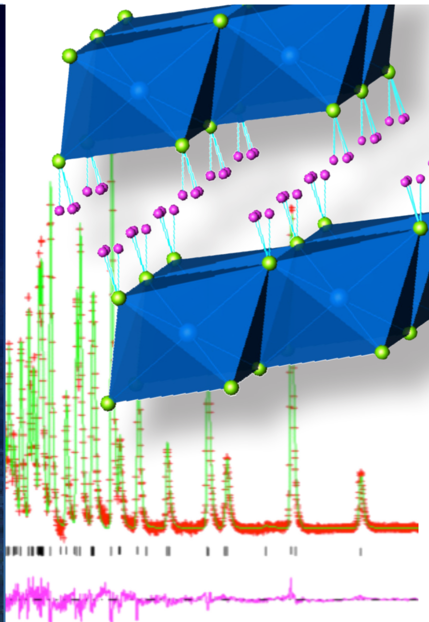
the Pulse AOT & LANSCE
February 2013
Approved for public release; distribution is unlimited.

INSIDE



Neutron diffraction pattern and crystal structure of deuterated brucite, $Mg(OD)_2$.

> *"Neutrons are ideal for detecting light elements, especially hydrogen."*

Photo by Sandra Valdez, IRM-CAS

Hongwu Xu

Using minerals and neutrons to unearth geologic solutions to global challenges

By Diana Del Mauro, ADEPS Communications

Hongwu Xu likes dreaming up new ways to use neutrons to solve problems in earth and environmental sciences. As he's simulating the planet's deep water cycle or reproducing the realms of buried nuclear waste, he uses neutrons to probe water-bearing minerals or complex oxide materials. His research often demands high-pressure, high-temperature conditions, nearly as extreme as what's found in Earth's mantle.

"Neutrons are ideal for detecting light elements, especially hydrogen," said Xu, who uses the Lujan Neutron Scattering Center at Los Alamos for his neutron diffraction studies. The community of geoscience researchers using neutron techniques is small, Xu said, partly because neutron facilities are in short supply compared with x-ray facilities.

The Mineralogical Society of America named Xu a 2013 fellow, paying tribute to his talents in neutron diffraction, conventional x-ray scattering, and synchrotron x-ray studies—complementary methods of exploring the atomic structures of materials and revealing their properties.

continued on page 3

> "This was my first Facility Centered Assessment here at TA-53, and during the process I learned a lot about our strong teamwork and our collective sense of a common goal of delivering reliable beam to the science community."

From Alex's desk . . .

Colleagues,

Recently, TA-53 went through a Facility Centered Assessment (FCA), led by David Funk (WX-DO). First, I would like to thank David and his team for their time and input. I also would like to thank TA-53 personal from all divisions for positively engaging with the team. The FCA team did a very comprehensive job in taking a look at all aspects of TA-53 operations. This was my first FCA here at TA-53, and during the process I learned a lot about our strong teamwork and our collective sense of a common goal of delivering reliable beam to the science community. Additionally, as in any large experimental facility, we also have areas for improvements. The FCA team did a great job in helping us identify areas for improvements. Now, the work is on our side. We have started discussions with TA-53 management on a measurable plan on how to address the FCA findings. One of the findings clearly articulated was the status of our facilities in general; in particular housekeeping issues. This is a topic I'm taking a particular interest in, and collectively TA-53 management will be intensifying MOVs related to housekeeping. We are also working on securing resources to address issues where a considerable amount of investment is needed. There are approaches, however, that can be done now and all of our help is paramount. Simple things such as office and lab space clutter can be addressed once a minimum amount of time is devoted to it. Yes, it can be done.

Please join me in welcoming Mark Bowden as the 2013 chair of the LANSCE User Group. Mark has served on the LUG since 2011 when he was elected as a user representative. Currently Mark is the Environmental Molecular Sciences Laboratory Capability Lead at Pacific Northwest National Laboratory. We also would like to take the opportunity to thank June Matthews (MIT Professor of Physics) for her service as 2012 LUG chair. June will remain on the LUG Executive Committee in 2013 as past chair. Additionally, we welcome Hillary Smith of the California Institute of Technology Department of Applied Physics and Materials Science as the elected student representative for 2013-2015. A LUG onsite meeting is now planned for the second week of March.

I also would like to bring to your attention the TA-53 WSST and its initiatives. I encourage you to meet/know and interact with your local WSST representative(s). Gary Sanchez (AOT-IC) is the new TA-53 WSST chair. The past chair, Eric Larson (LANSCE-LC), did such a great job that he is now the LANL Institution WSST co-chair. Gary continues the tradition of running an engaging meeting and our input to the TA-53 WSST effectiveness is paramount.

LANSCE Deputy Division Leader Alex Lacerda

Xu cont.

Inspired by time-tested minerals, Xu studies synthetic copies or analogues—mostly polycrystalline powder or ceramic chunks—of minerals. His studies, for example, potentially can be used for turning liquid nuclear waste into a rock-like ceramic that, when placed in a metal canister and buried, won't leach into the environment.

"We learn from nature," said Xu, of Earth System Observations (EES-14).

Since joining Los Alamos National Laboratory in 2004, Xu has fostered collaborations between the Earth and Environment Sciences Division and the Lujan Center. "New discoveries occur at the boundaries of different disciplines," he said. For five years, he has been a part-time instrument scientist assisting researchers at the national user facility and developing new research techniques. He is the only EES scientist who maintains an office at the Lujan Center.

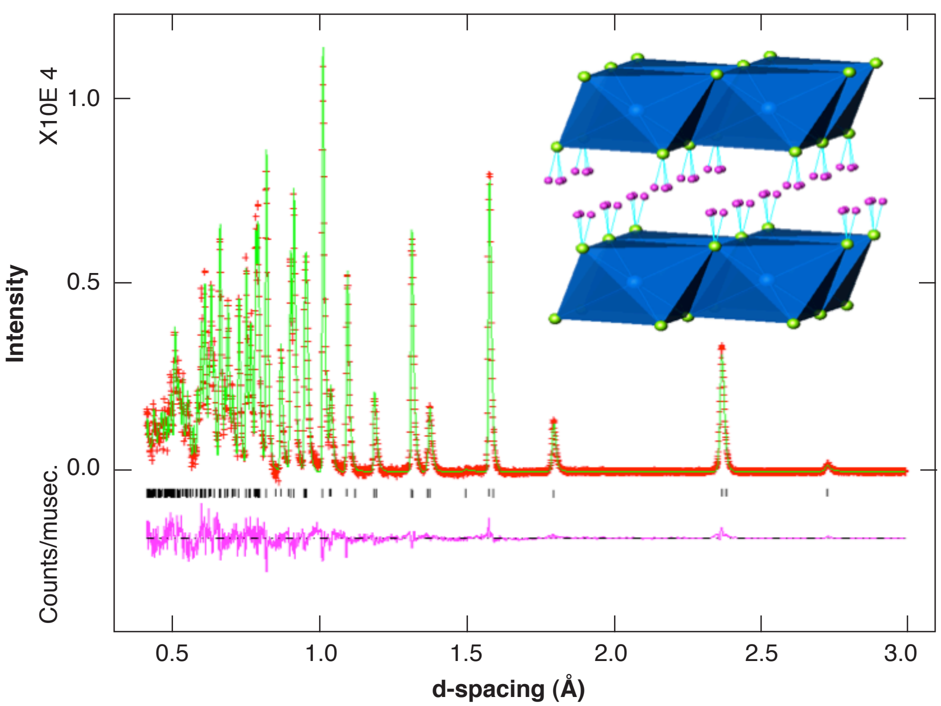
For HIPPO, the High-Pressure Preferred Orientation Diffractometer, Xu and his colleagues developed capabilities that combine high pressure–up to 20 GPa–with temperatures ranging from a low of 8 to a high of 1800 K. The benefits are two-fold: researchers can simulate situations deep in the Earth or other planets, or they can create new materials with new properties. "Only a few places in the world have these kinds of high-pressure neutron capabilities," Xu said.

Xu's knowledge of minerals and materials science, stemming from his PhD in geosciences from Princeton University, made him a key player on the Lujan Center team that pioneered in situ high-pressure neutron diffraction methodologies. Using high-pressure fluid cells, for instance, his team studies the stability and structures of clathrate hydrates, a family of ice-like solids filled with various gases that are stable at high-pressure, low-temperature conditions. Found in the ocean floor sediments, methane clathrate is a potential energy resource, however, during landslides or earthquakes methane release can negatively affect climate. Xu is unraveling the mechanisms and kinetics of how different gas clathrates are formed.

Xu plans to expand the capabilities of other Lujan instruments and apply the techniques to broader earth, energy, and environmental studies. For example, through neutron scattering and imaging measurements coupled with multiscale modeling, his team may assess the suitability of salt repositories, such as WIPP, for storing high-level nuclear wastes—an urgent challenge for sustainable nuclear energy.

As well, his work on high-pressure conditions could be applied to research at MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's proposed experimental facility for the discovery and design of advanced materials. "Broadly speaking, pressure is an effective tool for designing new materials or tuning existing materials for new properties," he said.

Xu has authored 82 publications in notable scientific journals and serves as an associate editor of *American Mineralogist*.



Neutron diffraction pattern and crystal structure of deuterated brucite, $Mg(OD)_2$. Brucite occurs as a component unit in the structures of complex hydrous minerals, which are potential hosts for water in the Earth's mantle. Since neutrons are sensitive to light elements, particular hydrogen, neutron diffraction is a powerful technique for studying hydrogen-bearing phases. Determination of the structures and phase equilibria of hydrous minerals at elevated pressure and temperature provides insights into mechanisms of water storage and transport in Earth's interior.

New precision measurements of the ^{235}U neutron-capture cross section at DANCE

The capture cross section for neutrons reacting with ^{235}U is of fundamental importance for understanding nuclear technology, including criticality and reactors, defense systems, and transmutation technologies.

Many measurements have been made over the past 60 years, yet this important quantity is still poorly known in the neutron energy range from 1 keV to 1 MeV, which corresponds to the energies with which roughly half of the neutrons from fission are produced. The uncertainties are estimated to range from 15% to 30%, far above what is needed for precise calculations of nuclear systems.

The main reason for this uncertainty is that capture is usually detected from the gamma-rays it produces, but the probability for creating fission, which also produces gamma-rays, is from 2 to 10 times higher than capture in this energy range. The probability for neutrons to scatter from ^{235}U into the detector is about 10 to 30 times larger than the capture probability, and these neutrons can also produce gamma rays that interfere with the measurement.

For accurate measurements of the cross section, it must be determined which reaction produced the gamma rays that are detected. Fission reactions can be identified using a "fission chamber" to tag the reaction, but a thin target (less than 0.5 micrometers thick) is required.

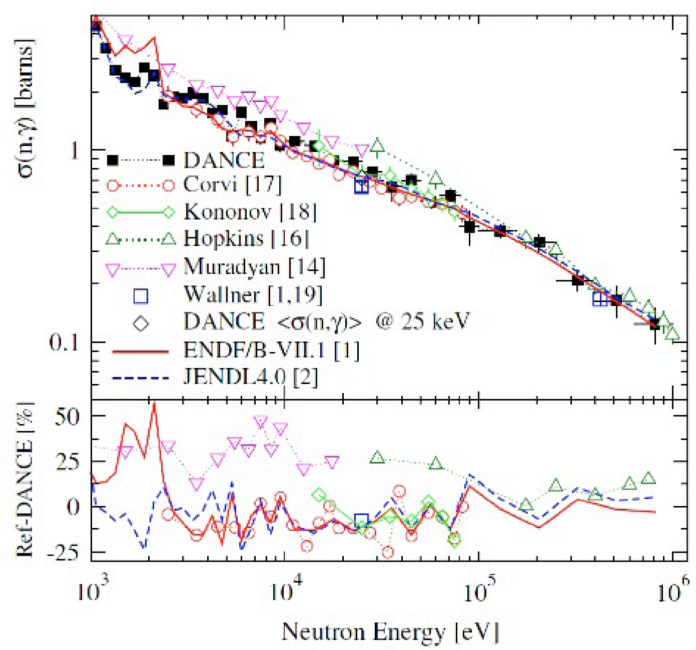
However, for good capture measurements, targets from 10 to 100 times thicker are needed. However, in a new experiment, recently published in *Physical Review Letters* (M. Jandel, et al., *PRL* **109**, 202506 [2012]), LANL and LLNL researchers led by Marian Jandel (Nuclear and Radiochemistry, C-NR), using the Detector for Advanced Neutron Capture Experiments (DANCE) at LANSCE, used two innovations to make measurements with 2% to 5% uncertainties. Both innovations are unique to detectors such as DANCE, which measure the total gamma-ray energy released during a reaction. In addition, the unique high segmentation of the DANCE detector (160 individual crystal detector elements) enables counting the number of individual gamma rays.

The first innovation involved measuring the fission gamma-ray spectrum as a function of neutron energy using a thin target, and then measuring the capture reaction using a thick target. The fission gamma rays were subtracted from the thick-target gamma ray spectrum by normalizing the fission gamma-ray spectrum to the thick-target spectrum for events with more than 6 gamma rays, a signature of fission.

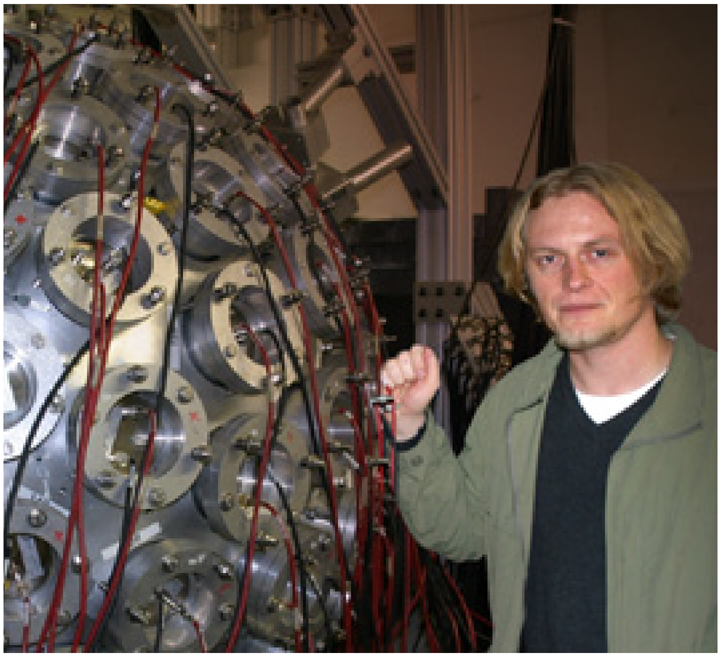
The second innovation involved measuring the spectrum of gamma rays due to neutrons scattering into the detector by using a ^{208}Pb target, which has a very small probability for neutron capture. The fission gamma-ray spectrum was measured using a 130 $\mu g/cm^2$ ^{235}U target mounted in a parallel-plate avalanche counter, which gave a signal for a fission event. The capture gammas were measured using a 26 mg/cm^2 self-supporting ^{235}U target, and the gamma spectrum from scattering was measured using a 120 mg/cm^2 ^{208}Pb target. Finally, since fission and capture were measured in the same target, the capture data were normalized to the very well known fission cross section, eliminating uncertainties due to target thickness and neutron flux measurement. More details of the experiment were given in the publication.

The results of the experiment are shown in the figure. The data from this measurement (black squares) are compared to two different data evaluations, the ENDF/B-VII.1 evaluation and the JENDL4.0 evaluation., as well as to other experimental results. The new data resolve the difference between the evaluations near 2 X 10^3 eV, and confirm the earlier data and evaluations above 10^4 eV. The uncertainty of the new measurement from 10^4 eV to 5 X 10^5 eV varied from 5% to roughly 10%. This data will provide new confidence in simulations for nuclear technology.

continued on next page



The top panel shows the $^{235}U(n,\gamma)$ cross section measured at the DANCE detector (black squares) compared to the ENDV/B-VII.1 and JENDL4.0 data evaluations, and earlier experimental measurements. The lower panel shows the percent difference between the current measurement and the earlier values.



Marian Jandel with the DANCE detector array.

DANCE cont.

This work benefitted from the use of the LANSCE accelerator facility and the moderated neutron source at the Lujan Neutron Scattering Center. NNSA Defense Programs support the LANSCE accelerator, and the Defense Programs Science Campaigns funded the DANCE spectrometer and experimental work.
Technical contact: John Ullmann

Neutron scattering contributes to understanding modern plastic solar cells

Plastic solar cells are being developed as a low-cost alternative to inorganic, mostly silicon-based, photovoltaics. They use conductive organic polymers and small organic molecules for light absorption and charge transport. However, many questions about the basic physics of light conversion by organic photovoltaics (OPV) persist.

Polymer-based solar cells consist of several polymer, copolymer, and mixed polymer/fullerene layers with thicknesses less than 100 nm, as shown in the figure. Because the layers are so thin, the properties of the interfaces dominate their electrical functions. Therefore, understanding the interface morphologies of the polymers used in these devices is required.

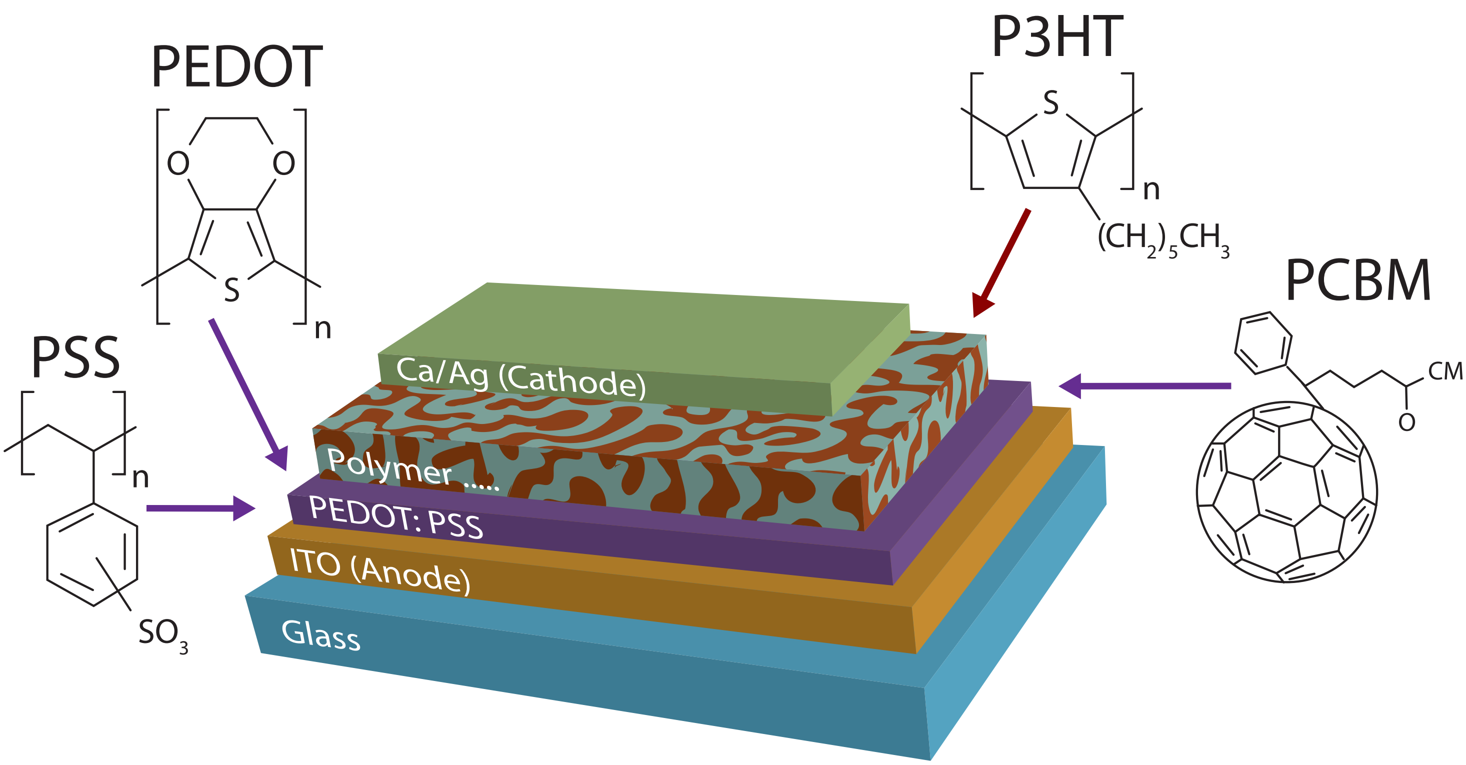
A multi-national group of investigators led by Professor Adam Moulé (University of California, Davis) demonstrated how neutron reflectometry can address the structural properties of various interfaces present in the OPV devices to improve their efficiency. Neutron reflectometry is well suited to address the structural properties of such polymer-based layers due to the excellent neutron scattering contrast between organic photovoltaic components, low absorption (which allows studying buried interfaces), and non-destructive nature of neutrons. *Advanced Functional Materials* published the research.

The materials distribution in organic photovoltaics greatly influences charge-carrier mobility. The researchers used neutron reflectometry and near edge x-ray absorption fine structure spectroscopy to examine the influence of heating, surface energy, and solvent additives on vertical segregation and doping in bulk-heterojunction organic photovoltaics. Neutron reflectometry enables measurement of the vertical concentration profile of a bulk-heterojunction under an intact metal electrode, avoiding any possible artifacts introduced by electrode removal.

The results indicate that the metal used as the cathode influences the bulk-heterojunction in ways not previously known. The vertical concentration profile changes drastically upon mild heating of the bulk-heterojunction layer due to interactions with the capping layer. The choice of metal capping electrode affects the vertical concentration profile through the surface energy and the Fermi energy difference between materials. Low work function capping metals donate electrons. This phenomenon contributes to the final vertical concentration profile of the bulk-heterojunction and to the current density-voltage characteristics of the organic photovoltaic devices. The solvent additives can alter the vertical concentration profile and the thermal stability of the

continued on next page

Cells cont.



Schematic of a typical polymer solar cell. (From top to bottom): a calcium/silver (Ca/Ag) cathode, a polymer:fullerene active layer consisting of a mixture of P3HT (electron donor) and PCBM (electron acceptor), a PEDOT:PSS hole-transporting layer, and an ITO anode on a glass substrate.

bulk-heterojunction morphology. The results reveal that surface energies and solvent additives greatly impact heat-induced vertical segregation. Current-voltage measurements show that self-assembly of interfaces affects the open-circuit voltage. The researchers conclude that it is necessary to consider samples processed with intact electrodes for all donor/acceptor pairs in order to understand the relationship between the morphology and device efficiency. Engineering the surface energy and electrostatic properties of the interfaces can lead to an optimized vertical concentration profile and open- circuit voltage, resulting in improvements to the power conversion efficiency.

Reference: “Self-Assembly of Selective Interfaces in Organic Photovoltaics,” *Advanced Functional Materials* (2012); doi:10.1002/adfm.201201874.

Researchers include Scott A. Mauger, Lilian Chang, Christopher W. Rochester, and Adam J. Moulé (University of California, Davis); Stephan Friedrich (Lawrence Livermore National Laboratory); Peng Wang and Jaroslaw “Jarek” Majewski (Lujan Center, LANSCE-LC); and David M. Huang (University of Adelaide, Australia).

This research benefited from the use of the surface profile analysis reflectometer (SPEAR) neutron time-of-flight spectrometer at the Lujan Neutron Scattering Center at LANSCE funded by the DOE Office of Basic Energy Sciences. The work supports the Lab’s Energy Security mission area and the Materials for the Future and Science of Signatures science pillars.

Technical contact: Jarek Majewski

It's so easy being green (or is it?)

It's that time of year, when we review our FY12 environmental accomplishments and communicate the ADEPS Environmental Action Plan for FY13. The ADEPS EAP team members are Steve Glick from P Division (the Directorate Point of Contact), Jim Coy from MST, Cathy Padro from MPA, and Frances Aull from LANSCE.

We had another strong year of environmental accomplishments in FY12. A sampling of our accomplishments:

- MPA and P collaborated to implement a short-fuse Pollution Prevention (P2) project to dispose of a total of 6 drums of chemicals, solids, toxic organic liquids, and corrosive liquids containing 204 gallons and weighing 275 kilograms in the "Chemical Cleanout" project.
- Four successful Helium Recovery projects were implemented at MPA's NHMFL, resulting in up to 72,200 liquid liters of helium recycled/re-used with a predicted annual savings of over $1.44M.
- In our efforts to reduce, eliminate, or reclaim sulfur hexafluoride (SF6), an extremely potent greenhouse gas, MPA fully removed its small amount of SF6, LANSCE-LC and MST (using a closed-loop system) are recycling the small amount that they use—and LANSCE plans to only keep one small cylinder for research purposes, if ever needed. P Division has the largest inventory of SF6; our FY13 EAP will include a target to address potential solutions to reducing P Division SF6 inventory.
- The MPA Methanol Recirculation and Recovery Loop (MRRL) project (from FY11) received one of the five top prizes, the "Star Award," in the P2 competition. The ADEPS EMS Team received a Bronze Award for its active involvement in the successful LANL "Recycle/Reuse" event. In addition, LANSCE received a P2 award for recycling of over 100,000 pounds of legacy metals.
- All divisions had extremely successful efforts to salvage unneeded equipment in a number of cleanout activities. Pallets full of electronic equipment were properly salvaged, as were 2 recycling bins filled with recyclable paper and books, boxes of cables, miscellaneous tools, and components. P Division's complete and total clean-out of the basement experimental area in 03-216 resulted in the removal of at least 30 years worth of collected equipment, materials, and chemicals. LANSCE disposed of 3 roll-off bins of metals for recycling, 1 refrigerator, 16 bins of recycled paper from office clean-outs, and 15 boxes of office supplies.
- We continue to improve on our goal of all managers performing at least 1 environment-related MOV per quarter. In FY12, over 61% of ADEPS managers met or exceeded that goal, with an overall average of >6 environmental MOVs per manager per year.

Environmental management will always be an ongoing effort. Our 2013 Environmental Action Plan addresses our impact on the environment and outlines steps we can take to reduce our impact and decrease the potential for and severity of any environmental damage.

In keeping with the three-pronged approach established in FY12, we have three objectives: Clean the Past; Control the Present; and Create a Sustainable Future. These objectives parallel the LANL institutional objectives, with the targets fine-tuned to fit our Directorate's needs.

Clean the Past: ***reduce environmental risks from historical operations, legacy and excess materials, and other conditions associated with activities no longer a part of current operations.***

Target 1: Focused inventory on out-of-date peroxide formers to ensure proper testing and potential disposal pathways

Target 2: Observe current institutional procedures for proper handling and transfer of research samples when the originator leaves the Lab.

Target 3: Reduce surplus equipment, chemicals, materials through effective salvage operations, reuse, and recycling.

Control the Present: ***control and reduce environmental risks from current, ongoing operations, missions, and work scope.***

Target 1: Managers will conduct at least one environmentally-focused MOV in each quarter

Target 2: Communicate environmental objectives

Target 3: Perform annual chemical inventories (90% of ChemLog entries inventoried)

Target 4: Complete MPA-11 P2 oil pump replacement project

Create a Sustainable Future: ***support institutional development and maintenance of high performance sustainable buildings and reduce or eliminate the use of SF6 by recycle/reuse or replacement activities.***

Target 1: Maintain a supporting role with local FODs and Utilities & Institutional Facilities to meet HPSB objectives for building 03-1415.

Target 2: SF6 reduction, elimination, and/or reclamation

continued on next page

Green cont.

We need you to turn off lights in offices, conference rooms, hallways, and labs when not in use. Get that leaking faucet/toilet/urinal fixed (contact your facilities coordinator). Turn off computer peripherals when not in use. Alter your purchasing habits–Purchase GREEN. Use the blue and green recycling bins. Share chemicals, minimize chemical inventories, purchase safer alternatives, recycle, and dispose properly. Salvage all unnecessary or unused (and not needed) equipment. Nominate a deserving colleague for a P2 Award!!

Document, Record & Report all significant environmental actions that you take that positively affect the environment. Remember, if it's not recorded, it didn't happen. Please send your environmental action updates to your Division's EAP contact (MPA: Cathy Padro at padro@lanl.gov; MST: Jim Coy at jcoy@lanl.gov; LANSCE: Frances Aull at aull@lanl.gov; P: Steve Glick at sglick@lanl.gov). This will ensure that our Directorate continues to get the recognition it deserves for our environmental efforts.

Steve Glick, POC for ADEPS EAP

Celebrating service

Congratulations to the following LANSCE and AOT Divisions employees celebrating service anniversaries recently:

Frank Krawczyk, AOT-HPE .... 20 years
Cynthia Heath, AOT-MDE.............................. 10 years
Jianzhong Zhang, LANSCE-LC...................... 10 years
Monika Hartl, LANSCE-LC .... 10 years

the Pulse AOT&LANSCE

Published by the Experimental Physical Sciences Directorate

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 lansce.lanl.gov/news/pulse.shtml.

Los Alamos NATIONAL LABORATORY EST. 1943

HeadsUP!

Icy spots? Take action!

Slips, trips, and falls are a leading cause of injury at the Lab, and many of these injuries occur during winter.

Removal of all snow and ice before employees arrive at work isn't always possible, so the Lab places bins with salt (de-icer) at convenient locations Labwide—especially in problem areas—so that employees can apply it on walkways leading to buildings as needed. The de-icer improves walking conditions, and there are no safety or health concerns associated with employees spreading de-icer.

See an icy, slippery spot on Lab property that you can't take care of yourself with de-icer? Report any unsafe spots or other hazardous conditions to the Snow Control hotline: 667-6111.

2013 call for Pollution Prevention Award nominations

The Environmental Stewardship (ENV-ES) Pollution Prevention Program is soliciting nominations for the 2013 Pollution Prevention (P2) Awards. The P2 Awards are presented annually in recognition of individual and team efforts that enhanced operations, saved money and/or reduced adverse environmental impacts. These awards demonstrate environmental improvement activities to the Laboratory and the surrounding community. The categories for the 2013 P2 Awards are the following:

- Comprehensive Energy and Fleet Management
- Cradle to Cradle for Pollution Prevention and Recycling
- Sustainable Acquisition
- Environmental Management Systems
- Integrative Planning and Design/Community Collaboration and Engagement
- Greenhouse Gas Management
- Change Agents/Sustainability Champions Living Laboratory/Health and the Environment
- Water Resources

For more information on the categories and for nomination guidelines, see int.lanl.gov/memos/2013/02/LANL_ALL2551.pdf.

Nominations must be submitted online by March 15.

LA-UR-13-21513
Approved for public release; distribution is unlimited.

Title: AOT & LANSCE The Pulse February 2013

Author(s): Kippen, Karen E.

Intended for: Newsletter
Web