

## Nano hopes are high

### ORNL's proposed Center for Nanophase Materials Sciences would adjoin the Spallation Neutron Source

ORNL is on the fast track for a national Nanoscale Science Research Center. DOE's Basic Energy Sciences program recently informed Laboratory researchers that their proposal to establish the Center for Nanophase Materials Sciences at ORNL is being recommended for Fiscal Year 2003 construction funding.

The \$50 million national research facility will be located at the Spallation Neutron Source and adjacent to the Joint Institute for Neutron Sciences, effecting what promises to be a productive marriage between neutrons and nanoscale science.

The Solid State Division's Doug Lowndes, who headed up the ORNL proposal team, says that a strong focus on partnering with universities, the Lab's interdisciplinary depth, and strengths in materials synthesis and computational science all were key to the success of ORNL's bid for a

nanoscience center. The Lab's location is ideal for building partnerships with growing nanoscience research programs in southern and eastern universities.



**Doug Lowndes and postdoc Anatoli Meleshko contemplate a carbon nanotube model in Lowndes' lab. ORNL's plans for a nanoscience center focus on university collaborations.**

Curtis Boles

"The center will have a strong educational function. It will help apply ORNL's unique research capabilities by creating partnerships in nanoscience research that don't exist now. These partnerships are needed to accelerate the advance in our knowledge of nanoscale phenomena," Doug says.

"We surveyed a lot of universities and asked for input on their needs—basically asking how, through forming a center, we could create the synergies needed to accelerate the discovery process and accomplish much more than we could by

operating separately."

Doug says the CNMS will be a valuable career-development tool for graduate students and

postdoctoral researchers who are delving into nanoscience, which comprises a mosaic of disciplines.

"Nanoscience requires working across boundaries, so nanoscientists will require training in two or more disciplines," he says. "In traditional scientific training, researchers might specialize in physics or chemistry or biology. But to work in nanoscience, you need the knowledge that's been generated in several of these disciplines. This new center will be structured to provide experience working at those interfaces, in multidisciplinary research groups."

If Congress, which has looked favorably upon the National Nanotechnology Initiative, abides by the Department's wishes, construction of the CNMS would begin in 2003, with a finish in 2005.

One vision of future nanotechnology is of complex assemblies of molecules acting as submicroscopic "machines," ordering themselves in ways that they can actually perform useful tasks. First, however, must come the basic groundwork of science. Neutron diffraction, for example, will likely be an exquisite and indispensable tool toward understanding how "self-assembling" materials work, and how they might be used to create functional arrays of other nanoscale objects.

(See NANO, page 5)

## QWE survey gives leaders sense of staff views, some surprises

Results from the recent Quality of Work Environment Survey are in. The remarks represent the opinions of about 60 percent of Lab employees—2,274—who responded to the survey.

Summaries of the survey results were announced and made available to ORNL staff on July 24.

"The survey data confirmed several things we anticipated and identified some issues we did not anticipate," says Lab Director Bill Madia.

"I am encouraged that ORNL is viewed with a good image, that staff are proud to be here and that the Laboratory is felt to be a safe place where a diverse work force is respected," Bill says. "Most staff who responded have a clear idea of their job responsibilities and confidence in decisions made by their immediate managers. They generally view their immediate managers as receptive, responsive, accessible and communicative. The majority of respondents indicated that recent organizational changes at ORNL have been relatively smooth."

Survey responses also brought forward issues that need attention, including views that management is "somewhat disconnected from staff problems," a significant number of employees who do not always feel respected and trusted and fear expressing opinions, a benefit program considered inadequate when compared with other DOE labs and anxiety over job security.

"Numerous respondents in written comments attached to the survey expressed dissatisfaction with our progress in reducing the cost of doing business at the Lab," Bill says.

In the most favorable comments, staff overwhelmingly agreed that they knew their job responsibilities and that their work area was safe. Employees gave high marks to co-workers, immediate managers and, on the topic of modernization, UT-Battelle.

The least favorable remarks regarded poor performers (many agreed with a statement that they are treated too leniently), management communication, retaining staff and employment security.

Responses broken down by directorate and divisions are being distributed to the respective organizations. Ombudsman Steve Stow has been given the lead in follow-up action on the survey.

The survey vendor, International Survey Research, a Chicago firm, will conduct a set of workshops—the first with the Leadership Team and a second workshop to include selected ORNL staff who will help communicate survey results and action plans.

"Changing deep-seated perceptions and cultural legacies requires time," Bill says. "Still, I want our response to the survey to demonstrate that we are serious about enriching the quality of life for Laboratory staff."—B.C. om1

# Mercury rising

## Environmental Sciences Division team studies cause of higher gaseous mercury levels in Arctic air

When the sun finally ends the perpetual Arctic winter darkness, the mercury climbs to unrivaled levels. But not in thermometers, where the silvery liquid records temperatures well below zero degrees Fahrenheit.

ORNL researchers and scientists from the National Oceanic and Atmospheric Administration are recording unusually high levels of reactive gaseous mercury, or RGM, in the atmosphere just after “Arctic sunrise,” and the toxic pollutant is making its way into regional wildlife populations.

A major portion of U.S. mercury pollution rises from the stacks of coal-fired power plants, yet there are no such sources of emissions in this remote corner of the world. Nonetheless, some of the atmospheric concentrations of RGM have actually been found to be higher in some Arctic regions than those measured directly downwind of power plant smokestacks. So how does the mercury make its way so far north?

Corporate Fellow Steve Lindberg and his associates George Southworth and Mary Anna Bogle from the Environmental Sciences Division are helping to explain this phenomenon.

Mercury is a relatively stable vapor in its elemental form ( $Hg^0$ ), with an atmospheric residence time of a year or more. This stability allows it to traverse long distances, creating a virtual canopy of global mercury.

Steve believes that gaseous  $Hg^0$ , which is relatively inert in air, is being converted by the severe ultraviolet rays after Arctic sunrise to a form of oxidized mercury—RGM. RGM is highly water soluble compared with  $Hg^0$ , and it has a residence time on the order of days, not years. Thus, it is easily deposited in Arctic snow.

The implication is that the less reactive  $Hg^0$  travels from distant industrial sources to the Arctic region, where intense sunlight converts it to RGM.

“This whole ecosystem, right at the point in time when it is entering its spring cycle and becoming active, is being bathed with this high concentration of mercury in snow-melt runoff,” Steve says.

Mercury is a severe neurotoxin. When people consume mercury-contaminated food, it essentially poisons the nervous system. Steve says the term “mad as a hatter” best describes some of the symptoms.

One of the most dramatic illustrations of human suffering attributed to mercury contamination occurred in the 1950s and 1960s in Minamata, a small factory town on the coast of Japan. Years of negligent industrial operation resulted in considerable discharges of methylmercury (a toxic mercury species) to the Minamata Bay and a corrupted supply of fish. Several hundred residents lost their lives during this period and several thousand more have since been diagnosed with what is now referred to as “Minamata Disease.”

Incidentally, Minamata will host the sixth Global Mercury Conference this October. Steve will be the

conference chair.

The Environmental Protection Agency recently reported that as many as 30,000 children each year in the United States are at risk for developmental problems as a result of their mothers’ consumption of mercury-tainted fish. Dismal tidings of this nature underscore the need for better scientific understanding.

“One of the problems with this RGM,” Steve says, “is that we don’t really know what compound it is. A unique chemistry occurs in the Arctic region when the sun goes down in December and it is dark for a few months. Certain compounds build up in the dark and, as soon as the sun comes up, they form by-products.”

One of these by-products is bromine monoxide ( $BrO$ ), a natural compound formed from photo-oxidation reactions with bromide ions in aerosol spray from sea salt. These aerosols are present in the atmosphere surrounding any marine environment. Steve believes that  $BrO$  is the culprit that converts  $Hg^0$  to RGM.

Ozone, another pollutant, also plays a role in this conversion. Here’s how it works: Reactive bromine is formed from sea salt interactions with light. It then reacts with ozone to form  $BrO$ . Steve and his team believe this compound further reacts with  $Hg^0$  to form RGM. This autocatalytic cycle—a vicious circle of reactions that propagates itself—continues until the ozone is gone.

Major depletion events in the tropospheric ozone layer have been found to correspond with high levels of  $BrO$  off the coast of Point Barrow, Alaska. Experiments in other parts of the world have also yielded the same type of correlation, possibly even in lower latitudes where 24-hour sunlight is not a concern.

Steve believes these findings are a key step toward a firmer grasp of the RGM mechanism: “This could explain why there have been unusual measurements of elevated levels of RGM in areas where there are no known pollution sources, even outside the Arctic. This phenomenon may also explain the mystery of unusually elevated mercury levels in Arctic biota.”—Jason Gorss [ornl](#)

*Jason Gorss has completed a brief but prolific stint as an intern in the Office of Communications and Community Outreach. Watch for his byline in upcoming issues of ORNL Review.*



Steve Lindberg basks in the Arctic sun. Ultraviolet rays from the Arctic sunrise may trigger high levels of gaseous mercury.

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Curtis Boles

The Chemical and Analytical Sciences Division’s Regina Violet (right) is helping to tackle a big task: Raising more than half a million dollars in this year’s United Way campaign. See the back page for more on UW volunteers.

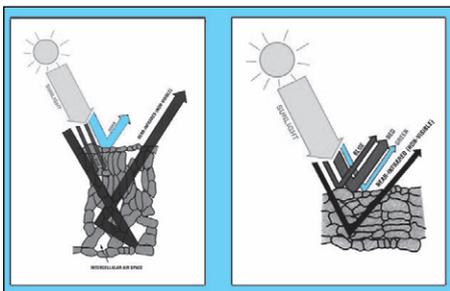
# Lab Notes

## Only mad dogs and ORNL researchers

A team of ORNL scientists has been venturing—Kipling-style—into the noonday sun for science and for the environment. David Reister of the Computer Science and Mathematics Division and Robert Washington-Allen of the Environmental Sciences Division recently went to a New Mexico area with a name that means “Journey of Death” to obtain spectrographic data on plants.

David explains that the bright sun is optimum for taking spectrographic readings on plants and looking for changes that might indicate how environmental stresses may be affecting them.

They’ve taken the instrument to



**Why leaves are green in the spring (left) and not in the fall (right)**

the area, near White Sands, N.M., that contains a Department of Agriculture research site that was subjected to an oil pipeline break. David and Robert want to look at plant life there and see how the spill may have affected it.

Sunlight has wavelengths ranging from ultraviolet to visible (blue, green and red) to infrared.

“The reason plants look green is that the chlorophyll in plants absorbs more blue and red energy (light) than green,” Robert says. “When leaves are stressed or change color in the fall, chlorophyll production decreases or stops. With less chlorophyll absorption in the red and blue, leaf colors change from green to red, brown or yellow.”

“We want to use this sensor to measure the reflectance of the plants and find correlations in the ones closest to the spill and farthest away,” says David. “What we expect in general is that there should be some shift in red edge—a move more into the red—when you see plants that are stressed.”

The CSMD-ESD team, which includes ESD’s Art Stewart, is supported by Chevron Oil and

DOE’s Office of Fossil Energy, National Petroleum Technology Office. The team is currently building a data set to compare with future readings. And good light—such as the New Mexico desert provides at noon—gives the team the most spectral data points.

Eventually, says David, oil companies would like to be able to monitor plant life near refineries, pipelines and installations and detect early signs of environmental stress in plants.

## Parking: First work carves new spaces

Changes in the Laboratory’s parking scheme loom ever closer. The temporary roping off of a portion of the east parking lot in July for core drilling was a taste of things to come for the hundreds of employees who use that lot. Another jolt: Early this month construction of a row of parking spaces along Sixth Street, facing the east side of Building 4500-North, will necessitate the closing of Sixth Street and the covered pedestrian entrance at Building 5506.

Staff members who use that rotogate will have to use other portals nearby until the 5506 entry reopens—but then just for a few months. Construction of new buildings in the east parking lot will ultimately close forever the 5506 rotogate and much of the east lot. That will happen later this year.

Still on its October 1 schedule is the activation of the new proximity reader system, the key event in the Revised Access Control program. Proximity cards have been issued to many staff members already. Come October 1, most portals and rotogates will be free access (you must still wear a badge), while entering a building will require activation of a proximity reader with a card.

The Revised Access Control program will figure into the parking scenario. Initially, lots inside the fence will be accessible to private vehicles with permits. Some lots inside the fence are being expanded, either sooner—such as the flagpole parking lot in front of Building 4500-North—or later as funds become available. That and other expanded parking lots, such as the “hill” lot above the current 6026 trailers, will help compensate for the loss of the east lot spaces (see the July *ORNL Reporter*).

## Kurchatov Institute seeks partnership

A delegation from Russia’s Kurchatov Institute visited the Lab in early July. The institute had proposed that ORNL and Kurchatov look into forming a joint institute for energy and environmental studies that would focus on collaborative research opportunities.

Bill Madia and Kurchatov Vice President Nikolai Ponomarev-Stepnoi signed an agreement to look into establishing the institute, which would include technologies ranging from neutron science to environmental sciences. ORNL will follow up with a visit to Moscow.

“I was very impressed with Kurchatov’s research agenda,” says Gordon Michaels, who helped host the group. “They are clearly one of the top energy R&D laboratories in the world—they have great staff and technologies. They are well on their way to diversifying their research mission into environmental, biology and sensor technology and were very interested in ORNL’s history in this regard.”

In the meantime, the visit was marked by the copious consumption of barbeque and “many toasts,” says Communications and Community Outreach’s Nancy Gray. Some of the visitors, who wanted to purchase items ranging from a fishing rod to health-food supplements, were treated to a trip to the local Wal-Mart. That probably left them a little overawed, as are we all.

*Reported by Bill Cabage*



**Madia and Ponomarev-Stepnoi shake on it.**



**President Bush has nominated John Marburger to be his science advisor. Marburger is the laboratory director at Brookhaven. U.S. Presidents have often called on the national laboratories for science advice. This photo shows a 1960 meeting of President Dwight D. Eisenhower’s Presidential Science Advisory Committee. Among those who advised Ike is Alvin Weinberg, then the director of ORNL, who is shown in the extreme right edge of the photo. The Environmental Sciences Division’s T.J. Blasing came across the photo in the March 1999 issue of *Physics Today*.**

# Cluster in a kit

## ORNL-developed OSCAR software package takes the tedium out of building your own supercomputer

A parallel processor in every lab, school or office—researchers at ORNL have had a leading role in developing a software product that could one day make that a fact.

Joined by several computer equipment manufacturers and schools, Stephen Scott of the Computer Science and Mathematics Division's Distributed Computing group has led an effort at ORNL to develop a software kit that enables users to link personal computers together into parallel-processing "clusters" capable of performing high-performance computing tasks.

"I work in a group at ORNL that does research on parallel and distributed computing. The cluster is one of the environments where our software must operate. I found building and maintaining our research clusters very frustrating," Stephen recalls.

"The rebuild and reconfigure cycle every time something changed became very monotonous and ate into my research time. Think about applying the same security patch 128 or more times. The generally accepted solution at the time for this problem was developed at university installations. Their solution was to hire low-cost undergrads to perform the redundant software installs on each of the cluster machines—not an option at ORNL.

"About this time our cluster program began to gain exposure and I started to field many requests for assistance in building clusters. I felt terrible as I ended the laundry list of what had to be downloaded, installed and configured for each machine. There had to be a better solution."

At a meeting at Argonne National Laboratory last

year, Stephen had a dinner discussion with Tim Mattson of Intel Corporation, who had the same idea: Using good software engineering principles, why couldn't this task be automated?

The result is a software product called OSCAR—Open Source Cluster Application Resources—a package that is freely available to all interested users. OSCAR, an amalgamation of Linux operating

*Most don't have the millions required to "run down to the bakery" and buy a supercomputer.*



system software and a suite of infrastructure programs including ORNL's Parallel Virtual Machine and Cluster Command & Control, or C3, greatly simplifies the task of setting up a cluster of computers.

OSCAR eliminates time and effort spent in downloading, installing and configuring the complex individual components of a cluster. In addition to

providing the cluster operating system installation, OSCAR provides the necessary components for cluster security, a programming environment, workload management and general administrative and maintenance of the system.

Stephen compares building a computer cluster to obtaining a cake: "You can bake it from scratch, buy a mix or visit a bakery." ORNL's Forrest Hoffman, Bill Hargrove and others took the first option several years ago when they built their Stone Souper-computer from castoff PCs. They had to start from scratch: No "mix"—such as OSCAR—was available at the time and they didn't have the millions required to "run down to the bakery" and buy a supercomputer.

Homemade systems such as Stone Soupercomputer, which was recently featured in *Scientific American*, are sometimes referred to as Beowulf machines after one of the first models, developed at NASA. Without a software package like OSCAR, Stephen explains, the builder has to deal with every computer as an individual machine.

The two key components that make OSCAR possible are ORNL's C3 suite and IBM's LUI (Linux Utility for cluster Install). LUI does the base operating system installation on the cluster machines, and C3 is used to initiate execution of the installation scripts on each of the machines—in parallel.

Working with Stephen on the C3 tools is Brian Luethke, an East Tennessee State University student. C3 is designed to provide what is termed a "single-system illusion" of the cluster. This is to be

## Advice to budding computer scientists shifts with dot-com market

Stephen Scott says the decline of the dot-coms has eased the tight supply of computer scientists in the job market somewhat, but it's still hard for a national lab to compete against the high salaries in industry. The Computer Science and Mathematics Division recently had a staffing representative assigned full-time to the division, which has a number of staff openings.

Stephen says, "At least we no longer have to compete against the dot-com "lottery ticket" (stock options). I tell prospective employees that ORNL stock options are better than those of most dot-coms—they are tax-free. Of course the joke is that ORNL stock options don't exist and many in industry owe taxes higher than their dot-com's stock value."

Stephen has his own tips for emerging computer scientists.

"During the dot-com days I advised computer science students to finish their undergraduate degree, then give the dot-com market a try for up to five years, as they have nothing to lose. If they aren't a millionaire by then, go back to graduate school for at least the master's," he says. Today, along with the dot-com market, his advice has changed. "I now tell students to get a year or two of good experience and then go back to graduate school for the master's and possibly the doctorate. I then emphasize that ORNL is a great location to get that experience."

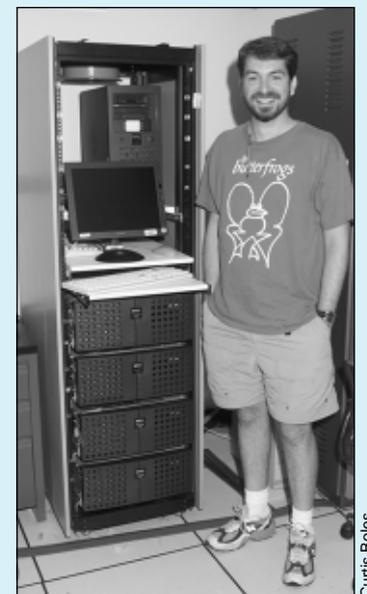
Stephen's work with clusters has involved several students who have made significant contributions to cluster tools, assembling OSCAR and building ORNL clusters. He believes that work will pay off for them.

"One of the things I do when I recruit students is have them work on projects that should allow them to publish," he says. "Two of the students I've worked with have gone on to graduate school at top-10 universities in computer science—and they both came out of small liberal arts colleges, which I've found to be a fertile field."

Stephen's own bachelor's degree is from Thiel College, a small liberal arts college in western Pennsylvania.

Staying abreast of a constantly changing computing scene keeps researchers like Stephen, who once had his own startup business, on their toes.

"I like to keep one foot in research and one foot in industry, always looking at how we can do this better or bigger as well as more efficiently," he says. "The work I do keeps me perpetually in the first three years of a high-tech startup. It is a very aggressive discovery-invention-release product cycle."



**Middle Tennessee State University graduate student Thomas Naughton sizes up the Dell cluster in the OSCAR lab.**

Curtis Boles

compared to the “single-system image” that is provided by a single machine. C3, for example, enables a single command password change or file copy to affect the entire cluster. OSCAR leverages this capability by using C3 to configure the cluster environment; C3 then remains on the cluster for use by cluster users and administrators.

Working with Stephen on OSCAR is soon-to-be University of Wisconsin graduate student Michael Brim. “Michael is responsible for much of the hands-on integration work that has resulted in the current OSCAR release. Michael used the C3 tools to automate the installation of the individual software packages that enable a group of machines to become a cluster,” says Stephen.

Partners with the ORNL group include the National Center for Supercomputing Applications, IBM, Dell, Intel, SGI, Notre Dame University, and Ericsson. Dell has used OSCAR internally for installations; Dell has also provided a cluster to Stephen’s group to further the OSCAR effort. NCSA is using OSCAR as a building block for its “-in-a-box” series of software.

“This software is open source; it’s freely available,” says Stephen. He cites several reasons why OSCAR is essentially at no cost: One is that it’s made up of open-source software, such as ORNL’s Parallel Virtual Machine, an award-winning ORNL product from the mid-1990s that enables computers to be linked together. CSMD’s AI Geist led that product’s development. At the same time, the redistributable software can be incorporated into commercial releases, so the potential of commercializing versions of OSCAR is there, too.

Besides, Stephen says, “With the open-source movement and associated free software, no one wants to pay for software anymore.”

In fact, one reason cited for the Internet’s explosive growth has been its “free to all” availability. Stephen believes clusters could become nearly as common. Manufacturers would like to see that happen. Setting up a cluster that links 64 personal computers together means, of course, that one needs to buy 64 PCs with at least one CPU in each.

Although Stephen isn’t tracking OSCAR users, he estimates from his e-mail traffic that the number of OSCAR users is in the hundreds. Already in development is OSCAR II, an upgrade that Stephen says will be more modular and thus more versatile. One of the goals for OSCAR II is to be more inclusive so that “anyone can join without increasing the work load of the OSCAR group.” OSCAR II is expected to be released at the Super Computer 2001 conference in November.

Stephen is also aiming to develop a Windows-based version of OSCAR (the current one is Linux-based.) The reason, he says, is that although a Windows version would obviously be less-than-open-sourced, it would enable colleges and universities who have Windows-based environments to teach parallel and distributed computing. Stephen’s group is working with Phil Pfeiffer of

East Tennessee State University to make it happen.

At ORNL, OSCAR has been used to set up a cluster for the Spallation Neutron Source. There is also a 64-node setup located in Building 4500-North. The main OSCAR lab, however, is a room in Building 6012, cluttered with hardware.

In time, OSCAR could make clusters as common as desktop computers.

“OSCAR is a time-saver. I look at it as making life

## Nano

*Continued from page 1*

Doug explains that, for example, some polymers have a self-organizing capability because of built-in chemical compatibilities and incompatibilities, and these can be further organized by applying electric or magnetic fields during their synthesis or subsequent heat treatment.

Nanofabrication techniques have raised much interest in quarters such as the semiconductor industry, which is perennially looking for ways to pack circuits more closely together to make smaller and faster devices. But understanding—much less developing and perfecting—new materials synthesis, processing and assembly methods is where the multidisciplinary focus of the new center will be key.

“One of the neat things we can do with nano materials and SNS neutrons is conduct time-resolved studies,” Doug says. “We’ll be able to study what happens as materials such as polymers, proteins and other macromolecules evolve throughout synthesis processes, or in reactions. Pulsed, high-intensity neutrons are well-disposed for such studies.”

One of the ORNL proposal’s three “scientific thrusts” is the study of so-called “soft” materials such as DNA, proteins, gels, polymers and even aerosols. The Chemical and Analytical Sciences Division’s Michelle Buchanan leads the soft materials thrust. The other two scientific thrust areas are complex nanophase materials systems, led by UT/ORNL Distinguished Scientist Ward Plummer, and a nanomaterials theory institute, led by UT/ORNL Distinguished Scientist Peter Cummings.

“We want to apply three strengths of the Laboratory—neutron science; our synthesis capabilities; and our theory, modeling and simulation abilities—together with many techniques for characterization of advanced and novel materials,” Doug says. “ORNL has tremendous breadth with special strengths in these areas, and you need combinations of these to make our knowledge of the nanoscale grow more rapidly.”

easier—for biologists, physicists, materials scientists and others who can benefit from high-performance cluster computing. With OSCAR they won’t have to deal with what software is needed, how to install and configure and how to debug a cluster,” Stephen says. “My goal is to make building and operating a cluster so easy that it does not require a computer scientist.”—B.C. [ornl](#)

The CNMS will have associated with it a new Nanofabrication Research Laboratory. The laboratory may also fill a research facilities gap that currently exists for universities located in the southeastern United States. The Southeast currently lacks a center capable of providing state-of-the-art nanofabrication resources to university users, even though a number of universities, including nearby Tennessee, Vanderbilt, Georgia Tech, Emory, Kentucky, Virginia Tech, and North Carolina, are

beginning to actively focus on nanoscale science and technology or have strong and closely related biomedical and health science programs. Currently, Cornell University in upstate New York is a university researcher’s closest state-of-the-art resource for fabrication of nanoscale devices.

“Of the seven universities in the Southeast with federal research expenditures of more than \$100 million per year, only one is more than a six-hour drive away from ORNL. In fact, three of them are less than three hours’ driving distance.

Having a nanofabrication research facility in the region will prove very attractive to researchers at these universities,” Doug says.

ORNL not only scored well with its proposal for the Nanoscale Science Research Center but also had two successful entries in another tier of DOE’s participation in the National Nanotechnology Initiative. Two Nanoscale Science, Engineering and Technology, or NSET, proposals, recently were winners in that competition: one team led by Solid State’s Lowndes and Plummer, the other team led by CASD’s Steve Overbury.

A planning workshop for the CNMS will take place this fall—probably the first of several—to flesh out research focus areas within the center’s three main scientific thrusts of soft materials; complex nanophase materials systems; and nanomaterials theory, modeling and simulation.

Doug confidently points out that the center’s completion ideally should precede that of the SNS. “We need to be ready with samples to study when the upgraded High Flux Isotope Reactor is fully operational in just two years, and well before the SNS is up and running in 2006,” he says.—B.C. [ornl](#)

*Having a nanofabrication research facility within driving distance will prove very attractive to researchers in the region’s large universities.*

# Protein modeling tool, heat pump water heater win R&D 100s

Two ORNL developments were among *R&D Magazine's* picks for this year's R&D 100 awards, a widely recognized annual showcase of technical achievement.

The "Protein Structure Prediction and Evaluation Computer Toolkit (PROSPECT)," developed and submitted by Life Sciences' **Ying Xu** and **Dong Xu**, and the "Drop-In Residential Heat Pump Water Heater," developed by Energy Division's **Van Baxter, Richard Murphy, John Tomlinson** and **Randall Linkous**, in conjunction with ECR International of Dunkirk, N.Y., and Arthur D. Little of Cambridge, Mass., were named to the 100.

PROSPECT is a suite of computational tools designed to predict three-dimensional structures of proteins from their amino acid sequences in a matter of hours, rather than the months or years current experimental approaches require.

## ORNL people

proteins from their amino acid sequences in a matter of hours, rather than the

The Residential Heat Pump Water Heater is a 50-gallon water heater that uses one-third as much electricity as a conventional electric water heater. The energy reduction is accomplished through the use of a small heat pump that extracts heat from the surrounding air, leaving it cool and dehumidified.

These two awards bring the total won by the Lab to 109, increasing its lead over other national labs and making the Lab second only to General Electric in the total number of R&D 100 Awards won since the competition began in 1963.

UT/ORNL Distinguished Scientist and condensed-matter physicist **Ward Plummer** is the 2001 winner of the Medard W. Welch Award, the American Vacuum Society's most prestigious award. The award recognizes Ward for his "development of novel instrumentation, its use to illuminate new concepts in the surface physics of metals and the mentoring of promising young scientists."

Ward will receive the award, which includes a \$10,000 cash prize, a gold medal and an honorary lectureship, at the AVS 48th International Symposium this fall in San Francisco.

Corporate Fellow **Steve Pennycook** of the Solid State Division has been named a fellow of the United Kingdom's Institute of Physics. He received the institute's Thomas Young Medal in January for his work in Z-contrast scanning tunneling electron microscopy.

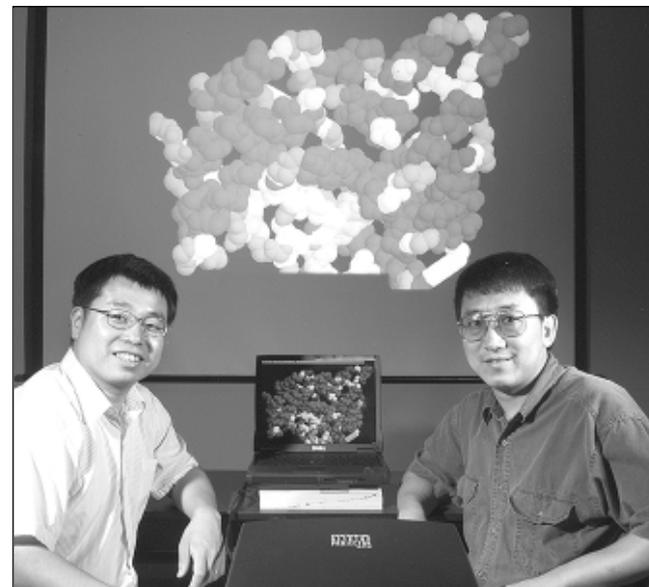
**Lynne Parker** of the Computer Science and Mathematics Division has been selected to participate in the National Academy of Engineering's seventh annual Frontiers of Engineering symposium. Lynne, a 2000 Presidential Early Career Award for Science and Engineering winner, will be among 81 of the nation's top young engineers to participate in the three-day symposium next month.



**Peggy Emmett** of the Computational Physics and Engineering Division and **Tom Kress**, an Engineering Technology Division retiree, were recently named fellows of the American Nuclear Society at the society's annual meeting. Peggy was recognized as being one of the original developers of the MORSE Monte Carlo Transport Code System and as the continuing software specialist for the MORSE family of codes. Tom was cited for his technical contributions to the field of reactor safety.

The Chemical Technology Division's **Michael Hu** has been invited to serve as an associate editor for the *Journal of Nanoscience and Nanotechnology*, published by American Scientific Publishers.

Chem Tech's **Tanya Kuritz** has been invited to serve on the International Microbiology Education Committee, a standing committee of the American Society for Microbiology International. She will be responsible "for developing and strengthening ties



(Left photo, from left) **Randy Linkous, Van Baxter, Richard Murphy** and **John Tomlinson** received an R&D 100 Award for the Drop-In Residential Heat Pump Water Heater. (Right photo) **Dong Xu** (left) and **Ying Xu** won for the Protein Structure Prediction and Evaluation Computer Toolkit.

with and facilitating the integration of scientists from the former Soviet Union and Middle East into ASM." Tanya was also selected by the International Science and Technology Center to be a technical auditor for the audit team that assessed progress on DOE and other U.S.-agency-funded projects in the Republic of Georgia. Georgia is still a repository for nuclear material.

**Yanlai Cho**, the technical director of the Spallation Neutron Source project, was recently elected a fellow of the American Physical Society, "for continuing excellent contributions to high-energy physics experiments and technology and to the design and commissioning of large accelerator facilities." Cho is also deputy associate laboratory director for Argonne National Laboratory's Advanced Photon Source.

## Tax legislation revises withholding tables

As a result of the recently enacted Economic Growth and Tax Relief Reconciliation Act of 2001, the Internal Revenue Service has revised the federal income tax withholding tables, effective for wages paid on and after July 1, 2001.

Only the four highest withholding brackets have been changed, dropping by 1 percent. The 28, 31, 36 and 39.6 percent rates decrease to 27, 30, 35 and 38.6 percent respectively. The 15 percent withholding bracket remains the same; therefore, some employees will not be affected by the changes to these tables. (Note that the 15 percent bracket will fall to 10 percent effective January 1, 2002. For 2001, the tax benefit of the 10 percent rate is being converted to a credit that IRS will rebate to taxpayers this summer.) A link has been provided from the Payroll Services home page, [home.ornl.gov/divisions/accounting/employeeacct/payroll/](http://home.ornl.gov/divisions/accounting/employeeacct/payroll/), for viewing the revised withholding tables.

If you are affected by these revisions and do *not* want to have your withholding reduced, you may want to file a new Form W-4 (also available as a link off the Payroll Services home page). You may claim fewer withholding allowances on line 5 or request additional amounts to be withheld on line 6.

The flat rate used for supplemental wages (lump sum payments) decreases from 28 percent to 27.5 percent, effective for wages paid on and after August 7, 2001.

## HBCU/MEI summer faculty program provides valuable time and resources for research

Divina Miranda and Ken Roberts teach at schools with a combined total enrollment smaller than the incoming freshman class of some major universities. Divina is associate professor of Chemistry at Southern University (La.) and Ken is assistant professor of chemical engineering at North Carolina A&T University.

Ken, Divina and several other visiting faculty from small, minority colleges are getting an opportunity to sink their teeth into some serious research at ORNL this summer.

The HBCU/MEI Summer Faculty Research Program, which is geared toward professors at historically black colleges and universities (HBCUs) and other minority educational institutions (MEIs), is a joint effort between ORNL and Oak Ridge Associated Universities to bring faculty from these schools to the Lab for a 10-week research appointment.

Both Miranda's and Ken's schools are classified as MEIs, and they carry with them a unique set of

*Programs like ORNL's allow the faculty from smaller schools to focus on research projects without the usual distractions.*

challenges. One of the chief obstacles facing the faculty at MEIs is the comparatively scant federal R&D funding these schools typically receive.

"At many of the smaller schools and minority schools, the faculty usually teach three or more classes

a semester," says Ken, "and they're still expected to do research. At the bigger schools they may teach one class a year. Programs like this allow the faculty from these smaller schools to focus on research projects for a while without the usual distractions."

Divina has been participating in similar programs for the past few years: "I usually look for opportunities to do research during the summer because my school is primarily a teaching university, and it's really tough to incorporate doing research when you're teaching 12 hours a semester."

"Smaller schools such as HBCUs don't receive as much money as the big research schools," Ken says. "We're not anywhere near them, in terms of numbers. But it's kind of a double-edged sword. If you apply for large-agency research support, they'll look at the school you're from and say, 'Well, we have specific programs for those schools, so you don't need to apply for this.' That can really hurt because it's hard to get the sustained funding you need."

Ken has also participated in other programs oriented toward MEIs. "These are really great opportunities for people who are willing to hustle

and do this type of research, even with all the other things we're expected to do," he says.

There are five other participants in the ORNL/ORAU-funded program at the Lab this summer, as well as 10 visiting scientists from MEIs in programs sponsored by individual divisions and schools.

The benefits of these programs extend beyond those afforded the participants, who are providing valuable research to further ORNL's mission. Both Ken and Divina are working in the Chemical Technology Division under the guidance of Michael Hu, and they are both doing research in the field of nanoparticles. Divina is synthesizing nanomagnetic materials and Ken is developing nanostructure catalytic materials—mainly for use in environmental applications such as fossil fuel desulfurization and carbon dioxide-based reactions.

"The big difference at ORNL is that this is a world-class research environment," says Ken. "ORNL has everything you could want as a researcher."—Jason Gorss [ornl](#)

## Service Anniversaries

August

**43 years:** John T. Mihalcz, Instrumentation & Controls; Patricia R. Hunsicker, Life Sciences

**35 years:** Kenneth R. Thoms, Engineering Technology

**30 years:** Brenda T. Hackworth, Communications & Community Outreach Directorate; Donald E. Todd, Jr., Environmental Sciences

**25 years:** Charles R. Ballard, Stephen W. Gardner, W. D. Hawkins and Karl Thatcher, Plant and Equipment; Nancy Y. Wright, Computing, Information, and Networking; John E. Cleaves, SNS Accelerator Systems; Margaret B. Nestor, Office of the Laboratory Director; Jack P. Adams, Environmental Protection & Waste Services; Richard M. Davis, National Security Directorate; Thomas W. Mitchell and Johnny H. Fairs, Technical Support Mgmt Systems Section, Instrumentation and Controls; Richard W. Leggett and Janet H. Swenson, Life Sciences; Walter L. Gardner, Fusion Energy; Vicky H. Wallace, Facilities & Operations Directorate; William G. Craddick, Energy

**20 years:** Karen C. Bills, Robotics and Process Systems; Eddie M. Shirley II, Research Reactors; Michael A. Green, Chemical Technology; Nestor L. Cacheiro, Life Sciences

## UT-Battelle gives \$3,000 to Oak Ridge Boys Club

UT-Battelle recently presented a \$3,000 check to the Oak Ridge Boys Club. The funds will be used for safety improvements at the Oak Ridge facility.

Kelly Beierschmitt, who leads the Environment, Safety, Health and Quality Directorate, presented the check to Lawrence Hahn, executive director of the Oak Ridge Boys Club. Kelly is also a member of the Oak Ridge Boys Club board of directors.

## CIGNA cards mailed, co-pay raises in effect

Members of the CIGNA/PHP medical plan should be receiving new ID cards in their mail at home. "Look for the envelope marked *CIGNA HealthCare*," says Benefits Delivery's Sally Jaunsen. "You should receive a separate card for yourself and each enrolled dependent."

Sally requests that members review the cards, assuring that name, ID number and PCP (primary care doctor) are correct for each person covered under the insurance. If corrections are necessary, call CIGNA Member Services. That number, which is found on the lower-right-hand section of your card, is 1-800-832-3211.

Any old cards should be destroyed once your new cards have arrived, says Sally. Old and new cards can be distinguished by checking the COPAYS line—doctor visits are now \$20.

In fact, as announced last April, several CIGNA co-payments increased in July. Office visits are now \$20; inpatient hospital co-payments are \$250, outpatient care surgery co-payments are \$100 and emergency room visits are \$100.

Merck-Medco prescription plan co-payments have also increased: Retail generic is now 20 percent and brand name is 30 percent. Unchanged are mail-service pharmacy co-payments, and there is still no deductible for the prescription mail-service program.

As always, call OneCall, 574-1500, for information about your benefits, or visit the Benefits Web site at [www.y12.doe.gov/benefits/bp-delivery/](http://www.y12.doe.gov/benefits/bp-delivery/).

## Deaths

Bea Washington, a reports and data assistant in Travel Services' accounting section, died suddenly on July 7. Bea was a Knoxville resident and had worked at Oak Ridge for 11 years. Employees have contributed to a fund, organized by Bea's co-workers in Travel Services, to purchase a motorized wheelchair for her daughter. Angie, 26, suffered a stroke as a small child. Bea is also survived by her son, Randall, and three grandchildren.

# Why give to United Way? It's local, it's efficient, it's accountable, it's expert ...

## ...and it helps your community.

BY HARVEY GRAY, UNITED WAY CHAIRPERSON

I'm proud to serve as chairman of ORNL's 2001 United Way Campaign—proud and confident that we can reach our goal of \$565,000—because so many of you have chosen to care. You care about your communities and your neighbors, and particularly about those who are in need. Because you care, United Way's member agencies in East Tennessee are able to help so many people lead better lives.

During my involvement with United Way, I've visited a number of area agencies and seen just how and why United Way works. Here are a few of the reasons:

- It's local. Your donations stay here in our communities, helping thousands each year.
- It's efficient. More than 90 cents of every dollar you give goes to helping those in need.
- It's accountable. United Way makes your caring count. Trained community volunteers decide which programs receive your money. They hold the agencies accountable, monitoring their budgets and the quality of their services.
- It's expert. United Way is a proven, organized system of caring that studies the diverse needs of our communities and allocates resources where they will do the most good.

I also have served on the Anderson County United Way funds distribution committee for the past three years and have seen firsthand the careful allocation and distribution of your money so that it makes a real difference for our neighbors in need. For example, if you gave just \$5 per week for a year, your donation would fund more than 1,800 pounds of food through the Second Harvest Food Bank; 20 nights of safe, affordable housing for a woman at the YWCA; or 20 weeks of hot meals delivered to a homebound elderly person through Mobile Meals. As you can see, your donation really does have a positive impact on the lives of people in our community.

If you currently give to United Way, we on the campaign staff thank you for your generosity. If you have not participated, or if you are a donor who is thinking of increasing your level of giving, we encourage you to consider the difference you can make in the lives of our children, families, elderly persons and communities in need.

I'm convinced that United Way really is the best way to help the most people. Thanks so much for your support.



Photos by Curtis Boles



ORNL United Way volunteers recently toured area agencies to see how our dollars help those in need. Regina Parks (top, left) and Linda Stansberry enjoyed visiting clients at Anderson County's Keystone Elder Daycare Center. Danny

Cantrell, Kahra Gilley and Tracy Bodine (center photo) spent time with this young lady at the Henry Center in Roane County. ORNL volunteers (bottom) got a close-up look at the Salvation Army's new facility in Knoxville.



**ornl** reporter

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