PPPL's
Bruce D. Kay

Page 2

DOE Pulse

Science and Technology Highlights from the DOE National Laboratories

Number 265 July 14, 2008

Research Highlights . . .

More evidence for a revolutionary theory of water

The traditional picture of how liquid water behaves on a molecular level is wrong, according to new experimental evidence collected by a collaboration of researchers from DOE's Stanford Linear Accelerator Center (SLAC), the RIKEN SPring-8 synchrotron and Hiroshima University in Japan and Stockholm University in Sweden. The team, involving SLAC scientist Anders Nilsson, used advanced X-ray spectroscopy techniques to create a more detailed picture of water's molecular behavior. They found that water is made up of tetrahedral groups, as had been previously noted, but they also discovered clear evidence for the dominance of a second, less defined structure in the mix. Published as the cover story in the April 22 online edition of *Chemical Physics Letters*, the findings could soon help overturn the established orthodoxy surrounding the substance most essential to life.

[Brad Plummer, 650/926-2282, brad.plummer@slac.stanford.edu]

New process makes Ti parts affordable

Whether for stopping cars or bullets, titanium is the material of choice, but it has always been too expensive for all but the most specialized applications. That could change, however, with a non-melt consolidation process being developed by DOE's Oak Ridge National Laboratory and industry partners. The new processing technique could reduce the amount of energy required and the cost to make titanium parts from powders by up to 50 percent, making it feasible to use titanium alloys for brake rotors, artificial joint replacements and, of significant interest now, armor for military vehicles.

[Ron Walli, 865/576-0226, wallira@ornl.gov]

ARTHR gives robots the brains to detect threats

U.S. soldiers and first responders could soon have their own version of a bomb-sniffing dog — a robotic payload named ARTHR developed at DOE's Idaho National Laboratory. The Autonomous Real-time Threat-Hunting Robot system enables commercial robots to search dangerous environments such as insurgent war zones, natural disasters and sites of radiological and chemical accidents. ARTHR creates its own maps, making barriers easy to read and color-coding safe and hazard zones. Traditional systems require command center units weighing up to 30 pounds, but ARTHR responds to lightweight PCs and handheld controllers such as Wii™ gaming remotes. In head-to-head tests, both novices and highly-trained military teams found ARTHR more reliable and easier to use than current systems.

[Nicole Stricker, 208/526-5955, nicole.stricker@inl.gov]

CDF sets constraints on the stop

Scientists know many reasons why the current theory of fundamental particles is incomplete. A possible extension of the standard particle theory is Supersymmetry, which predicts that every particle has its own superpartner—a sparticle. Scientists working on experiments at the Tevatron collider at DOE's Fermi National Accelerator Laboratory are looking for short-lived sparticles emerging from high-energy proton-antiproton collisions. In a new study, scientists of the CDF collaboration looked for the stop, the superpartner of the top quark. When the authors examined Tevatron collision events, they found no evidence for a light stop. Instead, they set new constraints on the proposed Supersymmetry theory.

[Kurt Riesselmann, 630/840-3351, 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).

Model gives insight to pandemic risk

A pair of researchers at DOE's Los Alamos National Laboratory have developed a mathematical tool that could help health experts and crisis managers determine in real time whether an emerging infectious disease such as avian influenza H5N1 is poised to spread globally.

In a paper published recently in the *Public Library of Science*, researchers Luís Bettencourt and Ruy Ribeiro of Los Alamos' Theoretical Division describe a novel approach to reading subtle changes in epidemiological data to gain insight into whether something like the H5N1 strain of avian influenza—commonly known these days as the "Bird Flu"—has gained the ability to touch off a deadly global pandemic.

"What we wanted to create was a mathematically rigorous way to account for changes in transmissibility," said Bettencourt. "We now have a tool that will tell us in the very short term what is happening based on anomaly detection. What this method won't tell you is what's going to happen five years from now."

Bettencourt and Ribeiro began their work nearly three years ago, at a time when the world was wondering whether avian influenza H5N1, with its relatively high human mortality rate, could become a frightening new pandemic. Health experts believe that right now the virus primarily infects humans who come in contact with infected poultry.

But some health experts fear the virus could evolve to a form that would become transmissible from human to human.

Bettencourt and Ribeiro developed an extension of standard epidemiological models that describes the probability of disease spread among a given population. The model then takes into account actual disease surveillance data gathered by health experts like the World Health Organization and looks for anomalies in the expected transmission rate versus the actual one. Based on this, the model provides health experts actual transmission probabilities for the disease. Unlike other statistical models that require huge amounts of data for accuracy, the Los Alamos tool works on very small populations such as a handful of infected people in a remote village.

In addition to its utility in understanding the transmissibility of emerging diseases, the new method is also advantageous because it allows public health experts to study outbreaks of more common ailments such as seasonal influenza early on. This can assist medical professionals in making better estimates of potential morbidity and mortality, along with assessments of intervention strategies and resource allocations that can help a population better cope with a developing seasonal outbreak.

Submitted by DOE's Los Alamos National Laboratory

Bruce D. Kay: Advancing Scientific Frontiers in Chemical Physics

Bruce D. Kay

Advancing scientific frontiers is not for the meek. So, it is not surprising that colleagues describe Pacific Northwest National Laboratory's Bruce D. Kay as audacious and insightful.

Kay joined PNNL in 1991 to lead the design, procurement, and fabrication of a state-of-the-art molecular beam-surface scattering laboratory at the Department of Energy's EMSL. A fan of Pacific Northwest wines and an avid cyclist, he decided to stay in southeastern Washington. Kay now leads the Laboratory's work in experimental chemical physics.

Chemical physics uses experimentation and theory to explain the forces in play in chemical reactions, such as the movement of water molecules through contaminated soil or the behavior of electrons on a new industrial catalyst. One ongoing project involves using nanoscale amorphous films to study desorption, diffusion and crystallization kinetics. This work, termed "beakers without walls," is furthering the understanding of deeply supercooled water and aqueous solutions.

"Bruce has a rare talent," said Bruce Garrett, director of the Chemical & Materials Sciences Division. "He combines meticulous experimental studies with careful theoretical analysis to yield profound insight into complex condensed phase systems."

His ability to present complex fundamental physical principles with scientific rigor, combined with real-world examples and a dynamic sense of humor, has led to more than 200 invited lectures worldwide.

Kay is a member of DOE's Basic Energy Sciences Advisory Committee, which provides recommendations on research priorities and other topics. He recently completed a three-year stint on the International Advisory Board, Academica Sinica Institute for Atomic and Molecular Science, Taiwan.

Kay is a Fellow of the American Physical Society, American Vacuum Society and the American Association for the Advancement of Science. He also is an affiliate professor of physical chemistry at the University of Washington and visiting professor of chemical physics at the University of Liverpool, England.

Submitted by DOE's Pacific Northwest National Laboratory