



Ames Lab's
Robert
Angelici

Page 2

Research Highlights . . .



Science and Technology Highlights from the DOE National Laboratories

Number 224

December 11, 2006

“Pseudogap” origin revealed

Research at DOE's [Brookhaven Lab](#) appears to resolve one mystery in the 20-year study of high-temperature (high-Tc) superconductors — the origin of a “pseudogap” in the energy level of the materials' electronic spectrum. The Brookhaven research shows that the pseudogap is the result of electrons pairing up above the transition temperature to the superconducting state. These pairs have strongly fluctuating phases, so they cannot behave collectively as soon as they are formed. Only by cooling the material to much lower temperatures do the phase fluctuations become suppressed. At a certain temperature, the phase becomes locked so the electron pairs act coherently — and the system becomes a superconductor.

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

Explosives Detection System to be installed at U.S. Air Base

A team from DOE's [Idaho National Laboratory](#) have spent the last four years perfecting an explosives detection system to assist Air Force security professionals detect the presence of smuggled explosives entering military bases. The award-winning Idaho Explosives Detection System will be installed at Ohio's [Wright-Patterson Air Force Base](#) for semi-permanent field testing. The system relies on a technique called pulsed thermal neutron generation. If nitrogen-based explosive signatures are detected, the IEDS will alert operators in about five minutes. The inspection time allows a large amount of statistical data to be captured, ensuring that the results are accurate to within 95 percent.

[Ethan Huffman, 208/526-0660,
Ethan.Huffman@inl.gov]

A new picture of the pion

Using the Continuous Electron Beam Accelerator Facility at DOE's [Jefferson Lab](#), scientists have snapped the most



Detectors in Jefferson Lab's Hall C.

precise picture yet of the pion. The pion is a common subatomic particle built of two quarks bound together by the strong force.

Also present is the quark-gluon sea, a strong-force driven bevy of quarks, anti-quarks and strong force glue particles called gluons. Studying the pion's relatively simple structure can provide new insight into the nature of the strong force. The experiment has thus far provided evidence that the quark-gluon sea does play an important role in the pion's basic structure.

[Kandice Carter, 757/269-7263,
krcarter@jlab.org]

Cold shot

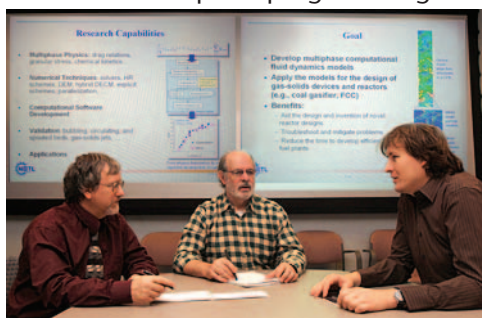
Scientists have long known that uranium salts glow greenish-yellow in ultraviolet light. An oddity about their UV glow, or fluorescence spectra: The resolution of the spectral fingerprint becomes sharper as the temperature falls. Scientists at DOE's [Pacific Northwest National Laboratory](#) are now applying cryogenic fluorescence spectroscopy to uranium in contaminated soil at a former nuclear fuel manufacturing site. After cooling the sediments to near the temperature of liquid helium, the team hit a UV laser on a contaminated sample to coax a uranium fluorescence intensity of more than five times that at room temperature. Other spectra absent at room temperature popped out when frozen, enabling researchers to distinguish different forms of uranium, including uranium-carbonate, which moves underground, threatening water supplies.

[Bill Cannon, 509/375-3732,
cannon@pnl.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).

NETL scientists developing next-generation multiphase flow software

Researchers at the **National Energy Technology Laboratory (NETL)** have developed a prototype of MFOAM, the next generation of multiphase flow software that will greatly increase the fidelity and speed of simulating fossil fuel reactors such as coal gasifiers and chemical looping systems. MFOAM permits combining the geometric fidelity available in commercial software with the source code access provided by NETL-developed MFIx (Multiphase Flow with Interphase eXchanges) software. MFOAM is composed of open-source components such as OpenFOAM (Field Operation and Manipulation) rather than being written from scratch — greatly reducing software development time and cost. MFOAM will have a scripting front end that will allow researchers to focus on physics and numerical algorithm development rather than computer programming issues.



MFOAM research group

A team of computational scientists led by NETL met recently at NETL, Morgantown, to formulate software design and development

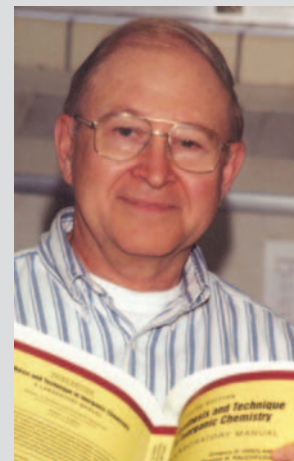
plans for the next-generation software for modeling multiphase flows. The team includes representatives from **Oak Ridge National Laboratory**, Fluent Inc., and Aeolus Research. The transfer of the capabilities in the existing MFIx software to MFOAM was discussed at the planning meeting.

The goal of the project is to improve the speed and accuracy of the simulations of complex multiphase flows commonly encountered in advanced power and process plants. Multiphase flows appear in fossil fuel processes in the form of gas-solids, gas-liquid, and gas-liquid-solids systems. These systems are notoriously difficult to design and scale up. Accurate models of these systems will enable the discovery of novel designs, speed up the design process, and save money. NETL has been a leading center for the research and development of this computational technology. The result of the project will be a software tool that researchers at NETL, other national labs, and universities will use to conduct research in computational multiphase flow.

Submitted by DOE's National Energy Technology Laboratory

AVOIDING FADS

Ames Laboratory inorganic chemist Robert Angelici is known for pursuing unique and challenging research problems and then developing fundamental concepts that may be applied to related fields. "I enjoy the thrill of exploring new ideas and directions," he says. If there is a 'fad' area, I'll avoid it and develop my own direction.



Robert Angelici

Angelici has made substantial contributions to the chemistry of the transition metals. He has used transition metals to stabilize molecules that would otherwise decompose. On the other hand, he has used transition metal complexes to increase the reactivity of otherwise unreactive molecules that are present in petroleum. He has also investigated catalytic conversions of petroleum and biodiesel components to potentially useful commercial products. Some of these studies involved a conceptually new type of catalyst consisting of a metal complex tethered to the surface of silica that also contains a different transition metal.

Currently, Angelici is pursuing two new efforts related to transition metals. One project examines the effects of transition metal binding on the shape and properties of curved carbon surfaces that are fragments of buckminsterfullerene. Another project focuses on the catalytic power of metallic gold, long considered a poor catalyst. Angelici now finds that this metal rapidly catalyzes reactions of carbon monoxide, amines, and oxygen. The DOE's Office of Science, Basic Energy Sciences Program, Chemical Sciences Division provides funding for both projects.

Committed to helping train new generations of inorganic chemists, Angelici developed the first textbook of inorganic laboratory techniques, *Synthesis and Technique in Inorganic Chemistry*, which is still used in many colleges and universities.

The text, first published in 1969 and now in its third edition, has had "a rather remarkable run," says Angelici.

An outstanding researcher and an inspiring teacher, Angelici will receive the American Chemical Society Award for Distinguished Service in the Advancement of Inorganic Chemistry at the 2007 ACS National Meeting and Exposition in March.

Submitted by DOE's Ames Laboratory