CHEMICAL SCIENCE AND ENGINEERING AT BERKELEY
Newsletter of the College of Chemistry, University of California, Berkeley
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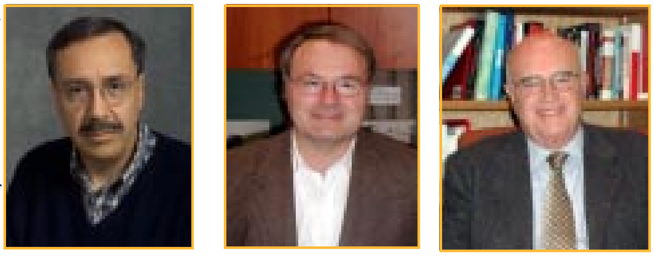
National Awards for Chemistry Professors

National Medal for Somorjai; NAS for Bustamante and Harris

Even for the highly decorated Berkeley chemistry department, it has been an exciting spring as faculty members were recognized nationally for their outstanding work. First came the news that **Carlos Bustamante** and **Charles Harris** are among the 72 new members of the National Academy of Sciences. Then **Gabor A. Somorjai** was named by President Bush to receive one of this year's 15 National Medals of Science, the nation's highest award for lifetime achievement in fields of scientific research. And, as we go to press, we learned that **Alex Pines** was elected Foreign Fellow of the U. K.'s Royal Society (to be covered in the next issue).



Berkeley Labs Photo Dept.

Carlos Bustamante, Charles Harris, and Gabor Somorjai. Bustamante and Harris are two of the newest members of the National Academy of Sciences and Somorjai will receive the National Medal of Science.

"The election of Charles Harris and Carlos Bustamante to the National Academy of Sciences and conferral upon Gabor Somorjai of the National Medal of Science is obviously a tribute to our outstanding faculty, and it is an even greater honor for Berkeley when you remember that two of these top scientists, Bustamante and Somorjai, were also graduate students here," said Dean Clayton Heathcock.

Gabor Somorjai

Somorjai is receiving his medal as "the world's leading authority in the development of modern surface science, having spent the last 40 years establishing the molecular foundation of many surface-

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Chatterjee (Ph.D. '71) to Speak at Commencement

This year's commencement speaker is **Dr. Nirmal Chatterjee**, vice president-environment, health and safety, and corporate engineering at Air Products and Chemicals, Inc. Dr. Chatterjee joined Air Products in 1971 after receiving his Ph.D. in chemical engineering from Berkeley under the direction of professor **David Lyon**. He is a member of the college's advisory board, which he chaired from 1996 through 1999.

Commencement will be held on May 25 at 2:00 p.m. in Zellerbach Auditorium. The graduating class this year (students finishing their requirements from summer 2001 through spring 2002) breaks down as follows:

B.S. Chemical Engineering—85
B.S. Chemistry—62
A.B. Chemistry—6
M.S. Chemical Engineering—4
M.S. Chemistry—10
Ph.D. Chemical Engineering—15
Ph.D. Chemistry—63

QB3 Receives Full Funding

The four California Institutes for Science and Innovation, including the Institute for Quantitative Biomedical Research (QB3), were fully funded by the state legislature in a mid-April vote.

QB3 is a cooperative effort among Berkeley, UC Santa Cruz and UCSF. It draws on the tools of the quantitative sciences, math, engineering, physics and chemistry, to help scientists better understand complex biological systems.

By fostering collaborations among scientific disciplines that have not traditionally interacted, QB3 hopes to encourage biologists, chemists, engineers and computer scientists to explore the big unanswered questions in health science. Some of the projects being tackled by college faculty involved in QB3 include exploring biological structures for new approaches to drug design and using combinatorial chemistry to develop molecular tools to analyze biological processes. The major portion of Berkeley's share of the funding will be applied toward the construction of an interdisciplinary research facility, to replace the current Stanley Hall.

100 Years of Iota Sigma Pi

Iota Sigma Pi (ISP), the national honor society for women in chemistry, will hold its centennial celebration here at Berkeley on June 12-15. Berkeley is the birthplace of ISP since the first chapter, the Hydrogen chapter, was formed here in 1902. There are now more than 10,000 members in 40 chapters nationwide.

According to secretary **Jennifer Sokol**, the local Hydrogen chapter is pleased to be hosting the meeting and will be organizing two poster sessions: one for presentation of the activities of all the chapters and one for presentation of research by ISP members.

ISP promotes the professional development and personal growth of women in chemistry and related fields through recognition, public outreach and the formation of support networks. The centennial meeting will combine perspectives of past and future; talks and posters sharing the rich and interesting history of ISP will be coupled with the latest news about current women's issues presented by the most knowledgeable female experts. For more information about the meeting, see the ISP home page at **http://www.cchem.berkeley.edu/~iota**.

Fleming Appointed Melvin Calvin Distinguished Professor

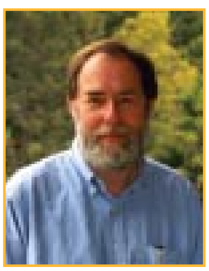


photo by Greg Butera

Graham Fleming has been appointed the first holder of the recently established Melvin Calvin Distinguished Professorship in the department of chemistry. This professorship was created with the intent that it be held by a scientist of exceptional caliber and achievement who has made major contributions to advancing chemical biodynamics or related fields.

Fleming and his group study dynamic processes in a range of complex systems, such as liquids, solutions and proteins. His research focuses particularly on the primary steps of photosynthesis and the transfer of light energy through reactions in plants to the reaction center. The major experimental tool for Fleming and his coworkers is femtosecond spectroscopy, which is combined with both theory and computer simulation to interpret data. His work has been recognized by his election as a fellow of both the Royal Society of London and the American Academy of Arts and Sciences.

Fleming is also director of the physical biosciences division of LBNL and is co-director at Berkeley of the institute being created under the QB3 initiative. (See story above.)

"I'm honored to receive the distinguished professorship and particularly pleased that it is named for one of the giants of photosynthesis research—a field I have worked in extensively during my five years at Berkeley," said Fleming.

The Melvin Calvin Distinguished Professorship honors the late Professor Calvin, who began his academic career at Berkeley in 1937 and served on the faculty until his death in 1997. Professor Calvin was a University Professor and received the Nobel Prize in 1961 for his elucidation of the path of carbon in photosynthesis. The cycle of reactions by which plants (and some bacteria) convert carbon dioxide into sugar and water is known as the Calvin cycle.

Chemistry Library Returning to Hildebrand Hall

By Mary Ann Mahoney, Head, Chemistry Library

After almost two years in temporary quarters in the campus's central library, Doe, the chemistry library will soon be back in Hildebrand Hall. In fact, part of the library is already there. The study area tables and chairs, carrels, and the artwork have all returned. The books, journals, and library staff, however, will move in after the spring semester is over. The library will close May 26th to prepare for the move, and will reopen at 1:00 p.m. on June 13th in Hildebrand Hall.

Hildebrand Hall, after the seismic improvements.

When the library reopens, the journals will be shelved alphabetically rather than by Library of Congress number. The other major change is the elimination of the closed reserves section that was located adjacent to the library staff work area. Those books have been moved out of the restrictive area and merged with the reference collection. The resulting enhanced reference collection will now be easily accessible to all users while the library is open and staffed. After-hours access to the library remains the same as it was before the move (by card access), and photocopying will also revert to the ID card procedures that were previously in place.

Other improvements to the library include a new data infrastructure and new high-speed data lines. Electrical lines were installed in the study area so that users can plug in their laptops, and study table reading lamps have been purchased to improve lighting at night. The library also has new flooring, a new ceiling with improved lighting, a new circulation desk, and new shelving in the study area. For increased safety and accessibility, there is a more streamlined entryway; a second, wider staircase to the mezzanine; a sprinkler system in the stacks area; and a wheelchair lift. With the elimination of the closed reserves section, the library staff will now be in one central room and no longer extend into the stacks at the back of the library. Finally, new paint and a general overall cleaning have really brightened the space.

The library will have an official opening sometime in the summer to celebrate the new space and to properly thank the many people who were involved in the project. In the meantime, everyone is invited to stop by the library when it reopens in Hildebrand to see the new facilities.

New Faculty Members for the Chemistry Department

The department of chemistry is happy to announce the addition of three faculty members for the upcoming academic year. **Stephen Leone** has been hired as a full professor and will become director of the chemical dynamics beamline at LBNL's Advanced Light Source. Leone, who is currently a fellow of JILA and of the National Institute of Standards and Technology, and an adjoint professor of chemistry and biochemistry at the University of Colorado, studies molecular dynamics and surface processes, including the use of lasers to probe semiconductor growth and etching; the dynamics of photofragmentation; and atomic force microscopy.

At the assistant professor level, two new faculty members, **F. Dean Toste** and **Haw Yang**, are joining the department. Toste received his Ph.D. from Stanford with Barry Trost and has worked on the development and applications of transition metal catalysts for organic synthesis, both at the graduate level and as a postdoctoral scientist at Caltech with Robert Grubbs. He is the recent recipient of the Nobel Laureate Signature Award of ACS, given in recognition of outstanding graduate work. Yang did his Ph.D. work here at Berkeley with **Charles Harris**, studying chemical reaction dynamics in liquids, and was a postdoctoral fellow at Harvard with Sunney Xie, studying complex biological systems.

Each of these scientists will be profiled in the August issue of the newsletter.

Batteries and Fuel Cells: An Interview with Professor Cairns

*Chemical engineering professor **Elton Cairns** studies electrochemistry and electrocatalysis and works to understand and improve electrodes used in rechargeable batteries and fuel cells.*

Where are high-performance batteries being used today?
They are used in portable devices such as computer laptops and cell phones, which require quite a lot of energy and need batteries that can store that energy and then be easily and effectively recharged. As these markets continue to grow, so will the demand for longer-lasting and more powerful batteries.

What aspect of battery technology are you currently working on?
Most rechargeable batteries are based on the lithium ion, which moves between the positive and negative electrodes as the battery powers a device and is then recharged. The electrode materials can accommodate the lithium ions in their structure with a minimum of structural rearrangement. In these batteries, the positive electrode is made of cobalt oxide, which is toxic, not friendly to the environment, expensive and in short supply. The battery industry is trying to build batteries for new applications such as for electric or hybrid cars, and the use of cobalt oxide is not feasible.

We are searching for a replacement of cobalt oxide for the positive electrode, and a good candidate is manganese oxide (Mn_xO_y), which is cheap and environmentally benign. One problem, though, is that Mn_xO_y batteries have a short life because the material loses its integrity too quickly. However, we found that by replacing a small percentage of the manganese with another metal, such as chromium, the lifetime of the battery can be greatly extended.

My group is investigating how the stability of Mn_xO_y is affected by small amounts of different metals. We are currently studying Mn_xO_y at the atomic level using spectroscopic techniques, including X-ray absorption spectroscopy in collaboration with professor S. Cramer at UC Davis and NMR in collaboration with chemical engineering professor **Jeffrey Reimer**. Through these techniques, we have found a few very important parameters in electrochemically stabilizing Mn_xO_y that explain why the best Mn substitute so far is chromium.

What other parts of the battery do you study?
My group is also looking at new materials for the negative electrode. The negative electrodes are usually made of carbon materials, which can pose a safety hazard since they are flammable. Also, the carbon electrode material is too slow in taking up the lithium ion, and lithium metal can be deposited on the electrode, which is extremely dangerous.

Fuel cells have been getting a lot of press these days as a replacement for gasoline engines in cars. How are fuel cells different from batteries?
Fuel cells are energy conversion devices that potentially will have higher efficiencies and greatly reduced emissions compared to internal combustion engines. However, there are some serious challenges that must be solved by chemical engineers before fuel cells are widely used in cars. Present-day fuel cells typically operate on H_2, so either an H_2-storage device or a complicated fuel reformer must be carried onboard the vehicle. Hydrogen is difficult to store, and right now the storage system weighs 30-50 times the weight of hydrogen. And it is not a good idea to store a flammable gas at high pressure on a vehicle.

What are some of the alternatives to storing hydrogen in the fuel cell?
One way to power the fuel cell is to pump liquid fuel such as methanol, (CH_3OH), into the fuel tank and then feed it into a system that would convert it into CO_2 and H_2. That way the hydrogen would be produced in the vehicle as needed. However, there are still some obstacles to this technology being implemented. The byproduct CO would need to be removed from the system because it is a poison to the platinum catalyst (as well as to people). Also, H_2 should really be produced only when the car is moving and not when the car is stopped.

We are hoping to circumvent these problems by developing an electrocatalyst that will act directly on the methanol and use very little energy in the conversion of CH_3OH to CO_2 and H_2 and electricity. It would also have to operate under mild conditions. So far, platinum alloys are the most promising. We look at the molecular species that are absorbed onto the fuel cell electrode to determine how the reaction takes place. By better understanding the electrochemical reactions, we can hope to design a better electrocatalyst.

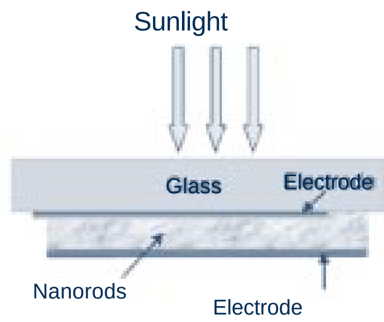
Technology Opens the Door to Plastic Solar Cells

by Robert Sanders

Scientists in the college of chemistry, led by chemistry professor **A. Paul Alivisatos**, have found a way to make cheap plastic solar cells flexible enough to paint onto any surface and potentially able to provide electricity for wearable electronics or other low-power devices.

The group's first crude solar cells have achieved efficiencies of 1.7 percent, far less than the 10 percent efficiencies of today's standard commercial photovoltaics. "Our efficiency is not good enough yet, but this technology has the potential to do a lot better," said Alivisatos, who is also a member of Lawrence Berkeley National Laboratory. "There is a pretty clear path to improve performance."

Alivisatos and his co-authors, graduate student **Wendy U. Huynh** and post-doctoral fellow **Janke J. Dittmer**, published their results in *Science*.



Schematic diagram of a hybrid "plastic" solar cell with a nanorod/polymer layer sandwiched between two electrodes.

The solar cell they created is actually a hybrid, comprised of tiny nanorods dispersed in an organic polymer or plastic. A layer only 200 nanometers thick is sandwiched between electrodes, and can produce, at present, about 0.7 volts. The electrode layers and nanorod/polymer layers could be applied in separate coats, making production fairly easy. And unlike today's semiconductor-based photovoltaic devices, plastic solar cells can be manufactured in solution in a beaker without the need for clean rooms or vacuum chambers.

The technology takes advantage of recent advances in nanotechnology, specifically the production of nanocrystals and nanorods pioneered by Alivisatos and his laboratory colleagues. These are chemically pure clusters of from 100 to 100,000 atoms with dimensions on the order of a nanometer, or a billionth of a meter. Because of their small size, they exhibit unusual and interesting properties governed by quantum mechanics, such as the absorption of different colors of light depending upon their size.

It was only two years ago that Alivisatos and colleagues found a way to make nanorods of a reliable size out of cadmium selenide, a semiconducting material. Conventional semiconductor solar cells are made of polycrystalline silicon or, in the case of the highest efficiency ones, crystalline gallium arsenide.

Huynh and Dittmer manufactured nanorods in a beaker containing cadmium selenide, aiming for rods of a diameter of 7 nanometers to absorb as much sunlight as possible. They also aimed for nanorods as long as possible—in this case, 60 nanometers. They then mixed the nanorods with a plastic semiconductor, called P3HT, which stands for poly-(3 hexylthiophene), and coated a transparent electrode with the mixture. The thickness, 200 nanometers, is a factor of 10 less than the micron-thickness of semiconductor solar cells. An aluminum coating acting as the back electrode completed the device.

The nanorods act like wires. When they absorb light of a specific wavelength, they generate an electron plus an electron hole—a vacancy in the crystal that moves around just like an electron. The electron travels the length of the rod until it is collected by the aluminum electrode. The hole is transferred to the plastic, which is known as a hole-carrier, and conveyed to the electrode, creating a current.

P3HT and similar plastic semiconductors currently are a hot area of research in solar cell technology, but by themselves these plastics are lucky to achieve light-conversion efficiencies of several percent.

"All solar cells using plastic semiconductors have been stuck at 2 percent efficiency, but we have that much at the beginning of our research," Huynh said. "I think we can do so much better than plastic electronics."

"The advantage of hybrid materials consisting of inorganic semiconductors and organic polymers is that potentially you get the best of both worlds," Dittmer added. "Inorganic semiconductors offer excellent, well-established electronic properties and they are very well suited as solar cell materials. Polymers offer the advantage of solution processing at room temperature, which is cheaper and allows for using fully flexible substrates, such as plastics."

National awards, continued from page 1

based technologies," according to the National Science Foundation. "Through his ingenious surface molecular chemical methodology, and his pioneering innovations and development of the requisite sophisticated instrumentation, Somorjai revolutionized the field, making possible the elucidation of processes at the molecular scale that occur at heterogeneous catalyst surfaces during the course of a chemical reaction," said chemistry professor **Alex Pines**.

"I cannot imagine an award that would be more important to me than this recognition by the United States of my work over the years," Somorjai said. "I came to this country as a 21-year old refugee (from Hungary) and have been lucky to make a life of science and teaching. My recent appointment as University Professor was a wonderful honor by the UC system for my research and teaching, and now the country has honored me. Both the University of California and the United States have been very good to me throughout my career, and I am gratified that I have been able to give something back through my work."

The National Medal of Science was established in 1959 as a Presidential Award to be given to individuals "deserving of special recognition by reason of their outstanding contributions to knowledge in the physical, biological, mathematical, or engineering sciences." This year's awards bring to 401 the total number of science medals awarded since their inception.

Somorjai has also been named the 2002 Faculty Research Lecturer by Berkeley's Academic Senate—recognition of his mentoring to generations of students who today constitute the leading lights of surface science and catalysis in academic institutions and industrial organizations worldwide. In addition to his position in the chemistry department, he is also a senior scientist of the materials science division and group leader of the surface science and catalysis program at the Lawrence Berkeley National Laboratory.

Carlos Bustamante

Bustamante, who is also professor of molecular and cellular biology and of physics and head of the advanced microscopies department in the physical biosciences division of LBNL, studies the dynamics, structure and kinetics of molecular motors and nucleo-protein assemblies using atomic force microscopy and optical tweezers, a laser-driven device capable of manipulating individual molecules.

Bustamante and his colleagues use these cutting-edge technologies to measure directly the forces that hold together molecular structures and the physical stresses and strains generated during the course of chemical and biochemical reactions. Their goal is to gain a better understanding of how biological molecules fold.

Charles B. Harris

Harris, who is also a faculty senior scientist in the chemical sciences division at LBNL, uses extremely fast, pulsed visible and infrared lasers to study the dynamics of chemical reactions in liquids and the properties of electrons on surfaces and at interfaces on the femtosecond timescale. In many cases he and his students also develop the theoretical basis for their experiments.

"It is an honor to be recognized," said Harris. "Of course, the greatest share of this honor should go to the outstanding students and postdocs whom I have had the pleasure of working with over the years."

Election to membership in the Academy is considered one of the highest honors that can be accorded a U.S. scientist or engineer, and is recognition of distinguished and continuing achievements in original research.

Whaley Studying Qubits

Birgitta Whaley, professor of chemistry, has recently received a $4.5M grant to lead a group of six investigators from physics, chemistry, and electrical engineering at Berkeley in studies to develop quantum information processing in the solid state. The grant is being awarded through the Information Technology Research (ITR) competition at NSF, and is entitled "Exploration and Control of Condensed Matter Qubits." It carries with it an outreach component, for which the researchers will hold workshops for science journalists in collaboration with the school of journalism.

Computers work by performing operations on bits, which store either a 1 or a 0. As computers get smaller, however, the ability to distinguish between the 1 or 0 state gets more difficult. Ultimately, in quantum computers, bits will be replaced by qubits, which are fundamental quantum logic units that can be both 1 and 0 at the same time. However, controlling qubits and harnessing them for computing ability is still a matter of active research.

College Updates and Noteworthy News

Chemical engineering professor **Alexis Bell** is the 2002 William G. Lowrie Lecturer at the Ohio State University.

Chemistry professor **Carolyn Bertozzi** is receiving the Irving Sigal Young Investigator award of the Protein Society at their national meeting in August.

Elton Cairns, professor of chemical engineering, gave an invited lecture at the Technical University of Graz in Austria in celebration of the 80th birthday of Karl Kordesch, a pioneer in fuel cell development.

Chemical engineering professor **Enrique Iglesia** gave the keynote lecture for the Symposium on Natural Gas Conversion held during the 2002 spring meeting of the American Chemical Society. He was also elected to serve on the National Research Council Committee on "Vision 21 Department of Energy Research and Development Program."

Assistant professor of chemistry **Jay Groves** has received the Searle Scholars award, which will provide $240,000 in research funds for his lab over the next three years. He will use this award to explore unifying principles that govern inter-cellular communications.

National Sciences and Engineering Research Council of Canada fellowships were awarded to graduate students **Jennifer Murphy** from **Ron Cohen**'s group and **Amanda Cole** from **Kristie Boering**'s group.

John Prausnitz, professor of chemical engineering, is the recipient of the Rossini Award of the Union of Pure and Applied Chemistry (IUPAC). He will present the Rossini Lecture at the international meeting of IUPAC in Rostock, Germany in late July.

David Schaffer, assistant professor of chemical engineering, received the Chemical Engineering Excellence Award for Academic Teaching from the Northern California AIChE.

Andrew Streitweiser, emeritus professor of chemistry, has received a three-year ACS Petroleum Research Foundation grant.

2001- 2002 Staff Retirees

After more than 33 years at Berkeley, 24 of them in the college of chemistry, **Virginia Mohler**, human resources manager for the college, will be retiring July 1st. "It has been an exciting place to work," she said, "but I'm ready to start a new adventure." She plans to keep busy and take some classes in her soon-to-be-free time.

Also, **Willie Weaver** retired October 1, 2001, after 40 years in the college. He worked in the storerooms and provided support for the undergraduate organic chemistry labs.

"We very much appreciate their decades of dedicated service and the very real contributions that Virginia and Willie made to the work of the college," said Dean Clayton Heathcock.

ChevronTexaco Undergraduate Research Symposium

The Coalition for Excellence and Diversity in Mathematics, Science and Engineering sponsored a symposium on May 2nd for the ChevronTexaco undergraduate research program. Faculty, staff and families of the students learned about some of the interesting research being done by the participating students.

The speakers were **Tomás Eggers**, civil engineering, who studied bioremediation; **Oscar Garcia**, chemical engineering, who worked with **John Newman** to measure reversible heat in rechargeable battery electrodes; **Abdul Kanu**, chemistry, who studied chelation of ions with **Kenneth Raymond**; **Evan Jorge Pineda**, mechanical engineering, who studied the new fabric Zylon; and **Amy Wong**, bioengineering, who worked with **Jay Groves** on spontaneous pattern formation at a membrane synapse.

Dr. Gary Masada, President of Chevron Research and Technology, and Professor Caroline Kane (far right) pose with the ChevronTexaco undergraduate researchers: Amy Wong, Oscar Garcia, Tomás Eggers, Abdul Kanu and Evan Jorge Pineda.

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@cal: A New Alumni Online Community

The campus has recently launched @cal, a new way for alumni to keep in touch with friends and colleagues from Cal no matter where they are.

The project started with the idea that Cal alumni should be able to affirm their lifelong connection to the university with a berkeley.edu e-mail identity. That idea spawned a full-scale online alumni portal with a suite of free services including e-mail forwarding with the berkeley.edu domain, an online directory, e-mail list discussion groups, and a career network.

The college of chemistry alumni can access the community through the main gate at **cal.berkeley.edu**, or through the chemistry@cal page at **chemalum.berkeley.edu**, which mirrors the campuswide site in look and feel but contains news and information geared towards chemistry and chemical engineering alumni.

Membership is free to Cal grads and attendees as well as California Alumni Association members. Eligible UC Berkeley students may participate in the career network.

Looking at the Water's Surface

The basic structure of water is well known: H_2O, held together by hydrogen bonds. But the short-lived structures formed when many millions of water molecules get together in a glass of water still remain a mystery—particularly as regards the liquid water surface, which covers 70 percent of our planet.

Scientists in the college of chemistry, using the Advanced Light Source at LBNL, have used novel spectroscopic techniques to examine the structure of water at the liquid surface. Using liquid microjet technology to introduce liquid water into a high vacuum X-ray experiment, chemistry professor **Richard Saykally**, graduate student **Kevin Wilson**, and their colleagues were able to characterize water molecules at the surface and they identified a new interfacial species: acceptor-only water molecules that have two free OH bonds and are in dynamic equilibrium with the vapor.

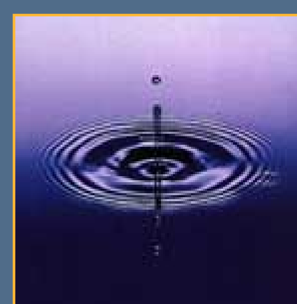

photo by Kelly Knudtson

They hope to use this new knowledge to develop a more detailed understanding of environmentally important surface processes such as evaporation, condensation, and uptake of gases.

The *NEWSLETTER OF THE COLLEGE OF CHEMISTRY* at UC Berkeley is published several times each year to support the college's mission of providing excellent teaching, research and public service in the fields of chemistry and chemical engineering.
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