SNL's Jim Miller

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Research Highlights . . .

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What makes quantum dots blink

In order to learn more about the origins of quantum dot blinking, researchers from DOE's Argonne National Laboratory, the University of Chicago and the California Institute of Technology have developed a method to characterize it on faster time scales than have previously been accessed. Quantum dots are being intensively investigated for applications such as light-emitting diodes, solid-state lighting, lasers, and solar cells. They are also already being applied as fluorescent labels for biological imaging, providing several advantages over the molecular dyes typically used, including a wider range of emitted colors and much greater stability.

[Eleanor Taylor, 630/252-5565, etaylor@anl.gov]

Dust defeats germ-killing fabrics

While researchers have found many ways to make fabrics that kill germs in the lab, the first field study of germ-killing fabric reveals that the real world is a tougher place. Research performed at DOE's Jefferson Lab shows that contaminants, such as dust and spilled coffee, can coat the surface of a germ-killing fabric and allow germs to thrive. Scientists speculate that germs settle on the dust that collects on top of the fabric; the dust thereby protects germs from the fabrics' germ-killing surface. The researchers are performing additional real-world tests to determine if periodically cleaning the fabric will protect its ability to kill germs.

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First-ever model beckons SNS test

An international collaboration directed by a researcher from DOE's Oak Ridge National Laboratory has performed the first-ever atomic-detail computer simulation of how proteins vibrate in a crystal. Jeremy Smith, who leads ORNL's Center for Molecular Biophysics, said experimental testing of the theoretical work will require the capabilities of the Spallation Neutron Source The model predicts the existence and forms of the protein crystal lattice modes.

"In doing so it throws out a challenge to next-generation neutron science to finally make the breakthrough and determine the forms and frequencies of the vibrations experimentally," he said. In other words, having overcome their computational hurdle, the lattice dynamics team is now ready for the SNS to test the simulation work and see if what is predicted is really there.

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Extending the Zinc(20) Family

Not long ago Ames Laboratory physicists discovered an exciting family of zinc(20) compounds that can be manipulated to take on the properties and behavior of other materials. The highly tunable zinc(20) series, RT2Zn20 (R=rare earth, T=transition metal, Zn=zinc), allows for many model compounds by substituting on either the rare-earth site or the transition metal site.

Now, expanding on that work, the research team has placed ytterbium, Yb, on the rare-earth site, making a half dozen YbT2Zn20 compounds. By putting ytterbium on the rare-earth site in the RT2Zn20 series, the group was able to make compounds that gradually lose their local moment magnetism at low temperatures.

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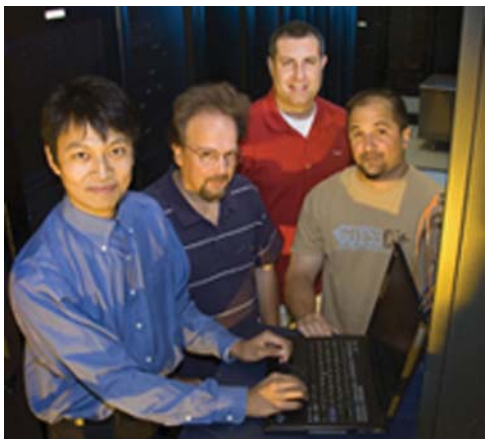
DOE Pulse highlights work being done at the Department of Energy's national laboratories. DOE's laboratories house world-class facilities where more than 30,000 scientists and engineers perform cutting-edge research spanning DOE's science, energy, national security and environmental quality missions. ***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).

TeraPaths to escort priority data through network traffic

You can think of the TeraPaths project as an HOV lane to keep physics data from getting stuck in a traffic jam.

With the quickly approaching start-up of the Large Hadron Collider (LHC) near Geneva, Switzerland, about 15 petabytes (15 million gigabytes) of data will be produced per year. The data from ATLAS, one of the LHC experiments, will be funneled in real time from the LHC directly to DOE's Brookhaven National Laboratory, which is the sole ATLAS Tier 1 computing facility in the United States. From Brookhaven, the ATLAS data will be further distributed to Tier 2 computing facilities at universities across the country. But with such an immense computing load traveling through the complex LHC network, congestion and competition for resources are expected.

That's where Brookhaven's TeraPaths project comes into play. The aim of this R&D project, whose collaborators include Stanford Linear Accelerator Center and numerous universities, is to supply efficient and reliable data movement in modern, high-speed networks. Because the LHC network is a shared medium, its default transport behavior treats all data flows with the same level of priority. But in reality, not all data flows should be treated equally, said TeraPaths Principal Investigator Dantong Yu.



The TeraPaths team includes Dantong Yu, Dimitrios Katramatos, John DeStefano, and Frank Burstein.

"Say I'm a physicist, and I want to present a paper at a conference, but I only have four weeks left for analysis," Yu said. "I have a few hundred terabytes of data that need to be analyzed, but all of the computing resources in my data hosting site are already booked up for several months. So I decide I want it shipped to a new site to do computing analysis within two weeks. That's possible with TeraPaths."

The TeraPaths project will allow the hundreds of US-ATLAS scientists to prioritize and protect specific data flows, and to schedule network bandwidth and usage. After a request is made, a path will then be "carved" to allow the data to travel unimpeded through the network.

"Like a fire truck or police car on the road, these data packages will have higher priority," Yu said.

Submitted by DOE's Brookhaven National Laboratory

Colleagues honor Sandia's Miller with Festschrift issue

The *Journal of Physical Chemistry* recently afforded a rare honor to Jim Miller of DOE's Sandia National Laboratories, publishing a Festschrift issue comprising a collection of articles submitted by combustion chemists to honor his long and productive career.

Jim Miller

He called it a highlight of his career, along with winning the Bernard Lewis Gold Medal from the Combustion Institute last year.

A Festschrift — German for celebration publication — is a book honoring a respected academic, usually in honor of an anniversary, retirement, or notable achievement.

"Jim is an intellectual leader and a guiding force for Sandia's energy science program and the Combustion Research Facility," says Terry Michalske, director of Sandia's Biological and Energy Sciences Center. "His Festschrift is a fitting recognition of his contributions to the international scientific community."

The introduction to the issue noted that "it is difficult to overestimate the impact that Jim Miller's work has had on the combustion community. But because of the rigor and detail of his chemistry contributions, his remarkable influence spreads beyond the sphere of combustion to the heart of fundamental gas-phase chemical reaction theory."

After earning a BS in engineering from the University of Cincinnati and a MEng and PhD from Cornell, Miller began working at Sandia in the spring of 1974 and helped open the Combustion Research Facility at Sandia's California lab in 1980.

Miller is working currently with former Sandian Stephen Klippenstein of Argonne National Laboratory to develop and implement a theoretical apparatus for studying chemical reactions involving multiple, interconnected potential wells. Such reactions are of paramount importance in the formation of aromatic compounds, polycyclic aromatic compounds (PAH), and soot in flames of aliphatic (non-cyclic) fuels.

Submitted by DOE's Sandia National Laboratories