BNL's Etsuko Fujita

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DOE Pulse

Science and Technology Highlights from the DOE National Laboratories

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Research Highlights . . .

Hydrogen truck rolls out

The Center for Hydrogen Research (the result of a collaborative effort between the Aiken County, South Carolina, Economic Development Commission and DOE's Savannah River National Laboratory) has unveiled its newly purchased eTec Hydrogen Internal Combustion Engine pickup truck, the first hydrogen vehicle to be registered in South Carolina. The truck will be used to publicly demonstrate the viability of using hydrogen in transportation, and will provide a real-world test bed for the development and evaluation of hydrogen storage systems, a critical link in advancing automotive hydrogen technology. Companies and research organizations, including SRNL, will be able to test hydrogen storage technology without having extensive modifications to a test vehicle.

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Proteins provide clues to nanomaterial toxicity

New research has revealed that proteins adsorbed onto nanomaterials play an important role in nanomaterial disposition and toxicity. A team from DOE's Pacific Northwest National Laboratory, the University of California-Davis and the University of Florida investigated the toxicity of two classes of nanomaterials: single-walled carbon nanotubes and spherical silica structures. They observed that albumin was the major protein adsorbed to carbon nanotubes and that it influenced the uptake of nanomaterial by cultured cells. "The data suggest that comprehensive knowledge of this behavior could help in understanding how complex biological systems process nanomaterials," said PNNL scientist Tom Weber.

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SSRL Beamline 13's first light

Last month, the first light shone into the newest beamline at the Stanford Synchrotron Radiation Laboratory, located at DOE's Stanford Linear Accelerator Center. Beamline 13, which has been under construction for the past two years, will allow new types of soft X-ray material science studies at SSRL. When it opens to users in 2009, this DOE-funded beamline will be configured with three experimental stations: Beamline 13-1 for scanning transmission X-ray microscopy, which will allow the study of condensed matter and surface science and magnetism at the nanometer scale; Beamline 13-2 for photoemission and X-ray absorption spectroscopy, which shows the angles and lengths of bonds both inside materials and at their surfaces; and Beamline 13-3 for resonant coherent scattering and diffraction imaging experiments, which can reveal structure at the nanometer scale.

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BIRC to support bioterrorism emergency response efforts

If you're an emergency response manager for a high-profile transportation facility and the biodetection system goes off, what do you do? One day soon you may be calling the BioWatch Indoor Reachback Center (BIRC) at Sandia. Since August 2007, a small group of Sandia/California researchers have been operating BIRC, part of the Department of Homeland Security's BioWatch program, an early warning system designed to detect trace amounts of biological materials at various U.S. public facilities. BIRC's role would be to provide scientific modeling support within two hours to decision makers responding to a public release of a biohazard agent.

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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).

'Exascale' computing envisioned by Sandia and Oak Ridge researchers

DOE's Sandia and Oak Ridge national laboratories recently launched the Institute for Advanced Architectures to lay the groundwork for a new computer that would perform a million trillion calculations per second.

An exaflop is a thousand times faster than a petaflop, which is a thousand times faster than a teraflop. Teraflop computers — the first was developed 10 years ago at Sandia — currently are the state of the art and perform trillions of calculations a second.

The institute is intended "to close critical gaps between theoretical peak performance and actual performance on current supercomputers," says Sandia project lead Sudip Dosanjh. "We believe this can be done by developing novel and innovative computer architectures."

Ultrafast supercomputers improve detection of real-world conditions by helping researchers more closely examine the interactions of larger numbers of particles over time periods divided into smaller segments.

An exascale computer would enable researchers to perform more accurate simulations in support of emerging science and engineering challenges in national defense, energy assurance, advanced materials, climate, and medicine, says James Peery, Sandia director of computation, computers and math.

The institute is funded in FY08 by congressional mandate at $7.4 million. It is supported by the National Nuclear Security Administration and DOE's Office of Science.

One aim of the institute is to reduce or eliminate the growing mismatch between data movement and processing speeds. Processing speed refers to the rapidity with which a processor can manipulate data to solve its part of a larger problem. Data movement refers to the act of getting data from a computer's memory to its processing chip and back again. The larger the machine, the farther away from a processor the data may be stored and the slower the movement of data.

"In order to continue to make progress in running scientific applications at these [very large] scales," says Jeff Nichols, who heads the Oak Ridge branch of the institute, "we need to address our ability to maintain the balance between the hardware and the software."

Submitted by DOE's Sandia National Laboratories

Building Better Catalysts for 'Artificial Photosynthesis'

Etsuko Fujita

Photosynthesis, the process by which green plants use sunlight to convert carbon dioxide and water into oxygen and carbohydrates, is the basis for all life on Earth: The oxygen makes Earth's air breathable, and the carbohydrates feed the entire food web. Many scientists would like to mimic this process to produce inexpensive fuels and raw materials using renewable solar energy. But copying Nature's chemistry is no simple matter.

"Nature has found a way to do this over eons," says chemist Etsuko Fujita of DOE's Brookhaven Lab. "It's very complicated chemistry."

That hasn't stopped Fujita and her colleagues from trying.

In one example, Fujita explains, "We would like to produce hydrogen — for use in fuel cells or other processes — from plain water and sunlight."

Recent experiments with a novel ruthenium-quinone catalyst discovered by Japanese colleagues have met with some success in mimicking what appears to be the rate-limiting reaction in the process of water splitting. The reaction, called water oxidation, is a step in natural photosynthesis that produces oxygen as well as protons and electrons from water. The protons and electrons can then be combined in a second reaction to make molecular hydrogen.

"We are combining theoretical and experimental studies to determine how this ruthenium complex with bound quinone molecules efficiently catalyzes water oxidation," Fujita says.

Fujita has also conducted pioneering work in understanding and advancing the catalysis of carbon dioxide reduction, a crucial step in transforming carbon dioxide to useful organic compounds such as methanol. Her systematic application of catalyst synthesis and advanced methods for determining key reaction pathways has demonstrated exceptional accomplishment in the face of great scientific difficulty.

Fujita's accomplishments span well over a decade, from early 1990s work that has become a cornerstone of the scientific foundation for solar activation of carbon dioxide, to recent innovations in bio-inspired photochemical processes that demonstrate creative new pathways to carbon dioxide reduction.

Submitted by DOE's Brookhaven National Laboratory