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### Research Highlights . . .

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 cuttingedge 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@hg.doe.gov, 202-586-5806).



## A low-cost, environmentally friendly solvent

A technology developed at DOE's Argonne National Laboratory will allow millions of pounds of toxic industrial solvents to be replaced by an environmentally friendly alternative. The "green solvent" can sufficiently reduce the cost of ethyl lactate to make it competitive in the marketplace against toxic solvents. Argonne's process, which received an Award for Excellence from the Federal Laboratory Consortium for Technology Transfer, cuts production cost nearly in half. "Our major breakthrough," said project manager Jim Frank, "is a new, patented advanced membrane-assisted process that minimizes byproduct formation and improves reaction efficiency." NTEC Versol will build a commercial demonstration plant using the Argonne process.

[Catherine Foster, 630/252-5580, [cfoster@anl.gov]

#### Bees may detect landmines

Bees gathering nectar and pollen may someday help protect the lives and limbs of people, if a landmine-detection demonstration at DOF's Sandia National Laboratories is successful. Sandia chemists are working with University of Montana entomologists and Pacific Northwest National Laboratory researchers to see if foraging bees can find residues of TNT, the primary ingredient of most landmines. As bees forage, they attract dust, soil, and pollen to their fuzzy, statically charged bodies and bring samples back to the hive. Those particles provide a chemical survey of an area extending a mile or more from the hive in all directions. Landmines leak small amounts of explosives into nearby soil or water, so the bees should pick up those traces. [Howard Kercheval, 505/844-7842, hckerch@sandia.gov]

### Work begins on "cool" rotary prototype

Scientists at DOE's Ames Laboratory are working on a prototype rotary magneticrefrigeration unit that, if successful, would be the first magnetic refrigerator capable of sustained operation. The technology is based on the magnetocaloric effect—the ability of some materials to heat when magnetized and cool when removed from the magnetic field. These materials provide an environmentally friendly alternative to the chlorofluorocarbons and hydrochlorofluorocarbons used in traditional vapor-cycle cooling systems. During the three-year prototype project, Ames Lab will concentrate on optimizing the performance of the alloys, and developing a magnetic source that is more cost-effective and convenient than superconducting magnets. The lab's industrial partner, Astronautics Corp. of America, will design, build and test the rotary prototype.

[Susan Dieterle, 515/294-1405, dieterle@ameslab.gov]

#### Pulp "fix-ion"

An obstacle to recycling water, energy and desirable chemicals in the pulp and paper industry is the presence of potassium and chloride ions in the process stream. A technology originally developed at DOE's Pacific Northwest National Laboratory to remove cesium from radioactive waste is being adapted to separate the potassium and recover valuable sodium in pulp and paper mills. Electrically Switched Ion Exchange uses membranes coated with a suitable electroactive ion exchange material. The membranes absorb the ions and then, when the polarity of the electrodes is reversed, the ions are unloaded into an appropriate waste stream.

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# DOE labs unite to advance computational materials science

B ruce Harmon is in the middle of a mission to both ease and advance the design, processing and production of better materials with more desirable properties. But he's not alone in the endeavor. It's a team effort that relies on people power and the super power of today's massively parallel computing machines.

Recognizing the tremendous potential computational modeling has for advanced materials development, Harmon, deputy director of DOE's Ames Laboratory and director of its Condensed Matter Physics Program, helped create and now serves as one of the coordinators for the new Computational Materials Sciences Network funded through DOE's Basic Energy Sciences office.

The CMSN resulted from interactions between Harmon and Iran Thomas, director of the BES Division of Materials Sciences, as well as the other CMSN coordinators: Chuck Henager of Pacific Northwest National Laboratory, Malcolm Stocks of Oak Ridge National Laboratory and Ellen Stechel of Ford Motor Co.

On Feb. 3, the CMSN coordinators launched the network at a special organizational workshop in Germantown, Md. The workshop brought together scientists from DOE labs, academia, industry and other government labs to formulate challenging materials science projects that could best be pursued through broad cooperative efforts.

"The materials science community has always operated in very small groups—single investigators or small collaborative efforts," Harmon says. "But larger, more complex problems require interdisciplinary teams. CMSN provides a means for the DOE community to coalesce and, if not speak with one voice, to at least work together where there's mutual interest in solving significant problems."

The opportunity has been well received. CMSN coordinators have already held three workshop meetings, and seven broad project categories have been identified for possible proposals to obtain network support:

- Polymers at interfaces
- · Understanding ductile and brittle behavior in fractures
- Excited-state electronic structure and response functions
- · Microstructural evolution based on fundamental interfacial properties
- Bridging basic and applied science in magnetic materials
- Oxidation
- · Microstructural effects on the mechanics of materials

Three of the categories—polymers at interfaces, microstructural evolution based on fundamental interfacial properties, and microstructural effects on the mechanics of materials—are competing for CMSN fast tracking. "We only have the green light to fund one of them," Harmon says. "But we hope we'll be able to do more next year. There's not much of the year left now, so that would be pretty soon.

"CMSN focuses on relevant, interesting and important science," Harmon continues. "These are not projects that someone could go back to his or her lab and do alone. They will require a concerted effort by a large number of people with different talents and different tools. To the extent that CMSN carries the excitement of the changes that are happening in computational materials science, we see projects like the ones we've identified not only being addressed, but being addressed with some degree of confidence that something valid will come out of it."

#### LASER LADY

The first impression of Dr. Michelle Shinn, at DOE's Thomas Jefferson National Accelerator Facility (Jefferson Lab) is one of barely contained enthusiasm. Michelle is responsible for the optics at the world's highest average-power laser, the Free Electron Laser (FEL) located at Jefferson Lab.



She is pioneering the use of specially coated mirrors that allow this very bright laser's light to be focused and directed.

Dr. Michelle Shinn

Michelle is also responsible for the initial "drive" laser that starts the FEL.

When asked about her career in science, Michelle replies that her interest began early. As a child she was always asking "why?" and science was the "why." To Michelle, physics is the science that fundamentally explains how things work.

Her interest in lasers? The world of lasers is a special blend of science: "It's practical, beneficial technology that derives from basic physics. That's the best place for me."

Michelle regularly takes her particular brand of enthusiasm to students of all ages. She volunteers for demonstrations and tours that put her in contact with people interested in science and FEL in particular. "I want to make sure that people understand how important science is to everyone, and one way is to spread the word myself".

Submitted by DOE's Thomas Jefferson National Accelerator Facility