the Pulse AOT & LANSCE

February 2014
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INSIDE

Photo by Sandra Valdez, IRM-CAS

A champion of neutrons for illuminating the properties and behaviors of materials, Olivier Gourdon uses neutron crystallography to study energy-related materials. Above, a schematic view of the High-Pressure-Preferred Orientation beamline at the Los Alamos Neutron Scattering Center. In the background, the atomic arrangement of a complex modulated intermetallic compounds of formulation $Zn_{212}Pd_{64}$ refined by Gourdon.

Olivier Gourdon

A crystallographer keen on showing off the revealing properties of neutrons

By Diana Del Mauro, ADEPS Communications

At Los Alamos's Lujan Neutron Scattering Center, crystallographer Olivier Gourdon shows visiting researchers some of the latest tricks that can be performed using this 100-year-old multidisciplinary science, which has a spectacular record of demystifying materials as varied as DNA and Martian rocks.

"Crystallography has the image of an old science. I'm trying to refresh that," said Gourdon, an instrument scientist for HIPPO, the High-Pressure-Preferred Orientation Neutron Diffractometer.

> **"With neutron diffraction, we can learn much more than where are the atoms."**

Since the 1914 Nobel Prize-winning discovery that crystals can scatter the light waves of x-rays, thereby revealing how atoms are arranged in matter, scientists have used x-ray crystallography to great effect.

Neutron crystallography, a related experimental technique, debuted in 1946. Also known as neutron diffraction or neutron scattering, the method involves immersing samples in neutrons rather than x-rays. It tends to be underused, though, because generating neutrons requires a sophis-

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From Alex's desk . . .

Colleagues,

Thanks to the hard work and dedication of many, LANSCE just finished a productive and intense run cycle—from our user programs to our scientific and programmatic impact. Although we had major production issues during the month of December, we were able to fix them and extend production to all areas for the month of January 2014. This is a great example of dedication and understanding of both the user's need and the importance of programmatic deliverables. The pRad team alone performed 34 dynamic shots, several of which were were Level 2 milestone experiments; the Lujan Center accommodated additional users; UCN made great use of the additional beam; WNR made good progress with experiments of the interest to the NNSA; and IPF made progress on a number of important R&D issues. Once again, thank you all!

We are now starting a very intense and relatively long scheduled maintenance period; work coupled with the Linac Risk Mitigation project. Upon completion of this stage, production beam to WNR will be at 100 Hz. There is a great level of programmatic interest in this milestone.

During times when we have many concurrent activities taking place, coupled with an intense workload adding to both internal and external pressures to deliver, work planning is no less than paramount. The bottom line is that at some level we are in control. Slow down; think of yourself your and co-workers before you "act."

On a different note, let me bring to your attention the recently updated TA-53 Visitor Tour Policy and Procedures, which can be found on MesaLib at *mesalib.lanl.gov/87256F35005D1024/All+Documents/1BB194A29F29422087257C7C005E185E/$file/ta53-st-121-001%203-vis-tours_w_sig.pdf*. Several changes were made. I encourage you to make yourself familiar with the new procedure. If you have questions, please contact: TA53tours@lanl.gov.

LANSCE Deputy Division Leader Alex H. Lacerda

"We are now starting a very intense and relatively long scheduled maintenance period. ... Upon completion of this stage, production beam to WNR will be at 100 Hz. There is a great level of programmatic interest in this milestone."

Alex

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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kkippen@lanl.gov.

For past issues, see lansce.lanl.gov/news/pulse.shtml.

Los Alamos NATIONAL LABORATORY EST. 1943

Celebrating service

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

Ronald Barber, AOT-MDE	35 years
Eric Larson, LANSCE-LC	30 years
Nathan Okamoto, AOT-IC	30 years
Anthony Balmes, AOT-RFE	15 years
Bjorn Clausen, LANSCE-LC	15 years
Rodney McCrady, AOT-OPS	15 years
Robert Moore, AOT-MDE	5 years
Katharine Page, LANSCE-LC	5 years
Nikolai Yampolsky, AOT-HPE	5 years

Gourdon cont.

ticated infrastructure, such as at the Los Alamos Neutron Science Center (LANSCE).

Gourdon (Lujan Center, LANSCE-LC) is a proponent of both techniques as together they sometimes paint the most vivid picture of all. With HIPPO, he guides users through the process of bombarding ground-up crystals with intense neutron beams and afterward deciphering the data for high pressure-temperature, texture, liquid-amorphous materials, or reaction-kinetic studies.

"With neutron diffraction, we can learn much more than where are the atoms. We can, in some conditions, understand the dynamics and the vibrations of some atoms," Gourdon said. Neutrons, for instance, can determine the internal strains and structure of deformed metal, telling the story of why metals give before they break.

He also encourages scientists to use the Lujan Center's complementary techniques, not just crystallography. "There is not a magic instrument that will give all the answers," he said.

Gourdon first experienced neutron crystallography as a 2004 Lujan Center postdoctoral researcher supporting users on the new HIPPO instrument and studying magnetic structures and hydrogen storage materials. Next, as an Oak Ridge National Laboratory instrument scientist for its neutron powder diffractometer POWGEN, he investigated structure-property relationships in materials for energy sources, such as batteries and fuel cells. And at Pennsylvania's International Centre for Diffraction Data, Gourdon built a materials database using neutron diffraction patterns as fingerprints and created software for diffraction data analysis.

Longing to return to hands-on science, Gourdon rejoined the Lujan Center in September. "He is without a doubt an extremely valuable addition to the Lujan Center and the HIPPO user program in particular," said HIPPO co-instrument scientist Sven Vogel, noting his former protégé's expertise in modeling crystal structures, fabricating samples, and analyzing neutron diffraction data. "His previous tenure [at HIPPO and POWGEN] allowed him to immediately contribute to our program."

When the LANSCE beam is on–about half the year–Gourdon dedicates himself solely to users. "We see so many kinds of people and so many kinds of science," he said. When the beam is off, he conducts energy-related research based on oxides and intermetallics. "Neutrons are more suitable than x-rays for studying batteries," he said, "since this ray can screen lightweight and heavy elements simultaneously."

Though Gourdon's first love was mathematics, he earned a PhD in materials chemistry and structural chemistry from the University of Nantes in France. "At the end of the day, crystallography is geometry, so it's math," he said. "I am somewhere between mathematics, physics, and chemistry. That's why the Lujan Center suits me well."

Olivier Gourdon's Favorite Experiment

What: Behavior of the lithium displacement in $LiMPO_4$ as potential battery material

When: 2013

Where: Lujan Neutron Scattering Center at Los Alamos National Laboratory

Who: With Gang Wu (Materials Synthesis and Integrated Devices, MPA-11) and Jiantao Han, Sven Vogel (Lujan Center, LANSCE-LC)

How: Using HIPPO, we were studying the behavior of the lithium in $LiMPO_4$ (for M=Fe and or Mn) at various temperatures using a furnace as a sample environment.

Why: We were hoping to observe the displacement of the lithium into the materials and, indirectly, the diffusion path. This information will lead to some understanding of the electrochemistry properties of these materials.

The a-ha moment: When we started to do the first refinement data we were able to see residues that we could associate with the lithium displacement in the material. This assumption was confirmed by further experiments. It is very exciting to see that neutron diffraction, which is traditionally used to understand static effects, could also be powerful for understanding dynamic phenomenon in such crucial research as battery materials.

New instrument aids fission-fragment yield measurements

SPIDER benefits weapons program research

Uranium undergoes fission with thermal neutrons. The fissioning isotope, ^{235}U, splits into two asymmetric fragments. The distribution of the mass of these fragments–the mass yield–is an important test for different theoretical models of nuclear fission. In addition, it provides important data to nuclear weapons diagnostics, provides a way to determine the burn-up of nuclear fuel, and calculate the source-term for spent fuel waste stream analysis. Future measurements of ^{239}Pu fission yields will provide a definitive answer regarding the energy dependence of ^{147}Nd, which is of importance to the weapons program.

In recent years, a new instrument has been developed by members of Nuclear Science (LANSCE-NS) to measure fission-fragment yields as a function of the incoming neutron energy, the fragment mass and charge, and the total kinetic energy of the fragments. The instrument, named SPIDER (SPectrometer for Ion DEtermination in fission Research), aspires to achieve 2-5% accuracy for incoming neutrons between 0.01 eV and 20 MeV. Determination of the masses of the fragments utilizes the “2E-2V” method. In this method, the energy of each fragment is determined by its energy deposition in an ion-chamber, and its velocity by time-of-flight. This method provides a mass resolution of better than 1 amu and approximately 1 charge unit for the light fragment.

An illustration of the spectrometer (without its case) is presented in Figure 1. Time pickoff detectors, which use an electrostatic field to focus electrons from a foil to a microchannel-plate detector, are evident on both sides of the fissile foil in the middle.

Figure 2 shows preliminary results from the measurement performed at the Lujan Center at LANSCE between October and November 2013. The graph shows the yield of fission fragments as a function of their mass. The characteristic asymmetric mass distribution in thermal fission of actinides is evident from the data; a light mass peak is observed around 95 amu and a heavy peak around 140 amu. Further work is needed before drawing conclusions about the agreement between the evaluated data (ENDDF/B-VII.1) and this experiment. An improved calibration of the instrument using radiation sources is planned at the end of the current LANSCE run cycle, and this might still change the experimental results slightly.

Future plans include the construction of 8-10 detector arms to enhance the acquisition rate and allow for the measurement of fast-neutron-induced yields.

The detector design, construction, and analysis was the result of a collaboration between Los Alamos, University of New Mexico, Colorado School of Mines, Slovak Academy

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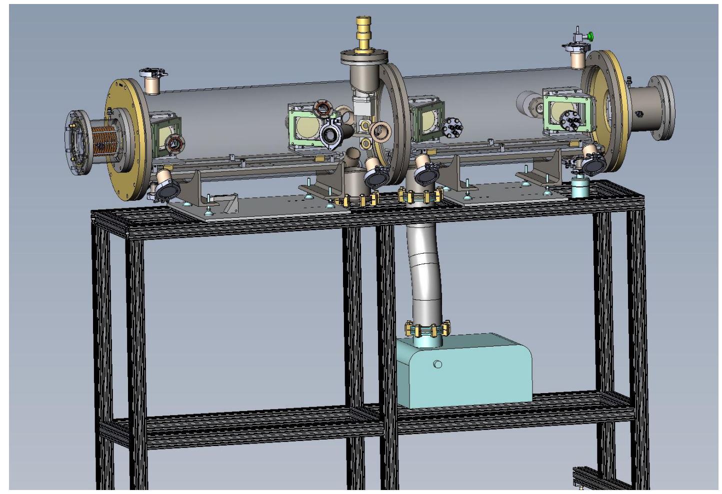


Figure 1: View of SPIDER spectrometer. The source is in the middle and the time pickoff detectors are evident on each side.

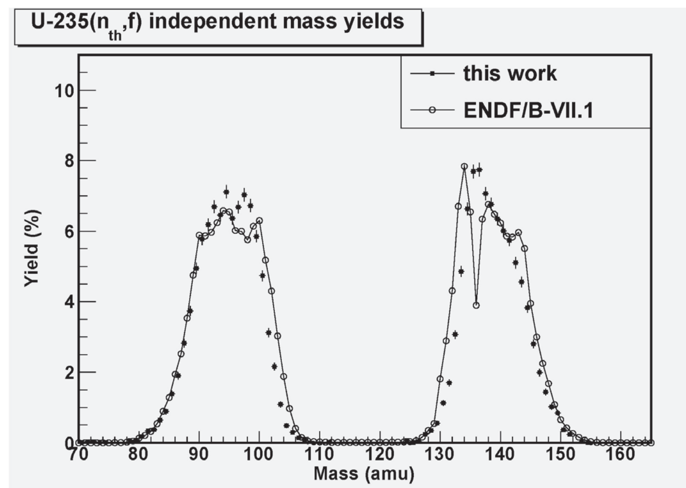
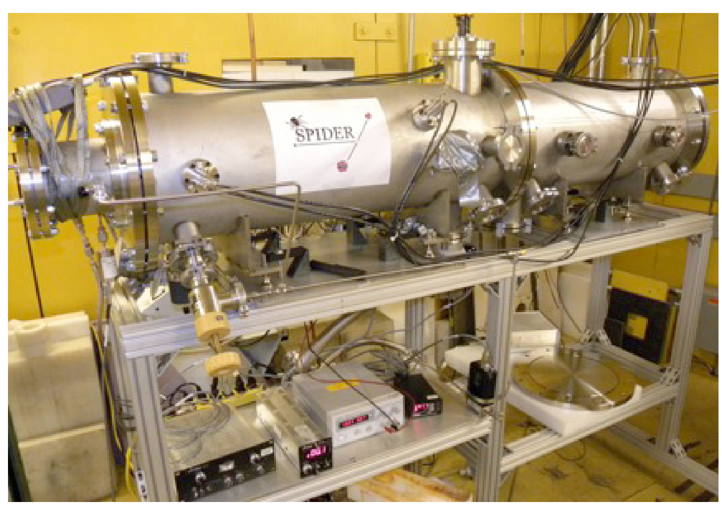


Figure 2: Mass yield results obtained with the SPIDER spectrometer to evaluated data taken from ENDF/B-VII.1



SPIDER at flight path 12 at the Lujan Center

SPIDER cont.

of Sciences, Lawrence Livermore National Laboratory, and Lawrence Berkeley Laboratory. Los Alamos participants include Fredrik Tovesson, Krista Meierbachtol, and Dan Shields (LANSCE-NS), Morgan White (Materials and Physical Data, XCP-5), Charles Arnold and Todd Bredeweg (Nuclear and Radiochemistry, C-NR), Justin Jorgenson (Applied Engineering Technology, AET-5), and Arnie Sierk (Nuclear & Particle Physics, Astrophysics and Cosmology, T-2).

Instrument construction and research, which supports the Laboratory's Nuclear Deterrence mission and Nuclear and Particle Futures pillar, was funded by the LDRD program.

Technical contact: Fredrik Tovesson

Former Rosen Scholar named American Physical Society Fellow

Markus Roth, a former Rosen Scholar at LANSCE, has been inducted into the 2013 class of American Physical Society fellows, Division of Plasma Physics. He was cited "for outstanding experimental contributions in laser-produced proton and deuterium beams, and their application to fast ignition and neutron beam generation."

Roth, a distinguished professor of physics at Germany's Institut für Kernphysik, Technische Universität, came to LANSCE in 2012 under a fellowship aimed at attracting visiting scholars in the fields of nuclear science, materials science, defense science, or accelerator technology. As a Rosen Scholar, Roth worked with LANSCE and Physics Division staff members to research novel, compact, high-brightness sources of neutrons using ultra intense lasers.

Using the Lab's powerful 200 trillion-watt short-pulse laser system TRIDENT, Roth was part of an international team that created the largest neutron beam ever made by a short-pulse laser, breaking a world record. They focused high-intensity light on an ultra-thin plastic sheet infused with deuterium. "So far only at TRIDENT has this new plasma acceleration mechanism been successfully implemented," Roth, the first author on the paper, said in a Los Alamos news release at the time. Five times larger than the previous record and requiring less than a quarter of the laser energy, this record neutron beam has the speed and energy range that makes it an ideal candidate for radiography and a wide variety of high energy density physics studies. His work at LANL was one of the Laboratory's top science news stories for 2013.

APS Fellows are selected for exceptional contributions to the physics enterprise, with fellowship a distinct honor signifying recognition by professional peers. APS represents more than 50,000 members, including physicists in academia, national laboratories and industry in the United States and throughout the world.

Technical contact: Alex Lacerda

Seeking design rules for efficient lighting sources

In the search for more efficient general lighting, down-conversion strategies based on inorganic light sources and phosphor conversion have emerged as a front-runner. Advantages include durability, long life, color stability, and an environmental footprint free of toxic heavy metals. In research published in *Chemistry of Materials*, scientists have examined the desirable properties of phosphor materials.

The oxide garnet $Y_3Al_5O_{12}$ (YAG), when substituted with a few percent of the activator ion Ce_{3+} to replace Y_{3+}, is a luminescent material that is nearly ideal for phosphor-converted solid-state white lighting. The local environments and distributions of the small number of substituted Ce_{3+} ions critically influence the optical properties of the phosphor, yet crystal-chemical guidelines for finding new and efficient phosphor compounds have not been developed. A user group, led by the University of California, Santa Barbara, and staff of the Lujan Neutron Scattering Center employed a combination of state-of-the-art scattering and spectroscopy techniques to determine the nature of these local environments and correlate them with the macroscopic luminescent properties of Ce-substituted YAG.

This study demonstrates the deep understanding that can be obtained for the composition-structure-property relationships of solid-state phosphors. This knowledge could aid the development of rational design strategies for the syntheses of efficient thermally stable light-emitting compounds with tunable colors. The researchers established the rigidity of the garnet structure, which plays a key role in the high quantum yield and in the resistance toward thermal quenching of luminescence. Local structural probes reveal compression of the Ce_{3+} local environments by the rigid YAG structure, which gives rise to the unusually large crystal-field splitting and yellow light emission. The results suggest that effective design rules for finding new phosphor materials require rigid, highly three-dimensionally connected host structures with simple compositions that manifest a low number of phonon modes, as well as low activator ion concentrations to avoid quenching. Reference: "Local Environments of Dilute Activator Ions in the Solid-State Lighting Phosphor $Y_{3-x}Ce_xAl_5O_{12}$," *Chemistry of Materials* **25**, 3979 (2013). Researchers include Katharine Page and Anna Llobet (LAN-

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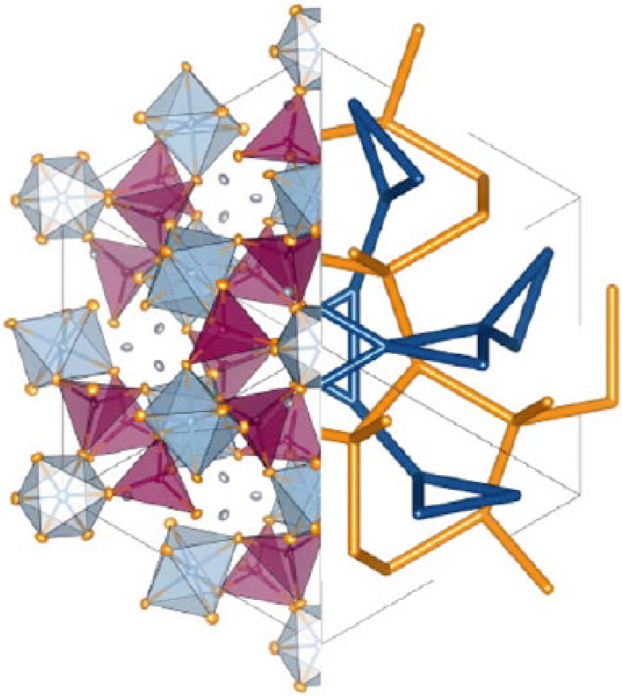


The crystal structure of YAG viewed down the (111) face of the unit cell with red, blue, gray, and orange spheres representing four-coordinate Al, six-coordinate Al, Y, and O atoms, respectively. The right half of the figure depicts the interpenetrating networks of Y and Al, which form a double-gyroid structure. The high connectivity of the lattice decreases the degrees of freedom available for phonon modes and enhances luminescence properties.

Design cont.

SCE-LC), Nathan C. George, Bradley F. Chmelka, and Ram Seshadri (University of California, Santa Barbara), Andrew J. Pell and Guido Pintacuda (Université de Lyon, France), Geraldine Dantelle (École Polytechnique, France), and M. Balasubramanian (Argonne National Laboratory). This work benefited from the use of the Neutron Powder Diffractometer (NPDF) and the High Intensity Powder Diffractometer (HIPD) at the Lujan Neutron Scattering Center, which the DOE Office of Basic Energy Sciences funds. The research supports the Laboratory's Energy Security mission area and Materials for the Future science pillar.

Technical contact: Katharine Page

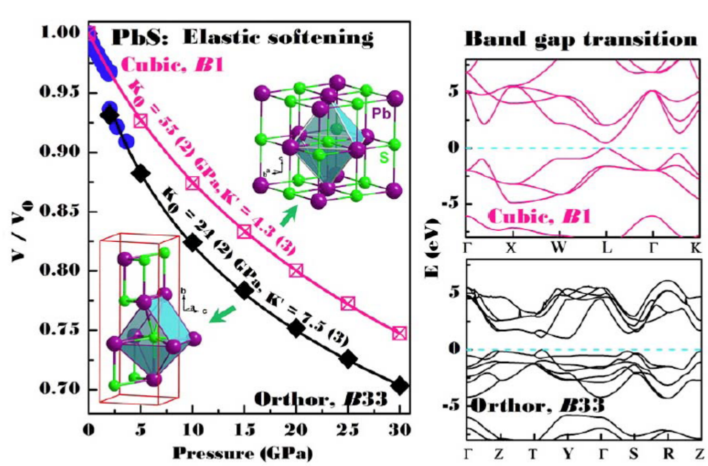
Improved understanding of a semiconductor used in infrared detectors

At the Lujan Neutron Scattering Center a combined study of high-pressure neutron diffraction, electrical resistance measurement, and first-principles calculation provides new insights into structural and electronic transitions in lead sulfide (PbS). PbS is a semiconductor used in infrared detectors. The material undergoes both structural and electronic phase transitions under pressure. However, the nature of the transitions remains a subject of debate. The experiments and complementary models published in the journal *Inorganic Chemistry* offer a description of the phase transition mechanisms and advance the understanding of lead-based semiconductors.

The researchers observed phase-transition induced elastic softening and direct to indirect band gap transition in PbS. First-principles calculations simulated the elastic properties and band structures of PbS. The scientists conclude that both cubic and orthorhombic phases are semiconductors, but they exhibit features of direct and indirect band gaps, respectively. Phase transition induced elastic softening in PbS is likely to be associated with enhanced metallic Pb - Pb bonding in the orthorhombic phase. Phase transition also leads to an anomalous drop in electrical conductivity in orthorhombic PbS, which the researchers attribute to the lower crystal symmetry and the enlarged band gap in the *Cmcm* phase. Based on the results and calculations, the team proposed a new model for the B1→B33→ B2 phase transitions. They suggest that the phase transitions paths involve translation of a trigonal prism in the B1 phase and motion of the next-nearest neighbor Pb atom into $\{SPb_7\}$ coordination and subsequent lattice distortion in the B33 phase.

Reference: "Phase-Transition Induced Elastic Softening and Band Gap Transition in Semiconducting PbS at High Pressure," *Inorganic Chemistry* **52**, 8638 (2013). Researchers include Jianzhong Zhang (LANSCE-LC), Shanmin Wang, Yi Zhang, Andrew Alvarado, Jeevake Attapattu, Liping Wang, Changfeng Chen, and Yusheng Zhao (University of Nevada, Las Vegas); and Duanwei He (Sichuan University, China). This work benefited from the use of the High-Pressure Preferred Orientation Diffractometer (HIPPO) instrument at the Lujan Neutron Scattering Center at LANSCE funded by the DOE Office of Basic Energy Sciences. The research supports the Lab's Energy Security mission area and the Materials for the Future and Nuclear and Particle Futures science pillars.

Technical contact: Jianzhong Zhang



(Left): Pressure-volume data from high-pressure neutron diffraction and ab initio simulations. (Right): Simulated band structures.

HeadsUP!

Taking charge of electricity usage

The UI-FOD has provided information on electricity usage in ADEPS buildings. While ADEPS staff share many of these buildings with folks from other directorates, the data is, nonetheless, revealing. We also note that in buildings with experimental areas, it is not surprising that all forms of energy usage may vary, sometimes greatly, from quarter-to-quarter and year-to-year.

As can be seen in the data, ADEPS electricity usage increased 5% from FY12 to FY13. Electrical usage has a significant monetary and environmental impact to our bottom line.

Please remember to turn off/unplug equipment when not in use, lower room thermostats in the winter at nights and when common areas (conference rooms) are unattended, and turn off office and common area lights if you are the last one out. Lastly, always look for energy-efficient alternatives when they do not affect mission delivery.

A good adage to follow: “If you do it at home (shut off lights and lower thermostats at nights and vacations), then why not do it at work too?” Take responsibility for protecting and sustaining our environment! Thank You.

Your ADEPS EMS (Environmental Management System) POCs are:

Steve Glick - Physics
Jim Coy – MST
Susie Duran – MPA
Frances Aull – LANSCE

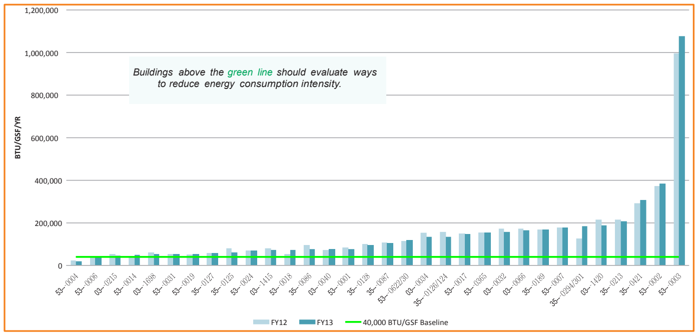
RAD Electricity Report

Fiscal Year Comparison – FY13 vs FY12

Account Number: RAD ADEPS

Billing Period: FY13

ADEPS Building Energy Efficiency – FY12 vs FY13

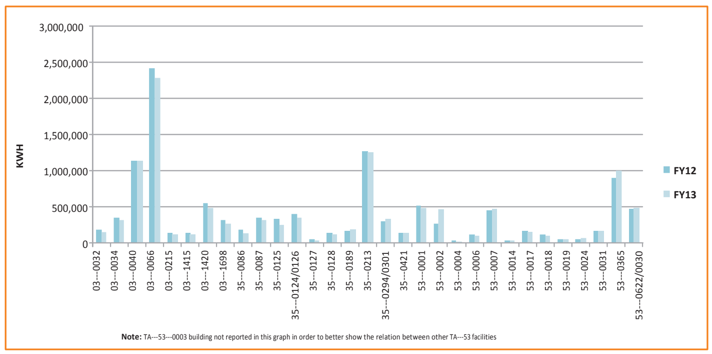


Building Energy Efficiency Comparison

This chart compares the energy efficiency of your RAD’s buildings this year with FY12.

*Energy efficiency can be measured by energy intensity—which for an office building is total energy use over time in relation to floor area, counting gas as well as electricity. The **green line** marks DOE’s standard for an efficient building: no more than 40,000 Btu/GSF per year or 10,000 Btu/GSF per quarter.*

ADEPS Building Electricity Use – Quarter 4 – FY12 vs FY13



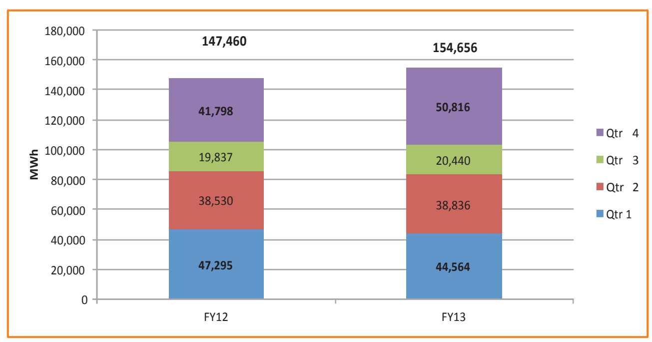
Building Electricity Use Comparison

Electrical consumption by your RAD’s buildings this quarter compared to the same quarter in FY12

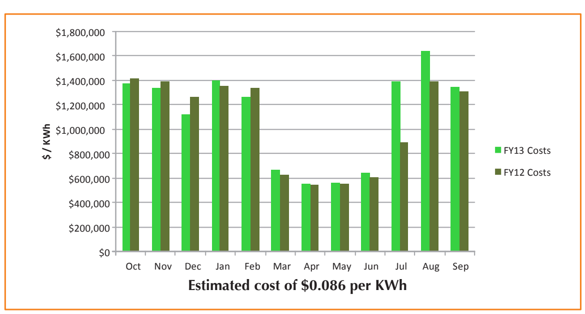
ADEPS Quarterly Electricity Use – FY12 vs FY13

Quarterly Electricity Use Comparison

Quarterly electricity use in megawatt-hours (MWh) for all metered facilities in your RAD during FY12 and FY12

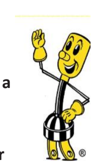


ADEPS Electricity Costs by Month – FY12 vs FY13



Individual Action Steps

- Unplug unnecessary electronics.
- Turn your monitor and the lights off when you leave for a meeting or the day.
- Put your computer to sleep or in power down mode when you’re not using it.



We hope this information helps you better understand and make better choices about your RAD’s use of electricity.

Questions? Need more information? Go to umetering@lanl.gov

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