NREL's Michael Crowley

Page 2

DOE Pulse

Science and Technology Highlights from the DOE National Laboratories

Number 267 **August 11, 2008**

Research Highlights . . .

Expanding the radiotracer tool kit

Using positron emission tomography (PET) to monitor the movement and interactions of radioactively labeled "tracer" compounds inside the human body, scientists have advanced the understanding of diseases such as cancer and drug addiction. But there are many more compounds scientists would like to label for tracking with PET. To this end, researchers at DOE's Brookhaven Lab have devised a simple, fast method for radiolabeling formaldehyde, a common organic chemical reagent. This radiolabeled formaldehyde can now be used to synthesize a wide range of carbon-chain molecules that can be administered to humans as radiotracers, greatly expanding the tool kit available to PET researchers.

[Karen McNulty Walsh, 631/344-8350, kmcnulty@bnl.gov]

Kinetic battery truly off the grid

Inventors at DOE's Idaho National Laboratory have collaborated with research partners at M2E Power, Inc., to successfully convert the power of motion into electrical generation and battery charging. This sophisticated technology, M2E motion-to-energy power generation systems, uses an innovative, optimized microgenerator with power management circuitry that kinetically charges mobile batteries from natural motion, such as walking. This breakthrough technology eliminates the need for recharging — taking mobile devices off the electrical grid. This changes the very nature of mobile power. No longer will people need to plug in to get the power needed for smart phones, digital cameras, gaming devices or mobile audio players.

[Keith Arterburn, 208/526-4845 keith.arterburn@inl.gov]

Argonne bottle cap thwarts wine counterfeiters

In the past few decades, bottles of rare premium wines have begun to command tens of thousands of dollars apiece at auction, and thousands of other wines retail for hundreds to thousands of dollars a bottle. Wine counterfeiting has grown into a booming criminal enterprise. To combat this problem, engineer Roger Johnston and his colleagues in the Vulnerability Assessment Team at DOE's Argonne National Laboratory have created a cap that fits over the bottle's cork. The cap contains a small circuit that completes when it is removed, which triggers an electric pulse that creates electronic evidence someone has tampered with the bottle. By connecting the cap to a laptop through a USB cable, the auctioneer or the consumer can check whether or not the wine has already been opened or altered.

[Jared Sagoff, 630/252-5549, jsagoff@anl.gov]

Fermilab zooms in on the Higgs particle

Scientists working on the CDF and DZero experiments at DOE's Fermi National Accelerator Laboratory have entered Higgs territory. For the first time, the two experiments directly restrict the allowed mass range for the elusive Higgs particle, which would explain why elementary particles such as electrons and quarks have mass. Prior to this result, particle physicists expected the Higgs to have a mass in the range of 114 to about 200 GeV/c^2. Now, CDF and DZero scientists have ruled out a Higgs mass of 170 GeV/c^2. The two groups expect to double their data sets in the next couple of years, improving their chance to observe the particle or to constrain its mass even further.

[Kurt Riesselmann, 630/840-5681, kurtr@fnal.gov]

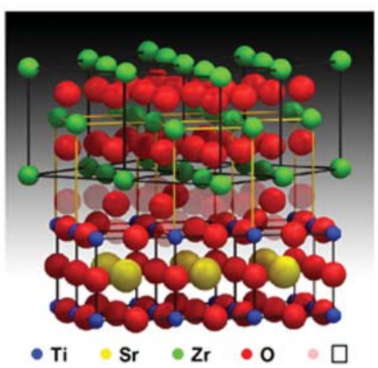
DOE Pulse highlights work being done at the Department of Energy's national laboratories. DOE's laboratories house world-class facilities where more than 30,000 scientists and engineers perform cutting-edge research spanning DOE's science, energy, national security and environmental quality missions. *DOE Pulse* (www.ornl.gov/news/pulse/) is distributed every two weeks. For more information, please contact Jeff Sherwood (jeff.sherwood@hq.doe.gov, 202-586-5806).

Z-contrast STEM shows how 'colossal conductivity' works

A new material characterized with ORNL's Z-contrast scanning transmission electron microscope could open a pathway toward more efficient fuel cells.

The material, a super-lattice developed by researchers in Spain, improves ionic conductivity near room temperature by a factor of almost 100 million, representing "a colossal increase in ionic conduction properties," says Maria Varela of DOE's Oak Ridge National Laboratory, who characterized the material's structure with senior researcher Stephen Pennycook.

The analysis was done with ORNL's 300 kilovolt Z-contrast STEM, which can achieve aberration-corrected resolutions near 0.6 angstrom, until recently a world record. The direct images show the crystal structure that accounts for the material's conductivity.



The molecular model of the ion-conducting material shows that numerous vacancies at the interface between the two layers create an open pathway through which ions can travel.

Solid oxide fuel cell technology requires ion-conducting materials—solid electrolytes—that allow oxygen ions to travel from cathode to anode. However, existing materials have not provided atom-scale voids large enough to easily accommodate the path of a conducted ion, which is much bigger than, for example, an electron.

"The new layered material solves this problem by combining two materials with very different crystal structures. The mismatch triggers a distortion of the atomic arrangement at their interface and creates a pathway through which ions can easily travel," Varela says.

The research team with Spain's Universidad Complutense de Madrid and Universidad Politécnica de Madrid produced the material and observed its outstanding conductivity properties, but the structural characteristics that enable the material to conduct ions so well were not known until the material was put under the Lab's ultra-high resolution microscopes.

The paper, a collaboration between researchers at the Universities of Madrid and at ORNL, was published Aug. 1 in *Science*. —*Sarah Wright*

Submitted by DOE's Oak Ridge National Laboratory

NREL's Michael Crowley helps researchers see nature at work

Michael Crowley

Its official name is cellobiohydrolase Cel7A. In Michael Crowley's award-winning animated version, it looks a Technicolor dinosaur fossil caught in the act of chomping on dinner.

In reality, Cel7A is just the opposite—it's a vegetarian molecule.

Crowley, a senior scientist, and his associates at DOE's National Renewable Energy Laboratory are modeling nature's primary agent for decaying plants. By precisely understanding how Cel7A does its job so well, they hope to bioengineer a version that will accelerate the process of making ethanol from woody plants and farm wastes.

Crowley's animation was awarded second place in DOE's Electronic Visualization competition sponsored by the Scientific Discovery through Advanced Computing program. He received the award at the program's meeting in Seattle. It was Crowley's first submission.

What makes the award especially noteworthy is the nature of the competition.

His animation was one of 52 submissions by national laboratories and universities. Moreover, nearly all of the contestants were visualizing the behavior of large-scale phenomenon like hurricanes and flames.

Instead, Crowley's work focuses on the behavior of a single molecule. While something like a storm can be very large and complex, the process of modeling them is relatively straightforward and can be divided into discrete sections and a logical sequence.

In contrast, Crowley said, animating Cel7A required finding ways to successfully model the interactivity of many atoms interacting dynamically with each other—simultaneously.

"It is very difficult to parallelize the process to run even on a huge computer," Crowley said. "You can have 1,000 processors and it's not easy to speed up."

Crowley is a native of Hempstead, Long Island, with a Ph.D. from the University of Montana. Prior to joining NREL 16 months ago, he was at The Scripps Research Institute in La Jolla, Calif., where he studied protein folding in human metabolism and helped develop high performance computer programming. He joined NREL and started his own high performance computer group after consulting with the Lab's biofuels program.

Submitted by DOE's National Renewable Energy Laboratory