on High Temperature Plasma Diagnostics, virtual

INSIDE

*Contractor Support **National Laboratory Detailee

Welcome to another issue of *Stewardship Science Today*. We conduct exciting research in the Stockpile Stewardship Program, and we attract top talent (read about new staff member Rebecca Lewis below). In this issue, we discuss highly-relevant work related to the synthesis of high explosive formulations that render high explosives less sensitive (more stable) when handled. This is a top challenge in our mission space, and work being conducted in the Explosives Science and Shock Physics Division at Los Alamos National Laboratory is breaking ground in understanding the impacts of making small, systematic, structural changes in explosive molecules and how these changes affect the handling sensitivity of high explosive formulations. This is fascinating research space with true, practical applications.

Also featured is the exceptional talent of our incoming Stewardship Science Graduate Fellowship and Laboratory Residency Graduate Fellowship classes. As you will read in their research statements, these graduate-level scientists already are making impactful contributions to our mission space. We look forward to seeing the results of their research and following their careers. Hopefully many of them will join the ranks of the top-tier scientists, engineers, and technicians at our national laboratories.

Lisa E. Gordon-Hagerty (left), Administrator of the National Nuclear Security Administration and U.S. Department of Energy's Under Secretary for Nuclear Security, toured Nevada National Security Site in early September. Above, she is pictured at the U1a Complex.

As this pandemic wears on, remember to take good care of yourselves and those around you. Remain diligent in protecting yourself, your loved ones, and your communities by wearing a mask and washing your hands. This is what the science is telling us to do.

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

RDT&E Welcomes Dr. Rebecca (Becky) Lewis to the Office of Experimental Sciences

Becky Lewis

Dr. Rebecca (Becky) Lewis, a member of the Stewardship Science Academic Alliances (SSAA) program from 2016-2019, joined the Office of Experimental Sciences in June as the Federal Program Manager for the Neutron Diagnosed Subcritical Experiments program. Lewis was funded by SSAA to perform her thesis work at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University (MSU), titled "Indirect neutron-capture cross sections for the weak r-process," and graduated in 2019 with a PhD in Nuclear Chemistry. While at MSU, she investigated techniques to indirectly constrain neutron-capture cross sections of exotic neutron-rich nuclei that cannot be directly measured due to the lack of a suitable target of short-lived nuclei or neutrons. As part of her research, Lewis spent a semester at Los Alamos National Laboratory, supported by SSAA, to collaborate with staff at the Los Alamos Neutron Science Center on an in-depth investigation of reaction codes used

Lewis and former postdoctoral researcher, now beam physicist, Mallory Smith preparing the Summing NaI (SuN) detector for an experiment at NSCL. Both Lewis and Smith were funded by an SSAA grant.

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Targeting Synthetic Functional Group Changes to Explosives to Modify Handling Sensitivity

by Virginia W. Manner, Nicholas Lease, Geoffrey W. Brown, Lisa M. Kay, and Marc J. Cawkwell (Los Alamos National Laboratory)

One of the most important properties of an explosive is its sensitivity, or how easily it can undergo violent reaction using stimuli such as shock, heat, impact, friction, or spark. The handling sensitivity of explosives, which is central to the National Nuclear Security Administration's missions, focuses on non-shock initiation mechanisms, such as dropping, pinching, or scraping an explosive. Although explosives have been developed for hundreds of years, the ability to predict and manipulate handling safety remains an important, yet elusive, goal. In 1979, Kamlet and coworkers wrote that a more detailed knowledge of fundamental chemical and physical properties would lead to "a unified theory of structure, sensitivity, and thermal stability of organic high explosives."[1] Almost 40 years later, Zeman and coworkers stated that "a single universal relationship between molecular structure and initiation reactivity does not yet exist."[2] In order to move towards this goal, Los Alamos National Laboratory (LANL) scientists in the High Explosives Science & Technology Group have been performing experimental studies with small, systematic, structural modifications to explosive molecules along with targeted modeling studies with LANL theoreticians to interpret experimental results.[3,4]

Recently, we have turned our attention to reducing the sensitivity of erythritol tetranitrate (ETN), an explosive that was developed in the 1800s and that has relatively poor handling safety. ETN contains nitrate ester functional groups (ONO_2), which are common energetic oxidizers that form explosives when combined with the carbon backbone "fuel" contained in erythritol (see Figure 1). To tune the sensitivity of this explosive, we have replaced the nitrate ester functional group with other energetic groups, such as more sensitive azides (N_3) and less sensitive nitramines ($NHNO_2$).

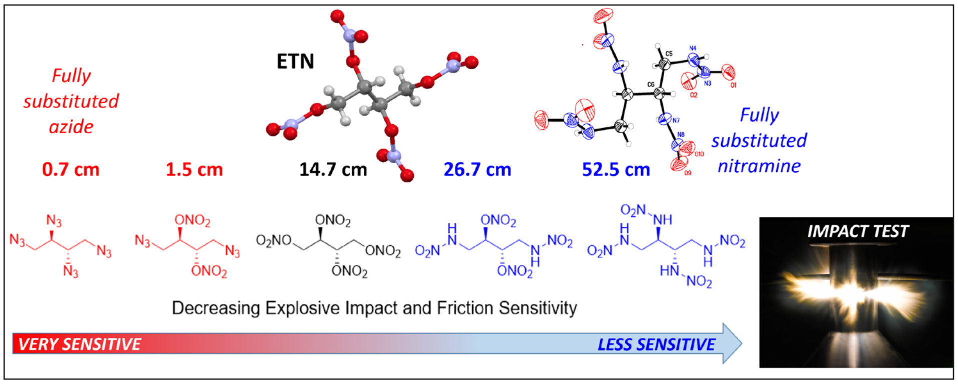

Figure 1. Derivatives of ETN with varying chemical groups and how they rank with respect to sensitivity. Impact values are given as the height (cm) at which initiation will occur 50% of the time from dropping a 2.5 kg weight onto a series of 40 mg samples. Higher values represent less sensitive (or more difficult to initiate) explosives.

Our intention was to modify the sensitivity of ETN by partially or fully replacing these groups.

Upon synthesis of the derivatives of ETN, standard sensitivity testing was conducted on all new molecules. Typically, these tests involve insulting the explosive by dropping a weight on top of a confined sample in a controlled environment (drop-weight impact testing). Less sensitive materials require dropping the weight from a greater height to observe a reaction. Other tests, such as friction and electrostatic discharge (ESD), are performed by scraping the explosive with grit or initiating it with a known amount of electrostatic discharge. Explosives can be ranked using these methods when the conditions are highly controlled.

Sensitivity testing showed that with the addition of the azide groups, the impact sensitivity of the materials increased dramatically compared to ETN. Conversely, the addition of nitramine groups decreased the sensitivity compared to ETN, and the impact sensitivity of compounds containing a mixture of two chemical groups was found to fall between the fully functionalized compounds (see Figure 1). Similar trends were observed in the friction sensitivity with less defined patterns in the ESD sensitivity. These results were exciting because we were able to tune the explosives as we predicted based on the model that certain facets of explosive handling sensitivity are controlled primarily by the energetic functional groups of the molecules. These studies could allow us to create a blueprint for the development of new explosives with specifically designed properties, especially with the aid of new computational studies that are able to rank drop height sensitivity and its dependence on chemical substitutions based on their effect on reaction rates.[5] The full article published on this work can be found in a recent issue of The Journal of Organic Chemistry.[6]

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The 2020-2021 Laboratory Residency Graduate Fellowship and Stewardship Science Graduate Fellowship Classes

by The Krell Institute

The Department of Energy National Nuclear Security Administration (DOE/NNSA) Stewardship Science Graduate Fellowship (SSGF) and Laboratory Residency Graduate Fellowship (LRGF) each will welcome five new students this fall. SSGF students are required to serve a 12-week practicum at an NNSA laboratory. The LRGF extends that to at least two practicums and encourages fellows to collaborate on their thesis research with lab scientists. All fellows receive tuition, a stipend, and other benefits. Summaries of the new fellows' research statements follow.

Laboratory Residency Graduate Fellowship

At the University of Texas at Austin, **Patricia Cho** models white dwarf star spectra. Using new codes, she's investigating atomic absorption line profiles that reflect advances in line-shape theory. Cho became familiar with Sandia's Z Astrophysical Plasma Properties collaboration and its photoionized silicon experiment which provided benchmark emission spectra suitable for evaluating discharges from accretion disks around black holes and similar compact objects. Some have iron abundances five to 20 times that of the sun, raising questions about the validity of atomic theory. Under advisor Don Winget, Cho will use her Sandia residency to resolve the super-solar iron abundance problem, collaborating on Z machine experiments and using the XSTAR astrophysical modeling code.

Kevin Kwock uses lasers and theoretical models at Columbia University to investigate lattice and electronic properties in atomically thin semiconductors, specifically transition metal dichalcogenide (TMD) monolayers. With advisor P. James Schuck, Kwock plans to use optical pump-probe spectroscopy to produce lattice-resonant phonons and examine effects on a second probe beam that produces high harmonic generation (HHG). At Los Alamos National Laboratory's Center for Integrated Nanotechnologies, he will enhance TMD optical properties through integration with nanophotonic devices to boost HHG efficiencies. Based on simulations of metasurfaces tuned to specific TMD resonances, he will fabricate optical devices, integrate the materials, and characterize the coupled optical emission properties. He hopes to demonstrate that efficient on-chip nonlinear HHG is possible.

A plasma-simulation conundrum occupies **Logan Meredith**, a PhD candidate at the University of Illinois at Urbana-Champaign. Fluid codes demand less computing power than others but make assumptions about the plasma. Kinetic codes track individual particles more accurately than fluid codes at low densities but demand more computing resources. Meredith and advisor Davide Curreli are devising a hybrid method that switches between the two in different parts of the domain. On residencies at Sandia National Laboratories in New Mexico, Meredith will apply their technique to aspects of pulsed-power experiments and use the resources of a lab team developing the EMPIRE hybrid code. "In addition," he writes, "cooperation with pulsed-power research groups will yield physical insights for guiding hybrid development and data for verification and validation."

John (Ryan) Peterson plans to work on a new laser-powered gamma-ray source using relativistic streaming instabilities to image high energy density (HED) experiments. His Stanford group recently demonstrated that a laser-driven electron beam, when shone on a background plasma, is unstable to filamentation, producing strong magnetic fields. "Synchrotron emission of beam electrons in these magnetic fields could reach tens of MeV," Peterson writes. With support from advisors Siegfried Glenzer and Frederico Fiuza, he'll work in residence at Lawrence Livermore National Laboratory's Jupiter Laser Facility, performing and analyzing simulations to advance techniques that use betatron and bremsstrahlung X-ray sources. He'll also explore filamentation-based schemes for generating X-rays, potentially producing a new diagnostic for HED science.

At the University of California, Santa Barbara (UCSB), **Ashley Roach** studies how internal pores in a crystal under external loads grow and deform –and possibly fail. She and advisor Irene Beyerlein will use experiments and simulations to grasp how pore growth depends on size and rate effects. UCSB has developed thin-film deposition techniques that allow small-scale mechanical testing and uses electron microscopy to observe discrete dislocation activity in real time. Roach plans to conduct pore-growth experiments at Los Alamos National Laboratory plus simulations using a lab-developed hydrodynamics code. "With the experimental investigation and material model informing each other," she writes, "a physics-based understanding of pore growth at critical length scales can be developed."

Stewardship Science Graduate Fellowship

Rice University's **Sophia Andaloro**, with advisor Christopher Tunnell, works with XENONnT, a time projection chamber (TPC) designed to detect dark matter and other rare events. Andaloro wants to characterize background radiation sources and reduce them to improve distinctions between detector interactions. She solves multidimensional fits for XENONnT's electronic-recoil backgrounds, focusing particularly on recombination fluctuations, when xenon captures ionized electrons before they reach a gas region in the detector. Using XENONnT calibration data, Andaloro will optimize parameters with machine-learning methods. To preserve low-energy data and exclude unwanted background events, she will develop waveform processing that minimizes redundant data storage and optimizes high-energy veto parameters. She hopes to make the techniques generalizable to noble-element TPCs.

At Stanford University, **Griffin Glenn** will work with Siegfried Glenzer to improve a cryogenic jet target for laser-generated neutron beams. The SLAC National Accelerator Laboratory's High Energy Density Science Division's cryogenic jet target creates thin sheets of free-flowing liquid deuterium for use with high-repetition petawatt lasers in neutron-generation studies. Glenn will develop brighter, more energetic ion and neutron beam sources. He'll field targets on high-repetition-rate lasers to probe the fundamental physics of laser-driven ion and neutron production. Results will be used to optimize laser and target parameters. As part of the work, Glenn will develop dedicated diagnostics for such beams.

Plasticity preoccupies **John Shimanek** at Pennsylvania State University. The multiscale nature of this key factor in metal machining and failure makes it difficult to model. With Allison Beese, one of his advisors, Shimanek will test and improve molecular dynamics models of the crystalline and atomic deformations behind plasticity. He'll incorporate the best model into a crystal plasticity finite element method to simulate single-crystal deformation and compare results with experiments. Shimanek will extend that method to polycrystalline deformation and perform simulations to predict stress-strain curves that relate to macroscopic deformation experiments. The research will look at face-centered cubic metal nickel, but the method should be applicable to other systems.

Sandra Strangebye of the Georgia Institute of Technology quantifies radiation's effects on nanocrystalline and ultrafine-grained materials. These substances resist radiation, but defects caused by radiation alter active deformation mechanisms. It's not well understood how these materials' high-density grain-boundary structures then evolve. With advisor Josh Kacher, Strangebye will test a hypothesis that irradiation-induced grain-boundary changes reduce dislocation mobility. Using facilities at Sandia National Laboratories' Center for Integrated Nanotechnologies, she will irradiate 100 nanometer-thick gold specimens and use tunneling electron microscopy to "characterize the new defect state induced by the radiation damage prior, during and after straining," she writes.

California Institute of Technology's **Christopher Yang** says machine learning (ML) and reinforcement learning (RL) can make a "spectacular impact" on inertial confinement fusion simulations. The commonly used multiphysics code HYDRA has difficulty with three-dimensional (3D) simulations due to entangling in its computational mesh to track fluid motion. In his work with advisor Andrei Faraon, Yang aims to replace manual meshing strategies with ML. He's already imitated a manual meshing approach to greater than 98 percent accuracy on 1,300 HYDRA frames. Yang plans to use RL to further generalize the algorithm for high-resolution and 3D simulations.

This work will be performed under the auspices of the U.S. Department of Energy / National Nuclear Security Administration under Cooperative Agreement DE-NA0003960. ◆

RDT&E Welcomes Dr. Lewis *(continued from page 1)*

to calculate neutron-capture cross sections in order to quantify the systematic uncertainty associated with the choice of reaction code.

Lewis presented her work at the 2017-2019 SSAP Symposiums, and was awarded "Outstanding Poster" honors in 2018 and 2019 for her research focused on the experimentally constrained neutron-capture cross sections of ^{73}Zn and $^{70\text{-}72}$Ni. After completing her PhD, she joined the 2019-2020 class of the NNSA Graduate Fellowship Program as a fellow in the Office of Defense Nuclear Nonproliferation R&D (DNN R&D), where she established a plan for assessing the impact of DNN R&D's research funding on sustained capabilities at the national laboratories, organized the Federal program needs component of the annual Workshop for Applied Nuclear Data Activities, and coordinated nuclear data needs for many applications across NNSA, DOE, and the Interagency. ◆

Lewis assembling a position-sensitive photomultiplier tube system at the NSCL with her advisor Sean Liddick (MSU) and graduate student Katie Childers.