INTERACTION POINT

April 16, 2004

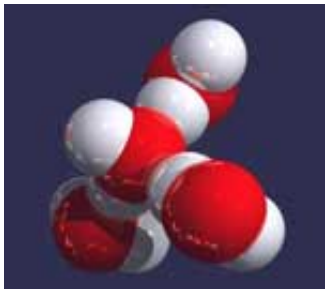
Back to SLAC Homepage

Back to TIP Homepage

In this issue:

Understanding the Structure of Liquid Water

By Davide Castelvecchi



Physicists of antiquity called it one of nature's fundamental elements; third graders know its chemical formula; and all known forms of life need it to exist. Yet what water really is—at least in its liquid form—is still, to a large extent, a mystery. A team led by scientists from SSRL and Stockholm University has now achieved a breakthrough in understanding the structure of liquid water.

See whole story...

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By Mason Inman

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See whole story...

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By Mason Inman

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See whole story...

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By Linda DuShane White

SLAC participated in the third annual Stanford Community Day, an open house to introduce people from the local area to the University. Combine this with the Founder's Celebration, mix in diverse activities such as science demonstrations, Dickens, the arts, the Stanford Band, food booths, lectures, a carnival, a petting zoo, Shakespeare and bicycle races and you have the perfect recipe for fun!

See whole story...

Bringing Science to Life: Second Talk in Public Lecture Series

By Kate Metropolis

Why do thousands of researchers from universities and industry come to SSRL each year? SSRL gives them a way of seeing real things at the level of individual atoms, and what they see helps to design therapeutic drugs, investigate living cells and viruses, and study pollutants and exotic materials.

See whole story...

The Stanford Linear Accelerator Center is managed by Stanford University for the US Department of Energy

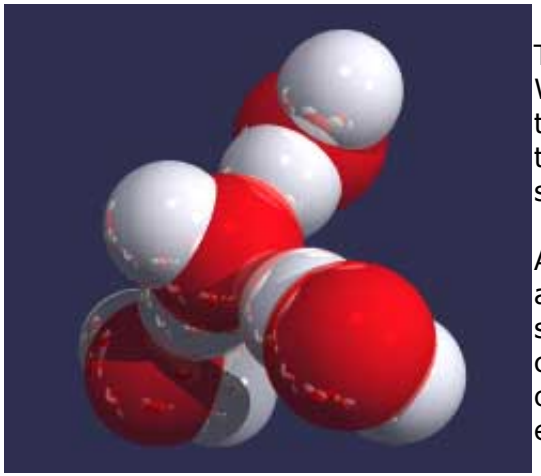
Last update Tuesday April 13, 2004 by Emily Ball

INTERACTION POINT
April 16, 2004

Understanding the Structure of Liquid Water

By Davide Castelvecchi

Physicists of antiquity called it one of nature's fundamental elements; third graders know its chemical formula; and all known forms of life need it to exist. Yet what water really is—at least in its liquid form—is still, to a large extent, a mystery. A team led by scientists from SSRL and Stockholm University has now achieved a breakthrough in understanding the structure of liquid water. They found that water molecules clump together much more loosely than previously thought.



A schematic of water molecules
(Image courtesy of Hirohito Ogasawara)

Their findings appeared in Science magazine's advance publication Web site on April 1. "The results overturn 20 years of research in the physical chemistry of water," says Anders Nilsson (ESRD), the team leader. "It's going to be a big shock in the whole field," he says.

As its H2O formula suggests, each water molecule is made of two atoms of hydrogen and one of oxygen. Water molecules tend to stick together in what chemists call hydrogen bonds. The oxygen can form two hydrogen bonds, so a molecule can link with up to four others—with two links through its oxygen atom and one through each of its hydrogens.

In ice, each molecule forms four stable bonds, while as a liquid, water bonds form and break a trillion times per second. The ephemeral patterns formed by bonding in the liquid are still far from being understood, but are thought to be responsible for the peculiar properties of water, including its relatively high boiling point, its high viscosity, and—last, but not least—its ability to sustain the chemical reactions inside a living cell.

The consensus among researchers has been that, at any given time, a molecule of water typically forms three or four hydrogen bonds—3.5 on average. "What we find," says Uwe Bergmann (ESRD), "is that there's not 3.5 hydrogen bonds, but only 2." Each molecule could still form up to four bonds, the research suggests, but two would be of different, much looser kinds.

The earlier 3.5 estimate was based on theoretical assumptions that became commonly accepted because

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

computer simulations gave results consistent with known properties of water. "Nobody had anything to object to the prevailing model, so it became the truth," says Nilsson.

The difficulty of 'seeing' the actual molecules in action meant a dearth of real data. "There has not really been new experimental information about water in the last 20 years, except for neutrons," says Nilsson. "The amazing thing," he says, "is that hardly anything is known about the microscopic origin for the unique properties of liquid water."

The new result now reopens the hunt for the structure of liquid water. "It resurrects models that were considered inappropriate," says Bergmann. One possibility, he suggests, is that water molecules could arrange in chains or even in closed rings. Eventually, the outcome could mean a better understanding of the chemistry of the cell, which is notoriously hard to imitate using different liquids. "Nobody has a clear answer to why water is essential for life," says Nilsson.

The research was the first to apply a technique called x-ray absorption spectroscopy to the local structure of water. The technique, developed by SSRL along with other research laboratories, bombards a material with x-rays that are finely tuned to excite particular electrons in a molecule's structure. Careful measurement of the scattered radiation reveals the motions of the excited electrons which, in turn, reveal what bonds molecules are forming. While SPEAR was being upgraded, the experiments used intense x-ray sources at Argonne and LBNL.

The team is now working on several projects to extend their results. "We want to study water in a whole range of pressures and temperatures," says Bergmann. "We propose to build a new facility at SPEAR3 where the structure of water would be a large part of the scientific drive," Bergmann says.

In addition to Nilsson and Bergmann, the other scientists from SLAC included in the five year long collaboration are Philippe Wernet (first author of the paper, now at the BESSY Laboratory in Berlin), Hirohito Ogasawara (ESRD) and Lars Naslund (Stockholm University).

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INTERACTION POINT
April 16, 2004

Scientists on Capitol Hill

By Mason Inman

In late March, Chris Roat (BABAR) took a break from lab work to go to Washington, D.C. as part of a delegation to represent high energy physics. Before his first meeting with a congressman, Roat was so nervous he couldn't eat. It turned out, however, that he found it easy to talk to most of the congressmen and their staffers. "People are generally supportive of science, but a lot of them don't know about what we do," Roat said. One point of the trip was to educate congressmen about research in their district funded through the DOE Office of Science.

Chris Roat (Photo by Diana Rogers)

The primary focus of this year's trip was to thank representatives who have been supportive of high energy physics centers including SLAC. "It's worth going every year," Roat said, "even if you won't have a direct impact that year."

Roat said his preparation for the meetings helped. All of the delegates—about 30 graduate and postdoctoral students as well as scientists from SLAC and Fermilab—had been given packets beforehand that provided background on science policy.

"We had to learn a lot about the people we were going to visit, what went on in past years, and how the budget gets determined," Roat said.

Roat and Caolionn O'Connell (ARDB), another graduate student who went on the trip, agreed that their experience as SLAC tour guides was also helpful. "We've spent a considerable amount of time trying to explain our work to people with no scientific background," O'Connell said.

It makes a big difference for policy makers to meet scientists in person, according to O'Connell. "To put a face on the science they fund is a good thing, and to show that we're passionate about what we do. I think that's persuasive enough for a lot of them."

The delegates appealed to people's interest in science, avoiding politics and questions of how to allocate

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

limited funds. "I was surprised by how supportive they were of basic research," O'Connell said.

Michael Wilson (BABAR), another graduate student on the trip, took the same approach. "I think not trying to play politics, and trying to talk freely about what I do—I think that's the most effective argument," Wilson said. "I like what I do and I think it's important. I just tried to convey that." In his discussions, Wilson also put research in a larger context. He pointed out that labs such as SLAC are a training ground for scientists, and that high energy physics is integral to many other areas of science.

Keeping the discussions open was also helpful, Roat said. "I try to make it a two-way conversation where they can ask questions and tell you what they know." He added, "Finding out whether they knew anything about science was a way to gauge at what level it was useful to talk with them." The trip was also an opportunity for the scientists to learn about science policy. "I definitely encourage people to go," Roat said. "It's a good way to learn something about your government."

O'Connell agreed, adding, "It was a civics lesson, definitely."

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Last update Thursday April 15, 2004 by Emily Ball

INTERACTION POINT
April 16, 2004

Let the Light Shine: SPEAR3 Up and Running

By Mason Inman

SPEAR3's shutters are open and users are getting their first taste of work with the completely rebuilt synchrotron radiation facility. The SPEAR3 upgrade is not yet complete as the current level is at 100 mA rather than the final 500 mA target. Like any new machine, it will continue to improve as it is broken in, users are already seeing improvements over SPEAR2.

Herbert Axelrod (Photo by Amanda Prado)

The top off injection technique is one improvement, in which more electrons are periodically injected at-energy into the synchrotron to keep the current high and maintain an intense x-ray beam. With SPEAR2, keeping the current high involved emptying the ring of electrons, refilling it at a lower energy, then increasing the ring energy back to 3 GeV, which could cause long down times for users.

"It's wonderful. We love SPEAR3," said Deanne Rudd (Stanford). "The best part is the top off."

Right now, the top off has to be done four times a day. As the synchrotron continues to run, however, the vacuum chamber that holds the electrons will become cleaner, making less top offs necessary and the beam more stable. "It's getting to be stable," said Ritimukta Sarangi (Stanford).

So far, SPEAR3 hasn't changed the nature of Sarangi's work on solutions of metal-containing proteins. She is already looking forward to this fall, when the electron beam is scheduled to be ramped up from 100 mA to 500 mA, which will allow Sarangi and fellow group members to collect data much more quickly.

For Frank Bridges (UC Santa Cruz), who uses EXAFS spectroscopy, the stability of the beam is crucial. "It looks good at this point," Bridges said. "The beam is very stable and the first few data traces look great."

Once Bridges starts taking data at the full beam current, the benefits of SPEAR3 should be immediate. He said the more intense x-ray beam will allow them to take high-quality data more quickly, partly because they can use smaller crystals in their experiments.

"The best crystals are often the smallest ones," Bridges said. Larger crystals have more imperfections and irregularities, which make the data less clear.

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

Along with the upgrade of SPEAR3, several robots were installed on the beamlines to help users.

"The robot is fantastic," said Herbert Axelrod (SG), about the machine that loads crystal samples into a cryogenic gas stream, produced by liquid nitrogen. Before, Axelrod had to load the samples manually, which was much slower and left him with chilly hands despite the use of gloves. "Believe me," Axelrod said, "it's pretty nice."

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Last update Monday April 19, 2004 by Emily Ball

INTERACTION POINT
April 16, 2004

PCD Improves Productivity Through Team Work

By John DiMaggio

Under the direction of department head Paul Bellomo, the Power Conversion Department (PCD) has achieved major productivity improvements in the manufacturing cycle for the High Voltage Power Supplies (HVPS). The HVPS provide power for PEP-II's klystrons, the microwave generators used to accelerate electron and positron bunches.

There are 11 HVPS in operation at PEP-II, one at SPEAR3, one in the Klystron Test Laboratory, one at Cornell University and PCD is building two more for PEP-II and there are plans for an additional three to be phased in over the next three years.

Klystron Test Laboratory, one at Cornell University and PCD is building two more for PEP-II and there are plans for an additional three to be phased in over the next three years.

John DiMaggio, project manager for the HVPS, supervised the implementation of the improvements, which required a team effort from many of the personnel within the department.

HVPS testing unit. *(Photo courtesy of John DiMaggio)*

As a starting point, a laboratory was set up in Bldg. 15 dedicated as an assembly area for the HVPS. The laboratory was refurbished by Power Systems Operations technicians, supervised by Serge Ratkovsky.

Ratkovsky and his group also refurbished Bldg. 647, dedicated to the storage of large parts and equipment for the HVPS. This was not an easy task because of the many 'treasures' stored there by engineers over the years. Some engineers even cried when their 'treasures' were sent to salvage. Steve Lowe, supervisor of Engineering Services, is having the roof repaired and a fresh coat of paint will spruce up the area.

Stephen Jenks, a senior technician in PCD, designed and built a new testing system. A comprehensive electrical diagram was developed by DiMaggio and Cliff Rogers, an associate engineer under Ponce Rodriquez in the Electrical Systems Design/Coordination group. Documentation support was provided by Joe Olszewski, supervisor of Electronic Coordination/Design.

DiMaggio and Rogers incorporated several design improvements to the HVPS blueprints. Bellomo designed a schedule system for manufacturing planning and control. Wayne Linebarger, PCD's Safety Officer, has

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

reviewed all building and facility changes to assure compliance to SLAC and OSHA safety standards.

The improvements achieved in the manufacturing cycle will result in large cost savings to PCD and SLAC. This will occur through efficiency in parts ordering and control, assembly and installation cycle and the general planning and schedule control of present and up-coming HVPS projects. These improvements were only achievable through the team effort of the PCD employees, who deserve a big 'Thank you.'

The Stanford Linear Accelerator Center is managed by Stanford University for the US Department of Energy

Last update Tuesday April 13, 2004 by Emily Ball

INTERACTION POINT
April 16, 2004

Bringing Science to Life: Second Talk in Public Lecture Series

By Kate Metropolis

Why do thousands of researchers from universities and industry come to SSRL each year? SSRL gives them a way of seeing real things at the level of individual atoms, and what they see helps to design therapeutic drugs, investigate living cells and viruses, and study pollutants and exotic materials.

Herman Winick, assistant director of SSRL and professor emeritus of applied physics at Stanford and SLAC, has been one of the leading developers of synchrotron light sources for three decades. At 7:30 p.m. on Tuesday, April 27, Winick will explain in lay terms what synchrotron radiation is, how it is made and how it is used to illuminate both fundamental science and societal problems. "Synchrotron Radiation: The Light Fantastic" is the second in the Lab's new public lecture series on science for the local community.

Herman Winick will explain how to see a molecule using an accelerator.
(Photo by Diana Rogers)

Winick joined the synchrotron radiation program here in 1973. He was superbly well qualified for the job, having just spent the past several months at Harvard identifying the weak points in the SPEAR proposal as a reviewer for NSF. "I was shocked out of my mind when SLAC offered me the position [leading design and construction]," he said.

In addition to keeping the Lab a leader in synchrotron light capabilities for 30 years and writing more than a hundred scientific papers, Winick has devoted considerable effort to the causes of human rights and international scientific collaboration. He conceived the idea of building a synchrotron light laboratory in the Middle East, with the hope that giving Israelis, Palestinians and people of other nationalities the opportunity to do world-class science together would increase mutual understanding and the chances for peace. In January 2003, ground was broken in Jordan for the UNESCO-sponsored project, called Synchrotron light for Experimental Science and Applications in the Middle East (SESAME).

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

After the talk, attendees can enjoy refreshments and chat with scientists who will be on hand to answer questions. Invite your family and friends! To help promote the public lecture series or put up posters in your community contact Emily Ball, Community Relations Coordinator (Ext. 2620, emily.ball@slac.stanford.edu).

For more information, see: http://www.slac.stanford.edu/lectures

INTERACTION POINT
April 16, 2004

Host a High School Student!

By Linda Alf

SLAC is participating in the Industry Initiatives Students in Math & Engineering (IISME) Program to host high school students this summer. These students will receive a stipend from a California grant so there is no cost to SLAC. The program's goal is to encourage and prepare girls and underrepresented minority students in pursuing course work and extracurricular activities that will lead to a college degree in science, technology, engineering or math (STEM).

Internships Start July 6

We would like the students to be placed in areas at SLAC where they can receive hands on experience with science, technology, engineering or math. Students will hold short internships for 16 hours per week for four weeks beginning July 6 (Tuesday -Friday, 4 hours per day). The students will be seniors next year and will have completed algebra I and II, geometry, chemistry, physics and (usually) biology.

The students are participants in a mathematics/science enrichment project that targets four Silicon Valley high schools, offering curriculum enrichment, summer internships, a summer science camp, high school engineering course (in development), visits to local colleges and science/technology complexes.

Sign up as a Host by April 23

Please respond before the April 23 deadline if you are interested in hosting an IISME Student. Contact Linda Ahlf (Ext. 2354, lahlf@slac.stanford.edu).

INTERACTION POINT
April 16, 2004

New On-line Databases...

Brought to you by the SLAC Library

Engineering Design Information

http://www.esdu.com

Come to the Demo at
10:00 A.M. on Tuesday, April 27
in the Orange Room

ASM Handbook

http://www.asmmaterials.info

Search all volumes as well as
the Alloy Center

Key to Metals

http://www.key-to-metals.com/

Nonferrous Metals Database

Key to Steel

http://www.key-to-steel.com/

Steel Property Database

INTERACTION POINT
April 16, 2004

From the Benefits Office:

Have Questions About Investing For Retirement?

Representatives from Fidelity, Vanguard and TIAA-CREF will be holding individual counseling sessions at SLAC. Please contact the companies directly to set up an appointment:

Fidelity
May 11, June 3
(800)642-7131

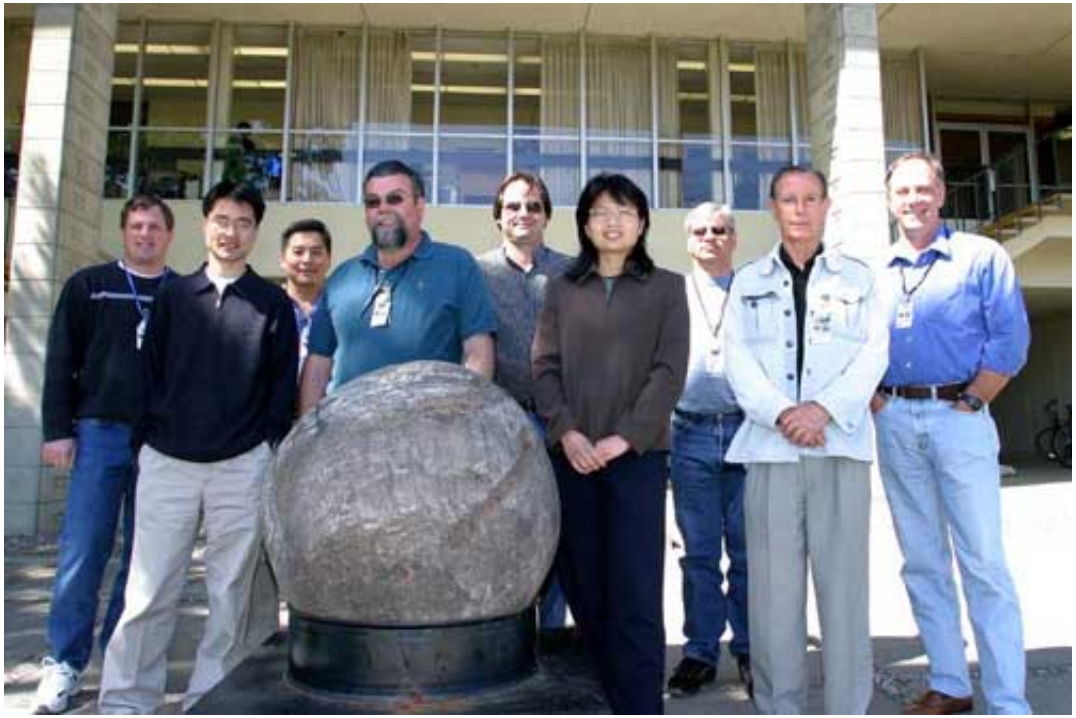
Vanguard
June 24
(800)662-0106, Ext. 14500
http://www.meetvanguard.com

TIAA-CREF
April 29, May 28
(800)842-2007
http://www.tiaa-cref.org/moc

All sessions will be held in:
Building 280A, Room 180

INTERACTION POINT
April 16, 2004

Welcome to New Employees



(Photo by Diana Rogers)

Welcome to the most recent new employees (left to right): Dean Zanardelli (ESD), Albert Nguyen (RD), Zhiyu Zhang (ARDA), Milorad Dragovic (ESRD), Tom Nieland (REG), Liling Xiao (ACD), Doug Plaza (MD), Bruno Brugnoletti (MD) and Leo Manger (REG).

INTERACTION POINT
April 16, 2004

What SLAC Does to Protect San Francisquito Creek

By Judy Fulton

The protection of San Francisquito Creek, which runs along most of the southern border of SLAC, is not the responsibility of any one person or organization. As noted in a previous article (The Interaction Point, February 20, 2004, http://www2.slac.stanford.edu/tip/2004/feb20/creek.htm), the issues and concerns are interrelated and overlapping and involve many different efforts. At SLAC the protection of the creek is not limited to one program or activity, but is part of a number of programs and, more importantly, is reflected in how each of us performs our job.

Programs

At the heart of the programs in place at SLAC to protect the creek is the minimization of any pollutant that could make its way into a storm drain:

The confluence of San Francisquito Creek and Bear Creek. *(Photo courtesy of Judy Fulton)*

• **Hazardous materials and waste management.** Through the proper use, storage, and disposal of hazardous materials and waste, SLAC minimizes the source of pollutants (https://www-internal.slac.stanford.edu/esh/wm/).

• **Pollution prevention and waste minimization.** Through thoughtful consideration of what materials to use, SLAC minimizes the toxicity and quantity of potential pollutants (https://www-internal.slac.stanford.edu/esh/wm/waste_minimization.htm).

• **Stormwater pollution prevention.** By using 'best management practices' (BMPs), SLAC ensures that pollutants will not make their way into storm drains (http://www.slac.stanford.edu/esh/epr/Stormwater/stormwaterBMP.html).

• **Spill prevention.** Through the quick response that comes from the careful planning contained in the Spill Prevention, Control, and Countermeasures Plan, SLAC can avoid releasing pollutants to a storm drain even in the event of a spill (http://www.slac.stanford.edu/esh/reference/SPCC.pdf).

Activities

The following are but a few of the ways that SLAC works to protect the creek

- Milestones

EVENTS

- You're Invited to the SLAC Education Fair
- SLAC Science at Stanford Community Day
- Atmospheric Experiments Highlight Balloon Fest
- Upcoming Events

ABOUT TIP

- Staff/Contact
- Submission Guidelines

• **Restoration and remedial action projects.** The clean-up of historic spills and contaminants is an important component of creek protection.

• **Stormwater monitoring.** SLAC monitors the stormwater of two storm events each year to gauge how well we are keeping pollutants out of runoff.

• **Secondary containment management.** Making sure our containment systems act as our first line of defense in the case of a leak or spill and that only rain water makes it into a storm drain.

• **Erosion and sediment control.** Sediment is a major pollutant and can have detrimental effects on wildlife in the creek. Controlling erosion and managing sediment is vital to reducing the flow of sediment to the creek.

• **Facility maintenance and housekeeping.** Normal maintenance of structures, utilities, and roadways helps prevent pollution from such sources as chipped paint, leaking water, and eroding asphalt. It is housekeeping, however, that makes the biggest difference on the day-to-day minimization of pollutants. Sweeping up debris, using drop cloths and drip pans to catch potential pollutants, covering materials, or storing them inside are the big hitters in our efforts to protect the creek.

Each of us can make a difference by being mindful of these programs and activities. If you want to know more about how you can protect the creek, please contact Judy Fulton, Environmental Protection (Ext. 4538).

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Last update Tuesday April 13, 2004 by Emily Ball

INTERACTION POINT
April 16, 2004

MILESTONES

Service Awards

5 Years
Datu, Martina (BSD), 4/26
Eaton, Betty (RP), 4/16
Luening, Katharina (ESRD), 4/30
Terebilo, Andrei (ASD), 4/15

10 Years
Carlson, Stephanie (SSRL), 4/19
Dayton, James (RAD), 4/1
Dorsey, Odell (KLY), 4/16
Fenske, (KLY), 4/11
Kim, Peter (EE), 4/1
Kurita, Nadine (SSRL), 4/13
Kwon, Joong (SEM), 4/11
Lauchner, Chester (SEM), 4/16
Loewen, Roderick (KLY), 4/16
Vanderzyl, Robert (KLY), 4/25
Villanueva, Vincent (PUR), 4/1

15 Years
Baumgartner, William (KLY), 4/24
Kim, Young (ESD), 4/17
Tran, Yen (ACC), 4/17

20 Years
Boyer, Roger (ESD), 4/4
Fant, Karen (MFD), 4/1
Mathew, Mary (ACC), 4/24
Rogers, Howard (REG), 4/16

25 Years
Gallego, Peter (SEM), 4/24

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

Retired
King, Tony (MET), 3/31

To submit a Milestone, see:
http://www.slac.stanford.edu/pubs/tip/milestoneindex.html

See Awards and Honors at http://www.slac.stanford.edu/slac/award

INTERACTION POINT
April 16, 2004

You're Invited to the SLAC Education Fair

By Linda DuShane White

What educational opportunities exist in the Bay Area? Want to learn about the SLAC staff tuition reimbursement program? These and other questions will be answered for SLAC employees and their families at the Education Fair on Tuesday, April 20, from 11:00 a.m. to 3:00 p.m.

As an educational and scientific institution, SLAC wants to encourage people to make this first-ever Education Fair a great success.

Coordinated by Pauline Wethington (HR/COM) and Lisa Noble (University of Phoenix-NCAL), the Fair will provide information on a wide range of career and educational prospects—and it will be fun.

Balloons, refreshments and drawings for prizes will create a festive air on the Green where representatives from 15 institutions will hand out literature providing information about admissions, majors, careers, financial aid, applications, degrees, certificates and more.

The following educational institutions will be represented, as well as SLAC and Stanford:

University of Phoenix-NCAL, UC Berkeley, San Jose State, University of San Francisco, Santa Clara University, UC Santa Cruz Extension, Golden Gate University, Menlo College, Tech Skills and the following community colleges: Foothill, West Valley, DeAnza and Evergreen.

No need to register for this fun, free and informative event. Just drop by on The Green and in the Breezeway to enjoy our Education Fair.

For more information see: www2.slac.stanford.edu/career/

INTERACTION POINT
April 16, 2004

SLAC Science at Stanford Community Day

By Linda DuShane White

SLAC participated in the third annual Stanford Community Day, an open house to introduce people from the local area to the University. Combine this with the Founder's Celebration, mix in diverse activities such as science demonstrations, Dickens, the arts, the Stanford Band, food booths, lectures, a carnival, a petting zoo, Shakespeare and bicycle races and you have the perfect recipe for fun!

A brave volunteer on the Bed of Nails. *(Photos by Diana Rogers)*

Curious visitors steadily streamed by the SLAC exhibits along the Packard Building patio and arcade. Questions were answered by a team of volunteers handing out Tour SLAC buttons, Future of Science mirrors and posters. They also provided information about tours and public lectures.

The Kavli Institute's Ask-an-Astronomer team was accompanied by a special exhibit staff ed by Sonoma State NASA Education and Public Outreach with special GLAST giveaways. A cosmic ray detector and a cloud chamber were set up in the darkened arcade where people were given an explanation of what they were seeing by a team of physicists.

A crowd-pleasing physics lesson was Keith Jobe's (NLC) chocolate chip ice cream made with liquid nitrogen, handed out to onlookers as a treat after each dramatic demonstration.

Our most flamboyant demonstration—the bed of nails—was flanked by crowds every time guest physicist Michael (MO) Olson (St. Norbert College) took up his bullhorn to announce another show.

Surprisingly, plenty of volunteers agreed to lie between two beds of nails with a cement block placed on top (see photo). The block became a cloud of dust when demolished by a sledge hammer and volunteers arose unharmed to laughter and "aahhs" from the crowd.

Special thanks go out to the many Ambassadors to the Community who supported this event from Nina Stolar (PAO) and Barry Webb (ER). The months of planning and hard work paid off. Stanford Community Day was an ideal venue to publicize the educational and scientific programs, tours and talks available at

- **Milestones**

EVENTS

- **You're Invited to the SLAC Education Fair**
- **SLAC Science at Stanford Community Day**
- **Atmospheric Experiments Highlight Balloon Fest**
- **Upcoming Events**

ABOUT TIP

- **Staff/Contact**
- **Submission Guidelines**

SLAC.

To see more pictures of the event look under Special Events for 2004, at: www-project.slac.stanford.edu/slacpix/index.htm

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Last update Tuesday April 13, 2004 by Emily Ball

INTERACTION POINT
April 16, 2004

Atmospheric Experiments Highlight Balloon Fest

This year's Balloon Fest attracted almost a dozen teachers and 30 high school students to Paso Robles to participate in atmospheric research experiments. Seven teams from three high schools registered for this year's Endeavor Academy to conduct experiments and prepare reports on their observations.

Pictured in the front row (left to right) are Lowell Klaiser (GLAST), Hartmut Sadrozinski (UCSC) and Terry Schalk (UCSC) with Gordon Spear (Sonoma State) and Kabutur Team member Pedro Flores (Paso Robles High School). *(Photo by Rose Schalk)*

The April 3 event was graciously hosted by parents Clair and Lance Silver in the meadows of Tobin James Cellars and supported by SCIPP, UC Santa Cruz, COS (Calspace), GLAST (NASA) and QuarkNet. For information on Balloon Fest, see: http://scipp.ucsc.edu/outreach/balloon/index.html