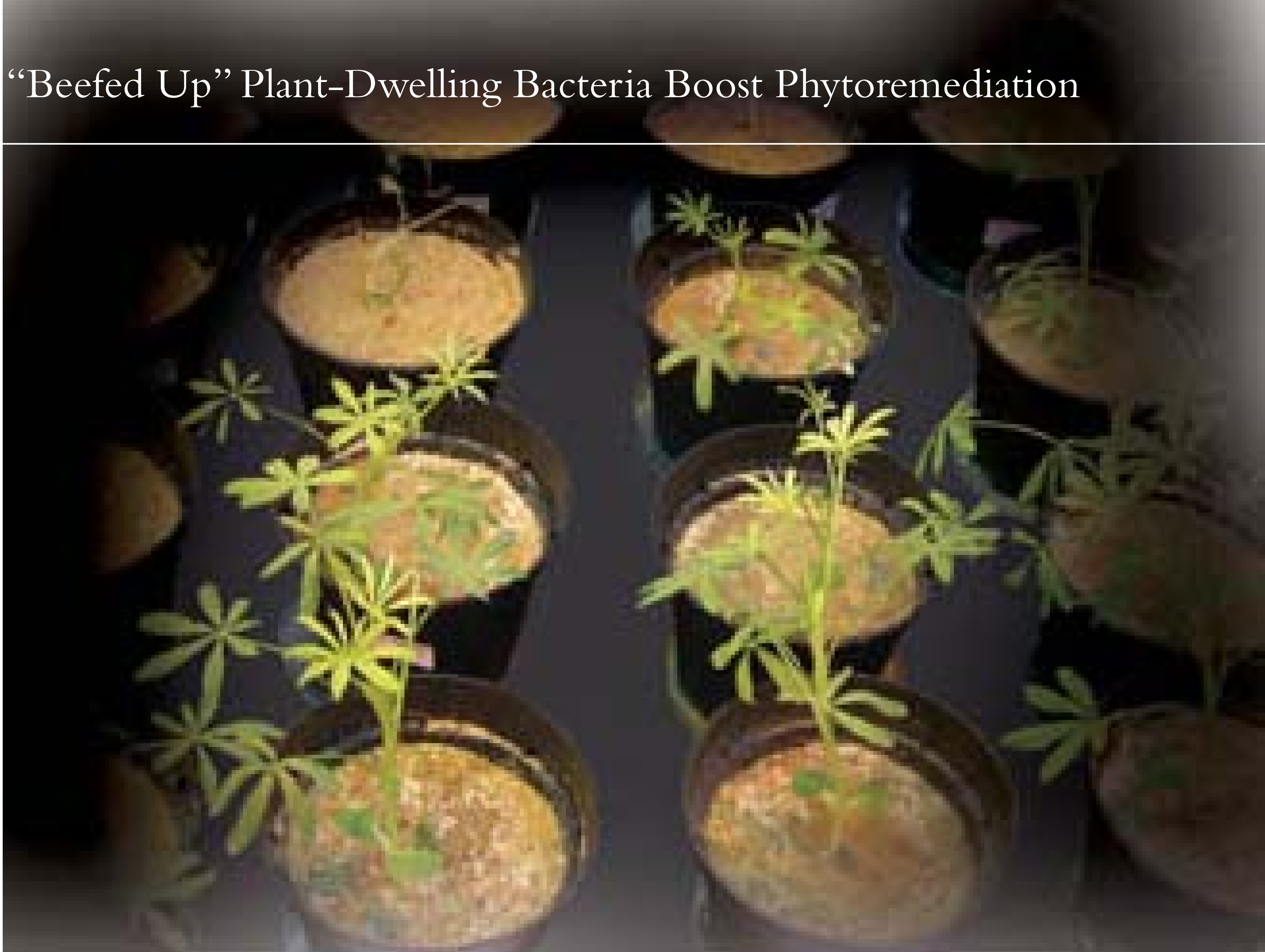
In This Issue

Spring 2005

"Beefed Up" Plant-Dwelling Bacteria Boost Phytoremediation



Brookhaven biologists and their collaborators in Belgium think they've found a way to improve plants' use in environmental cleanup: transfer genes from pollutant-degrading bacteria into bacteria residing in the plants so the resident bacteria can help the plants break down the pollutants. — Karen McNulty Walsh

Using plants to soak up and degrade environmental pollutants, a strategy known as phytoremediation, can be more successful in theory than in practice. The accumulated pollutants or their metabolites sometimes kill the plants or evaporate via the leaves back into the atmosphere. But scientists at Brookhaven Lab and their collaborators in Belgium think they've found a way to improve the process: transfer genes from pollutant-degrading bacteria into bacteria residing in the plants so the resident bacteria can help the plants break down the pollutants.

In a recent test study, plants inoculated with the "beefed-up" bacteria survived in toluene-contaminated soil and increased the degradation of the pollutant. The research, which was funded by the European Commission, the Ford Motor Company, and Brookhaven Lab, appeared in the May 2004 issue of the journal *Nature Biotechnology.*

"By introducing genes for the appropriate degradation pathways into natural plant-dwelling bacteria, known as endophytes, we should be able to tailor-make plants capable of cleaning up a variety of organic pollutants," said Brookhaven biologist Daniel (Niels) van der Lelie, one of the lead authors on the paper. He also envisions introducing pollutant-degrading pathways into bacteria that live in crop plants to reduce the residues of pesticides and herbicides that make their way into our food.

> "By introducing genes for the appropriate degradation pathways into natural plant-dwelling bacteria, we should be able to tailor-make plants capable of cleaning up a variety of organic pollutants." — Niels van der Lelie

Van der Lelie maintains that the technique should win widespread acceptance because it uses only naturally occurring bacteria and natural gene-transfer methods.

Niels van der Lelie, top right.

Left: Plants innoculated with endophytic bacteria that had acquired a toluene-degradation pathway from natural soil-dwelling bacteria were tolerant of toluene and best at removing the pollutant from soil.

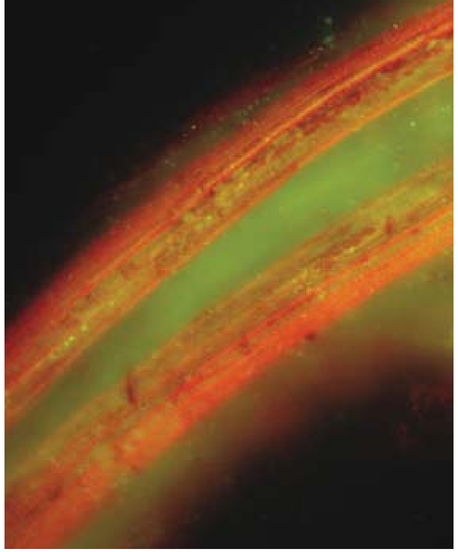
The scientists started with a type of bacteria that naturally colonizes the roots and stems of their test plant, yellow lupine. They mixed these bacteria with a related soil-dwelling strain known to degrade toluene. This allowed the strains to share genetic material through a natural process known as bacterial conjugation.

They then selected the endophytic bacteria that had acquired the capability to grow on toluene, and used this strain to inoculate yellow lupine plants. After allowing the inoculated plants to grow for 21 days, the scientists analyzed the bacterial content of their roots and shoots using selective growth media containing toluene to confirm plant colonization by the so called "endegrader" bacteria.

The scientists then compared the ability of these plants to grow in an environment containing toluene (both hydroponically and in non-sterile soil in greenhouse studies) with that of non-inoculated plants and plants inoculated with the soil bacteria. They also measured the amount of toluene released from the plants' leaves via evapotranspiration.

Plants inoculated with endophytic bacteria that had acquired the toluene-degradation pathway were able to grow in the toluene-contaminated environment under both hydroponic and greenhouse conditions, even when the levels of toluene present killed the other test plants. Furthermore, plants inoculated with the toluene-degrading endophytic bacteria released three to four times *less* toluene into the atmosphere.

"These results confirm our hypothesis that endophytic bacteria, when equipped with the appropriate degradation pathway, can help plants survive under conditions with elevated levels of pollutants, and improve the performance of plants



The root of a poplar tree, (magnified 1000X) colonized by endophytic bacteria containing a green fluorescent protein to mark their presence. Equipped with metabolic pathways that enable them to degrade environmental pollutants, these microbes can increase the plants' effectiveness in phytoremediation.

used to remove these contaminants from the environment," van der Lelie said.

The next step will be to test the technique in poplar and willow trees, deep-rooting species already used in phytoremediation. "In trees, the time between the uptake of the pollutant by the roots and its arrival in the leaves can take several hours to days, allowing sufficient time for efficient degradation by endophytic bacteria in the plant tissue," van der Lelie said.

Already, the researchers have identified 150 bacterial species that live as endophytes in poplar, and they are starting experiments to see which species will be most amenable to gene transfer. Then, they will select bacteria able to grow in the contaminated areas that need to be cleaned up, and mix those bacteria with the endophytes to encourage gene sharing. New strains that result will then be inoculated into poplar and tested for their ability to clean up pollutants in field studies.

more information —

- Niels van der Lelie, vdlelied@bnl.gov or (631) 344-5349; Safiyh Taghavi, taghavis@bnl.gov or (631) 344-5306
- http://www.biology.bnl.gov/cellbio/vanderlelie.html

Meet Daniel (Niels) van der Lelie and Safiyh Taghavi

Niels van der Lelie, a pioneer in the field of microbial ecology, first came to Brookhaven Lab in 2001 at the urging of his partner in research and in life, Safiyh Taghavi. The scientists, who met at the Belgium Nuclear Research Centre (SCK-CEN) as collaborators on a project using microorganisms to detoxify land contaminated by years of zinc smelting, were invited to Brookhaven because of their advances in using microbes to seek out and demobilize chemical pollutants.

"My wife really pushed me," van der Lelie said. "She saw that the research opportunities in the United States were much better than in Belgium." So the two came to check it out, and decided to stay.

"Over the years we have become a very efficient team, where we both emphasize our strong technical and management skills," said Taghavi, a native of Iran who went to Belgium in 1971 for her university studies and stayed afterward.

Their research at Brookhaven focuses on the development of new genomic tools to study the functioning of microorganisms, both on the level of the individual organism and on the level of complex microbial communities. This work is of direct importance to several societal issues, such as the cleanup of pollution, the production of bioenergy as an alternative for fossil fuels, and the identification of pathogenic bacteria.

Van der Lelie earned his Ph.D. in mathematics and sciences with a specialization in biology from the University of Groningen, The Netherlands, in 1989. He conducted postdoctoral research in molecular biology at Transgène in Strasbourg, France, and then joined SCK-CEN and subsequently the Flemish Institute for Technological Research (VITO), created out of SCK-CEN for all non-nuclear research activities. There he conducted basic, long-term research on the fundamental genetics of soil bacteria, particularly those resistant to heavy metals and other pollutants, as well as applied research on environmental management and remediation using plants and microbes.

Safiyh Taghavi joined SCK-CEN in 1984 as an industrial engineer, working first as a chemist in the metallurgy department and later in collaboration with microbiologists and geneticists on the development of bacteria-based whole cell biosensors. As part of her ongoing education during her employment, she earned her Ph.D. in molecular biology and biotechnology from the University of Brussels in 1996, for functional and genetic studies of heavy-metal resistance in microbes. She collaborated with van der Lelie on the research mentioned above.

Van der Lelie and Taghavi were married in 1992 and have two daughters, Roxane and Danielle. Both scientists maintain joint appointments at Brookhaven and VITO, and have benefited from a partnership between Brookhaven and Belgian scientists that dates back to World War II. SCK-CEN was the first nuclear research center outside the United States to focus on civil applications for nuclear technology. Belgium got access to this technology as gratitude for supplying the uranium used for the Manhattan project.

"SCK-CEN looks like a mini Brookhaven, so when we came to Brookhaven we immediately felt at home," Safiyh said.

Though they miss Belgian beer, cheese, and haute cuisine, they are enjoying their time on Long Island and have discovered that certain North Fork wines are, in their best years, as good as those from Europe. In their spare time, they like to cook, entertain their friends and colleagues, and spend quality family time on the beach of Shoreham Village, where they are presently living.

"Over the years we have become a very efficient team, where we both emphasize our strong technical and management skills."

— Safiyh Taghavi

Radioisotopes and Nuclear Imaging Help Track Effects of Soil Contaminants

Niels van der Lelie's team in Brookhaven Lab's Biology Department is collaborating with scientists in the Chemistry Department to gain a better understanding of how the introduction of contaminant-eating bacteria might alter normal plant function. Their approach uses some of the techniques developed for medical imaging in human and small animal studies to track the allocation of nutrients and other biochemical compounds within the plants.

"Since the endophytic bacteria rely on the host plant for most, if not all, of their nutrients, we believe that some of the plant's resources — including carbohydrates and amino acids — will be reallocated to sustain the energy-consuming biodegradation chemistry carried on by the bacteria," says chemist Richard Ferrieri.

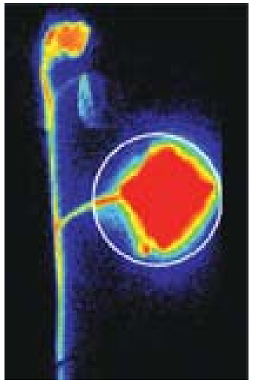
To monitor these changes, Ferrieri and colleague Michael Thorpe have developed novel techniques to study plant physiology using radiotracers — substances made with short-lived radioactive versions of ordinary chemical elements, such as those used to image brain chemistry. For example, under tightly controlled, closed environmental conditions, the scientists can administer discrete pulses of carbon dioxide gas tagged with radioactive carbon-11 or ammonia gas tagged with radioactive nitrogen-13 directly to leaves on intact plants. They then track the movement and biochemical interactions of the radioactive sugar and amino acids derived from these nutrients using non-invasive imaging techniques such as positron autoradiography and positron emission tomography (PET).

These tools will allow the scientists a unique opportunity to unravel the complex biochemical pathways involved in normal plant functions, including maintaining carbon and nitrogen balances for growth, and to see whether this balance changes over time from exposure to contaminants or the presence of endophytic bacteria.

Because the radiotracers used have very short half-lives (they decay in a matter of minutes), the radioactivity is quickly cleared from the plant. This allows repeated monitoring of the same plant over time. No other techniques afford this opportunity.

Additionally, the team plans to radiolabel key environmental contaminants such as carbon tetrachloride and trichloroethylene, again using carbon-11, to provide a unique look at the dynamics for uptake and transport of contaminants throughout the plant, and to gain greater insight into the mechanisms of biodegradation.

These developments will draw on Brookhaven's strength as a world-class laboratory in the synthesis of radiotracers. The current work is supported by a seed grant from Brookhaven's Laboratory Directed Research and Development Program.



By administering carbon dioxide labeled with the radioisotope carbon-11 to a single plant leaf (circled), scientists can track the distribution of radioactive sugar derived from that carbon over time, and study how the distribution varies with exposure to challenges such as contaminants. Red shows the highest level of the carbon-11 radiotracer; blue the lowest.

Scientists Create and Manipulate Nanoscale "Water Wires"

Scientists at Brookhaven Lab's National Synchrotron Light Source are studying how protons move in water at the nanoscale with an eye to implications in other areas of science. Hydrogen fuel cell technology may be one of the beneficiaries.

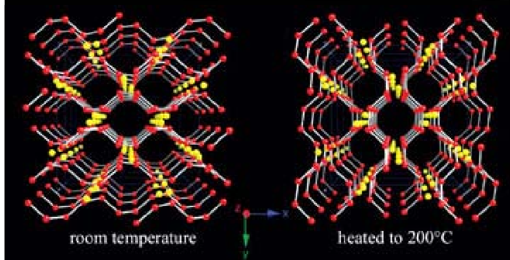
— By Laura Mgrdichian

Tiny strands of water or "water wires" may give scientists a new view of the properties of water. Brookhaven scientists have created the strands measuring less than one nanometer (a billionth of a meter) in width to look at very small quantities of water, such as that found inside cells, which behave differently than water at the macro-scale.

"Water in cells is distinct from bulk water as we know it," explained physicist and principal investigator Tom Vogt. "For instance, it can take the form of long chains of single water molecules, which we call 'water wires' or 'water polymers.' But scientists know very little about water in this form."

They do know, however, that water wires are responsible for proton transport across cell membranes, which is one step in the fundamental process by which most organisms produce energy. Scientists understand how proton conduction occurs in bulk water, but not yet in water at the nanoscale. Studying water wires may shed light on the mechanism.

"In order to understand the biological role of water wires, we must relate their structure to the properties they display, such as their stability and how they transport protons," Vogt said. "Confining very small amounts of water inside minerals and glasses is a good way to model and thus learn about water polymers."



The orientation of the water wires (water molecules are shown as red balls) at room temperature and 200 degrees Celsius. When the wires are heated, they change direction. The yellow balls represent sodium ions.

Vogt and his fellow researchers placed a sample of the mineral natrolite inside a diamond anvil cell, a device that applies very high pressure to a sample using the polished faces of two diamonds. In this case, the pressure was applied after the researchers first surrounded the natrolite sample with a water/alcohol solution. As the high pressure altered the natrolite structure, it also forced water molecules into its empty spaces — a process called pressure-induced hydration. Like tennis balls inserted into a canister, the water molecules nestled one-by-one within the structural framework, forming water wires.

As pressure was continually applied, it nudged the oxygen atoms in adjacent water molecules closer together than oxygen atoms in bulk water. This suggests that the wires may be good proton conductors, since protons travel in water by "hopping" from one molecule to the next, choosing the path of least water-to-water distance.

Next, Vogt and his group heated the sample to 200 degrees Celsius. Under pressure and heat, the natrolite structure expanded non-uniformly — more in one direction than the other. As a result, some water molecules moved closer together while others moved farther apart. This shifted the direction of the shortest water-to-water distance, creating a new preferred hopping route for protons. Because the direction of proton hopping is what defines the water wires, this shift also changed the wires' orientation.

Understanding proton transport at the nanoscale in water wires could be useful in the development of applications such as hydrogen fuel cell technology, which also involves proton transport. It may also help scientists better understand biological processes that depend on proton transport, such as the production of adenosine triphosphate, the compound that provides the energy for many cellular functions. The scientists followed the natrolite's structural changes at National Synchrotron Light Source (NSLS) beamline X7A.

This research was funded by a grant from Brookhaven's Laboratory Directed Research and Development (LDRD) program. Brookhaven's Yongjae Lee, C. Dave Martin and John B. Parise from Stony Brook University and Joe Hriljac of the University of Birmingham, United Kingdom, also participated in the research.

Meet Thomas Vogt

Physicist Thomas Vogt enjoys playing golf, but it's hard to believe he has time for it. Since coming to Brookhaven Lab, Vogt has continually taken on new leadership roles and research projects in his field — the study of inorganic materials.

When he arrived at the Lab in 1992, Vogt developed and operated a neutron powder diffractometer — a device that measures how neutrons interact with material powder samples — at the High Flux Beam Reactor, Brookhaven's former neutron facility.

Later, he began studying powder samples using a different type of probe: beams of highly focused x-rays. In 2000, he became the powder diffraction group leader in the Physics Department, and assumed responsibility for an NSLS x-ray workstation, or "beam line."

More recently, Vogt established the Physics Department's Materials Synthesis & Characterization group. He has also been involved in the scientific planning of Brookhaven's upcoming nanoscience facility, the Center for Functional Nano-materials (CFN), which will become operational in 2007.

The materials he studies include hydrogen storage materials, which may find use in environmentally smart, renewable hydrogen fuel cells and batteries, as well as metal compounds. Using x-ray, neutron, and high-pressure techniques, he investigates the atomic structure of these materials, determining how the structures relate to the materials' properties.

Vogt also investigates metal oxide materials — metal compounds that contain oxygen — because they tend to have interesting or unusual electronic behaviors.

"These studies are fascinating because they help identify materials that may be good candidates for many practical applications, such as reusable batteries or electronic devices," Vogt says.

Vogt received his Ph.D. from the Eberhard-Karls Universität in Germany, in 1987.

"Understanding proton transport at the nanoscale in water wires could be useful in the development of applications such as hydrogen fuel cell technology." — Thomas Vogt

science under pressure

Applying very high pressure to a material is one of the most useful methods of learning about its properties and behavior. Why?

High pressure causes materials to take on forms they otherwise would not, allowing new properties or behaviors to emerge. High-pressure devices can simulate the hot, dense conditions deep within the Earth, providing a glimpse of what happens to metals, rocks, and minerals in those extreme environments.

Additionally, high pressure forces materials to mix in interesting ways, such as forcing molecules of one material between layers or into open spaces of another, or causing chemical bonds to break and new ones to form.

Using high-pressure devices, scientists can study these processes in a controlled way. One device commonly used to apply high pressure is the diamond anvil cell (DAC), which uses the polished faces of two diamonds to squeeze a small sample. This setup, enclosed in tiny chamber, is surrounded with water or another liquid, which evenly transmits the applied pressure to all sides of the sample.

A DAC can apply pressures equal to millions of pounds per square inch. Samples are also often simultaneously heated to very high temperatures, up to thousands of degrees, using lasers. To follow the effects of pressure and/or temperature on the sample, such as chemical bond changes or the shifting of atoms, scientists bombard it with a beam of highly focused x-rays, such as those produced at the National Synchrotron Light Source (NSLS). The x-rays scatter and bounce off the atoms, emerging from the sample in a particular pattern. Using computers, scientists analyze the patterns to model the sample's changing structure as pressure increases.

The NSLS contains three workstations capable of high-pressure research, which draw scientists from all over the world. Some of the materials studied there are:

- Glasses made from metals, such as zirconium, which are often stronger and more resilient than traditional glasses, and may have applications as materials in medical and sports equipment
- Minerals, crystalline metal oxides called zeolites, ceramics, and other materials similar to those within inner Earth
- Metals, such as sodium, which can yield information about how free electrons behave under high pressure
- Gases, such as hydrogen, which take on new, ordered structures when compressed.

more information —
- Thomas Vogt, tvogt@bnl.gov or (631) 344-3731
- http://www.nsls.bnl.gov/newsroom/science/2004/06-Vogt.htm

Brookhaven Scientists Sample the Skies

To get the big picture on air pollution and climate, scientists have to think big — and small. Last summer, scientists from Brookhaven and other Department of Energy labs criss-crossed the skies above Western Pennsylvania to track the tiniest particles of air pollution.

— By Karen McNulty Walsh

Down-to-earth climate scientists agree that the level of atmospheric carbon dioxide (CO_2), the best known "greenhouse gas," is on the rise. But how much a given rise in CO_2 will raise our planet's temperature is still the subject of intense research — and heated debate.

One complicating factor is a lack of understanding of the influence of atmospheric aerosols, tiny particles released into the air from industrial processes like fossil-fuel combustion at the same time as CO_2. Aerosol particles scatter and absorb light and modify the properties of clouds, making them brighter and thus able to reflect more sunlight before it reaches Earth's surface. Aerosols could therefore be masking some or even much of the influence of the greenhouse gases — to the point where we might be seeing only the "tip" of the greenhouse effect "iceberg." But no one knows just how much global warming is "hiding beneath the surface."

To make more accurate estimates of the magnitude of warming we may face in the future, scientists need more information about the role of aerosols.

As part of the effort to gather that information, scientists from the three Department of Energy national laboratories — Argonne (ANL), Brookhaven (BNL), and Pacific Northwest (PNNL) — took to the skies above Western Pennsylvania for a month of air-sampling flights in the summer of 2004 to track the levels of aerosol pollutants.

The research was part of the International Consortium for Atmospheric Research on Transport and Transformation (ICARTT) experiment, an effort by many separate institutions and government agencies like the National Atmospheric and Oceanographic Administration (NOAA), the National Aeronautics and Space Administration (NASA), the University of New Hampshire, and others in Canada and Europe, to conduct a joint regional air quality and climate study of unprecedented scope.

"One main goal is to understand how pollutants from the Northeastern U.S. affect climate and air quality as they spread over the North Atlantic Ocean," said Peter Daum, lead researcher for the Brookhaven/DOE team.

The DOE scientists, funded and coordinated by the Office of Biological and Environmental Research (OBER) within DOE's Office of Science, focused on evaluating the effects of aerosol pollutants on Earth's radiation balance and climate forcing for a portion of the study known as the NorthEast Aerosol eXperiment (NEAX).

From July 20 to August 15, 2004, the DOE team launched regional air-sampling flights from Latrobe Airport, located about 25 miles east of Pittsburgh, Pennsylvania. Their aircraft, a G-1 Gulfstream operated by PNNL, carried research-grade instruments developed at both BNL and PNNL. Measurements gathered by additional ground-based instruments, which were deployed by ANL and PNNL scientists, provided complementary data.

"This large multi-agency study is a good example of how organizations with common goals can collaborate, pool resources, and accomplish something that they cannot do by themselves," said Daum.

Aerosols such as sulfur compounds result from emissions by fossil-fuel-burning power plants and other industrial sources. By themselves, and by affecting the brightness of clouds, they may increase the amount of incoming sunlight that is

Peter Daum, center, with other members of the research team in front of the G-1 Gulfstream research aircraft, also shown on the opposite page.

Meet Peter Daum

Peter Daum's research has its ups and downs – like when flying at 300 feet on a hot summer day. On such flights, some scientists lose their lunch; Daum seems to have the stomach for it. "I've never gotten sick, just a little queasy," he says.

Flying is actually one of the easy parts of his job. As lead researcher on a variety of multiagency air-quality and climate studies, Daum helps to design the specialized equipment that collects complex data on everything from aerosol absorption to ozone concentrations and ultraviolet radiation.

He also figures out when and where to fly to capture data that will make sense of our atmospheric soup – that is, so scientists can understand how the ingredients in the mix affect air quality and Earth's climate. "Deciphering the meaning of the data is the biggest challenge," he says, "but also the most important part, because that's what decision makers need to effectively regulate air pollution."

Daum got his start as a chemistry major at the Drexel Institute of Technology, earning his bachelor's degree in 1965. He went on to earn a Ph.D. in 1969 from Michigan State University. Daum then joined the faculty of Northern Illinois University before joining Brookhaven Lab's Atmospheric Sciences Division in 1980, a division he now heads.

In 1991, the Department of Energy sent Daum to the Middle East to study the environmental effects of the oil fires set by the retreating Iraqi Army during the Persian Gulf War. Closer to home, his studies have investigated pollutants above Nashville, New York, Phoenix, Philadelphia, Houston, and the Northeast.

When he gets a chance to stay on the ground, Daum likes to garden, cook, and play golf.

reflected back into space, thereby exerting a partial cooling effect on Earth's climate.

"But because their concentrations are highly variable and because they are removed from the atmosphere fairly quickly, it is difficult to assess these effects and the impact of aerosols on climate without collecting data in the ambient atmosphere," said Daum.

So the scientists participating in NEAX were particularly interested in aerosol formation and growth in plumes from point sources such as power plants, and in urban plumes with different characteristics. They also conducted air mass scale studies to see how the chemical, microphysical, and optical properties of aerosols evolve as the air mass ages and is transported to the east away from its sources.

Much of the data is still under analysis but it is already apparent that voluntary summertime reductions in power plant emissions are having an effect on the amount of ozone transported from western Pennsylvania to the Northeast. Ultimately, the scientists hope to characterize how much aerosols and aerosol precursors in the Midwest contribute to the aerosol burden over the western North Atlantic Ocean.

"Lack of knowledge regarding how aerosols are formed and distributed in the atmosphere and how they change the properties of clouds is one of the key factors preventing more accurate predictions of climate change," Daum said.

Findings from this study should help uncloud the climate picture.

"Lack of knowledge regarding how aerosols are formed and distributed in the atmosphere and how they change the properties of clouds is one of the key factors preventing more accurate predictions of climate change."

— Peter Daum

High-Tech Lab With Wings

DOE's air-quality/climate studies rely on a specially outfitted Grumman Gulfstream G-1 aircraft owned by Battelle, a manager of both Brookhaven and Pacific Northwest national laboratories. From the outside, the twin-turbo-prop looks like any other small aircraft, except for a few small probes mounted on the nose cone and fuselage. But inside you'll find $3-4 million worth of specialized equipment to sample the atmospheric stew, plus navigational and meteorological tools to track where the samples are coming from and the conditions under which they were collected. Some of the high-tech tools include:

- UV fluorescent instruments to monitor carbon monoxide levels
- Pulsed fluorescence spectrometers to track sulfur dioxide
- Ozone chemiluminescent instruments to measure nitrogen oxides
- Gas chromatograph for monitoring volatile organic compounds
- Integrating nephelometer for measuring aerosol light scattering
- Light scattering and particle mobility instruments for measuring the number and size of particles in the atmosphere
- Mass spectrometers and liquid sampling techniques for determining the chemical composition of aerosols in the mix
- Pyranometers to measure ultraviolet and visible radiation
- Thermometers, chilled mirrors, and gust probes, for monitoring air temperature, dew point/frost point, and wind direction and speed
- GPS (global positioning system) and a barometer for tracking the plane's position and altitude
- Differential pressure transducer for keeping tabs on air speed

Monitoring the instruments inside the Gulfstream G-1 ensures accurate data collection during time-sensitive study flights.

more information —

- Peter Daum, phdaum@bnl.gov or (631) 344-7283
- http://www.bnl.gov/des/ecd.htm

Research on "Holes" May Unearth Causes of Superconductivity

High-temperature superconducting materials could revolutionize electronics, computing, and electric power transmission — that is, once scientists understand how they work. Brookhaven Lab physicists have discovered that "holes" may hold a valuable clue.

— By Laura Mgrdichian

The mysteries of high-temperature superconductivity, a phenomenon in which the electrical resistance of a material disappears below a certain temperature, may one day be unlocked with the help of a recent discovery. In a superconducting compound, scientists found evidence of a rarely seen arrangement of "holes" — locations where electrons are absent.

The researchers were studying a compound made of strontium, copper, and oxygen (which they've dubbed SCO) that is one of the "cuprates," a family of compounds that contain copper oxide. In SCO, the scientists found evidence of a "hole crystal" — a rigid, ordered arrangement of holes. Holes are positively charged and, like electrons, may interact with each other to produce a superconducting current.

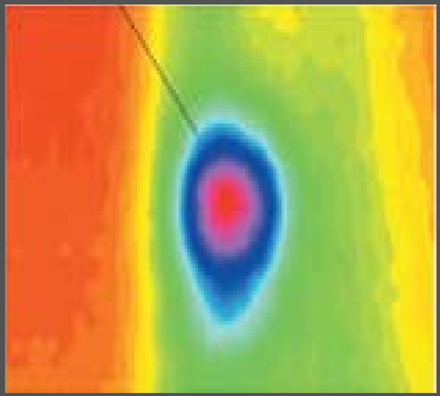
> "A hole crystal is a very unusual phenomenon."
> — Peter Abbamonte

"A hole crystal is a very unusual phenomenon," said Brookhaven physicist Peter Abbamonte, the study's lead researcher. "Its existence is a direct result of the correlations between holes, which are believed to produce superconductivity in other cuprates."

SCO consists of one layer of strontium atoms sandwiched by two sheets of different copper oxides. In one sheet, the copper-oxide molecules form long, parallel chains. The other copper-oxide layer, which contains the hole crystal, has a ladder structure, resembling chains that are linked horizontally.

A hole crystal is just one type of arrangement of electric charge in a material. These arrangements are important because some researchers believe that superconductivity is the result of a particular arrangement, or occurs when a superconductor approaches a boundary between two arrangements. In other cuprates, for example, scientists are studying a charge arrangement in which ribbons of holes and magnetic regions form alternating "stripes."

"We believe the hole crystal and stripes may be linked," said Abbamonte. "Specifically, the hole crystal in SCO may be a 'low-dimensional' precursor to stripes, meaning it exists only along the copper-oxide ladders, rather than in an entire copper-oxide plane."



An image of the hole crystal reflection

The Superconducting Phenomenon

Superconductors are remarkable materials that conduct electricity without any resistance. They perform far better than everyday conductors like the copper wire inside electrical cables and the tungsten filament inside light bulbs. Many scientists are studying superconductors to learn how they can improve many familiar devices and services.

What can they be used for?

Superconducting materials have an almost unlimited number of potential uses, such as:

- Electric cables: Making electric cables with superconducting wire could drastically reduce the amount of cable needed to power cities and regions. It could also reduce the size of power plant generators, cutting costs for the consumer.
- Medical imaging: Medical imaging techniques like magnetic resonance imaging (MRI) scanners use superconducting magnets to produce sharper, more detailed images of the body.
- Computers and electronics: Superconductors may lead to smaller, faster computer chips and ultra-fast computers. Other electronic devices like cellular phones can be improved by making circuits with superconducting materials.
- Transportation: Superconducting magnets may enable systems of levitating trains that are fast, quiet, and efficient. This technology, known as Maglev, was developed in the 1960s by Brookhaven scientists, and is being tested in Japan, Germany, and China.

How do they work?

To understand superconductors, it is first necessary to understand conventional conductors.

Inside a conductor, many electrons are not attached to any particular atom. Instead, these "free electrons" scatter about as they are repelled by the bound electrons and drawn to the atoms' positive nuclei. But constantly changing direction prevents the electrons from gaining momentum.

He and his collaborators studied SCO using x-rays from the National Synchrotron Light Source, a facility at Brookhaven Lab that produces x-ray, ultraviolet, and infrared light for research in a variety of scientific fields. They placed an SCO sample in the path of an x-ray beam, varied the wavelength of the beam, and watched how the x-rays reflected away from the sample.

At a particular energy, the sample reflected back the x-rays very intensely. The research group discovered that this reflection was caused by the holes, which led them to determine that the holes formed an ordered lattice since randomly placed holes could not have produced such a strong reflection.

Abbamonte and his collaborators plan to continue this research by varying the chemical composition of SCO to see if it changes the hole crystal. They will also examine another cuprate to see if its stripes are related to the crystal.

"Clearly, more research needs to be done to study these phases and their possible link to superconductivity," said Abbamonte.

The research was funded by the Office of Basic Energy Sciences within the U.S. Department of Energy's Office of Science, the National Science Foundation, Bell Laboratories, the Dutch Science Foundation, and the Netherlands Organization for Fundamental Research on Matter.

Inside a hot conductor, the atoms begin to vibrate, further hindering the free electrons' motion. For this reason, conductors perform better at colder temperatures.

To conduct electrons with no resistance, superconducting materials must be cooled to extremely low temperatures — approaching the coldest temperature possible, called "absolute zero," which is equal to about minus 460 degrees Fahrenheit (°F), or zero Kelvin (K). When a superconducting material is very cold, its atoms barely vibrate and its electrons behave as if they no longer repel each other. As a result, masses of electrons flow without any obstacles. This happens at a different temperature for each superconductor.

Where is superconductor research headed?

Currently, many superconductors must be cooled to nearly zero Kelvin using complicated cryogenic systems. Scientists are studying materials that exhibit superconductivity around 100K, or about -280° F, but this is still a very cold temperature to achieve. Scientists are hoping to discover materials that perform as superconductors at "room-temperature" and could be integrated into our everyday lives.

more information —

- Peter Abbamonte, abbamonte@bnl.gov or (631) 344-8406
- http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=04-94

Meet Peter Abbamonte

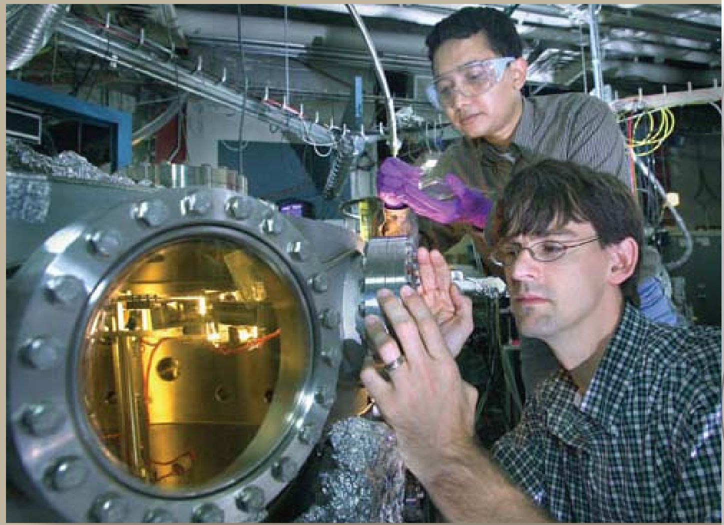
Peter Abbamonte's research activities, both past and present, showcase the usefulness of x-rays , extending beyond medical imaging into the frontier of materials science and physics.

As a physicist at the National Synchrotron Light Source (NSLS), Abbamonte uses x-rays to study how electrons behave in many types of materials — liquids and metals, for example. He has even used x-rays to image electrons splashing about amongst water molecules, creating a movie that covers a time span of less than one millionth of a billionth of a second!

He is currently investigating superconductors, remarkable materials that conduct a nearly limitless electric current. His research will help increase our understanding of how superconductors work.

Abbamonte began using x-ray light as a research tool in graduate school. He became an NSLS user and helped develop a new x-ray analysis technique called resonant inelastic x-ray scattering, for studying charge movement in superconductors. After earning a Ph.D. in physics from the University of Illinois at Urbana-Champaign in 1999, he spent two years at the University of Groningen in the Netherlands, developing the x-ray techniques he used to perform his superconductor hole crystal work (see article). He then worked in a biophysics group at Cornell University for one year, studying how energy is transported in light-harvesting bacteria.

Abbamonte joined the NSLS as an Assistant Physicist in 2003, and is now the spokesperson for one of the facility's x-ray beam lines.



Peter Abbamonte (bottom) and student researcher Andrivo Rusydi

Taking Charge of Molecular Wires

Linking single molecules together produces . . . long molecules. Yes, but scientists at Brookhaven view them as much more. They see "molecular wires" — tiny electron conductors with huge potential.

— By Laura Mgrdichian

Someday, "molecular wires" may replace silicon in micro-electronic circuits and components in solar energy storage systems. Brookhaven scientists and their colleagues at the University of Florida have uncovered information that may help this happen while studying how electric charge is distributed in polymer molecule chains several nanometers, or billionths of a meter, in length.

"Long molecules that can act as molecular wires, of which there are many variations, are one type of nanoscale object with the potential to lead to new technologies, due to their ability to conduct electricity and very small size," said Brookhaven chemist John Miller, the study's lead scientist. "But unlike conventional metal wires, polymer nanowires need assistance in order to conduct."

"Using a cluster of high-energy electrons from an accelerator, we can quickly add an extra negative or positive charge to a polymer molecular wire," Miller said. "When the end of the wire contains a chemically-attached 'trap' molecule, one where the electrons will be at a lower, more stable energy, the charge moves to it. This allows us to 'see' that the wire conducts electrons quickly, and over long distances."

One potential application for this finding is in the solar energy industry, particularly in a new field called "plastic solar." In conventional solar cells, incoming solar energy is transferred to the electrons in a semiconducting material, such as silicon, which knocks many of them loose. These electrons are guided to an electrode, creating a current that can be drawn off and used.

"Long molecules that can act as molecular wires are one type of nanoscale object with the potential to lead to new technologies."

— John Miller

The plastic solar movement aims to replace materials like silicon with polymer nanowires, which are cheaper and lighter. Another advantage of plastic solar cells is their physical versatility. Due to the flexible, bendable nature of polymer materials, plastic solar cells could be placed in areas of greatly varying size and surface type. Conventional cells are rigid and costly, and the current production method limits their size.

In plastic solar cells constructed to date, electrons must jump from one polymer wire to another in order to reach the electrodes. But as the electrons leave one wire in order to jump to the next, they encounter barriers, which require larger amounts of energy to traverse than the barriers that hinder electron movement within typical nanowires. This slows down the electrons.

Miller and his collaborators want to learn how to eliminate the barriers. But first, they must understand how the electrons move within single polymer wires — the amount of energy the electrons need, for example. Later, this information can be used to choose the best polymer conductors and design structures for plastic solar cells.

The group observed electrons move down a polymer wire by immersing the wire in an organic fluid and shooting high-energy electrons through the fluid. The electrons were supplied by Brookhaven's Laser-Electron Accelerator Facility (LEAF), which accelerates electrons to high energies for research applications. The energetic LEAF electrons either kick away some of the fluid molecules' electrons or allow the molecules to give up "holes" — mobile, empty spaces that carry positive charge. As a result, the submerged nanowire receives one of these electrons or holes.

"This new method injects extra negative or positive charges into the wire and allows us to observe the charges quickly diffuse across it. This observation is a key step toward developing polymer nanowires that are good conductors," Miller said.

In the future, Miller and his group also plan to look for ways to increase the conduction efficiency of the wires.

This research was funded by the Office of Basic Energy Sciences within the U.S. Department of Energy's Office of Science. Researchers included Alison Funston and Norihiko Takeda from Brookhaven Lab and Kirk Schanze and Eric Silverman from the University of Florida.

LEAF,
Chemistry's Newest Branch

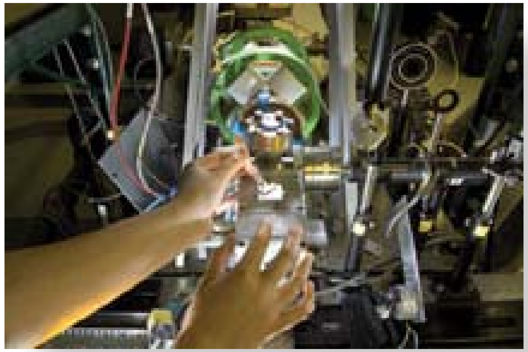
With the construction of the Laser-Electron Accelerator Facility (LEAF) at Brookhaven, the Lab's Chemistry Department has begun research in many exciting areas.

LEAF is a key component of the department's Center for Radiation Chemistry Research, which aims to closely study chemical reactions by bombarding samples with tiny clusters of high-energy electrons. This technique allows scientists to "see" chemical processes that occur on very, very short time scales.

Chemists working at LEAF are currently working on several cutting-edge research projects, and plan to delve into others. Materials they are studying, or plan to study, include:

- Ionic liquids — organic liquid salts with very interesting properties. For example, they remain in a liquid state over a wide range of temperatures, are exceptionally good solvents, and do not produce any measurable amount of vapors. They may become environmentally friendly replacements (called "green" solvents) for many harsh chemical solvents now used in industry.
- Aryl Halides — a class of molecules containing one of the "halogen" elements (fluorine, chlorine, bromine, iodine, and astatine) bound to a six-carbon, six-hydrogen ring molecule, known as a benzene ring. Studying how the halogen atom breaks away from the benzene ring, an extremely quick event, is a good way to learn about very fast bond-breaking reactions, which underlie the manufacture of many industrial products. These studies may, as a result, help improve the efficiency of and reduce the waste associated with industrial production.
- Dendrimers — a class of polymer molecules characterized by their unusual structure: multi-branch "limbs" radiating from a central core, somewhat like a tree with no trunk. Certain members of the dendrimer family are unusually good at storing light energy. When they absorb light, the electrons in the branches become energized and move to the central core, where they cluster for long periods of time. With further study of this behavior, dendrimers could be incorporated into efficient solar-energy systems.

Loading a sample into LEAF for analysis



Meet John Miller

How John Miller became interested in studying molecular wires is a great example of the power of education. While studying chemistry in college, he learned that electrons can "tunnel" through a string of molecules that don't conduct well in order to reach an acceptor molecule at the end. In graduate school, he found that tunneling provided an explanation for puzzling phenomena in glassy materials, while biological scientists were uncovering its role in photosynthesis.

"This was exciting, wonderful research that, for example, provided insights into how the sun's energy is captured by plants in photosynthesis, an exquisitely engineered natural system," says Miller. "I was hooked."

As a result of this early interest, Miller ultimately turned his attention to the electron accelerators at the U.S. national laboratories, where electron tunneling through molecules, and eventually along molecular wires, could be studied. In fact, with applications in molecular electronics in mind, scientists had already begun developing long molecule chains that rapidly transferred electrons.

Miller was intrigued. "I wondered about using molecular wires to develop simple, affordable solar energy systems. Brookhaven's Laser Electron Accelerator Facility seemed an ideal tool to investigate the wires' potential for converting solar energy to electrical energy."

Now, at the facility, Miller is doing just that. Through his research, he is helping to advance the "plastic solar" movement, which aims to create polymer-based solar energy panels that are inexpensive, physically flexible, and efficient.

Miller received his bachelor's degree at Oregon State University in 1966 and a Ph.D. in Chemistry from the University of Wisconsin in 1971. He then worked for several years at Argonne National Laboratory and came to Brookhaven Lab as a Senior Chemist in 1998.

more information —

- John Miller, jrmiller@bnl.gov or (631) 344-4354
- http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=04-79

DISCOVER BROOKHAVEN is published periodically by the Community, Education, Government and Public Affairs Directorate of Brookhaven National Laboratory

Editor: Kay Cordtz

Writers: Laura Mgrdichian, Karen McNulty Walsh

Photographer: Roger Stoutenburgh

Graphic Design: Theresa A. Esposito

DISCOVER BROOKHAVEN is also available at www.bnl.gov/discover

BROOKHAVEN NATIONAL LABORATORY

Office of Science U.S. DEPARTMENT OF ENERGY