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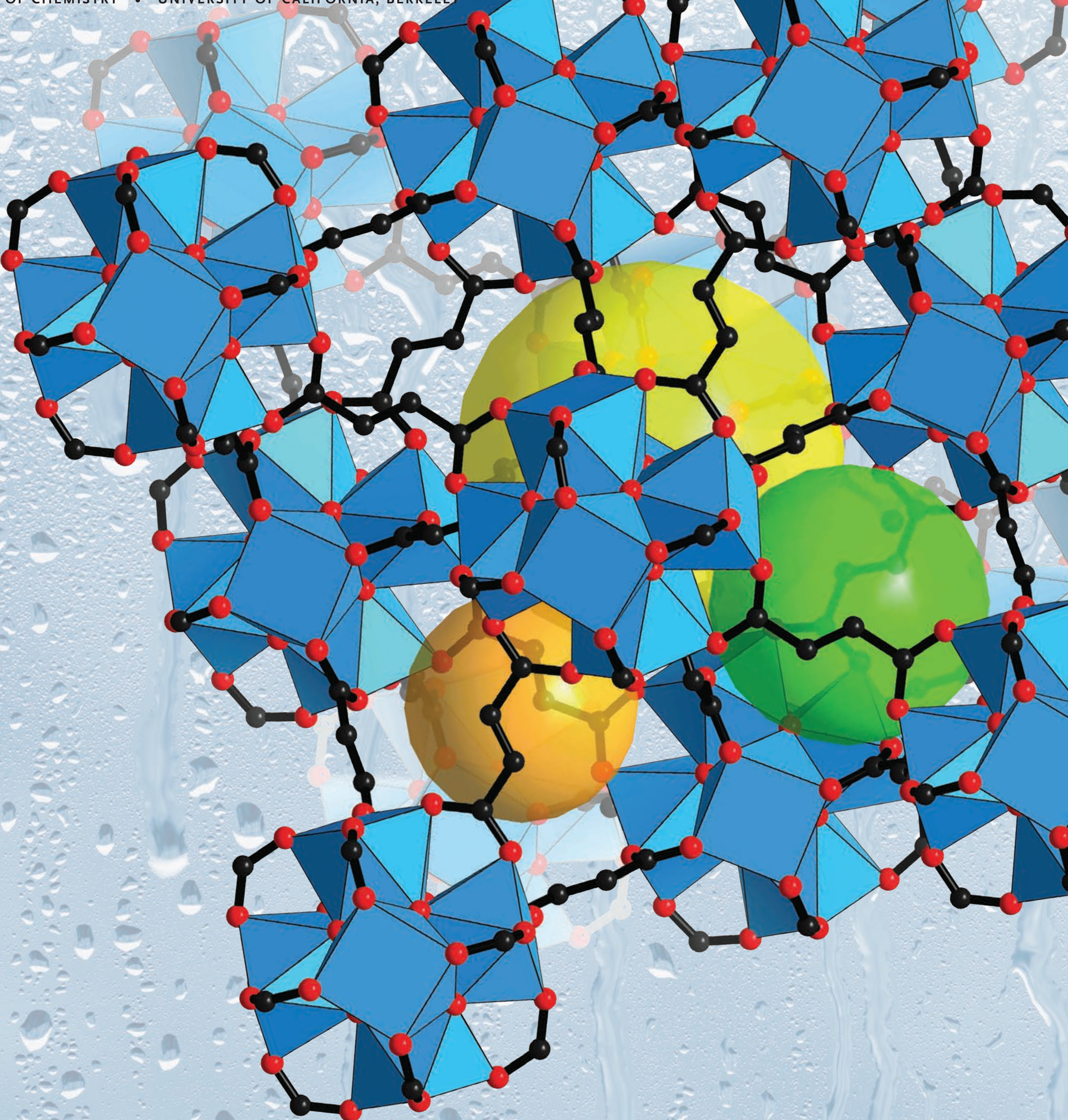
Catalyst

Spring/Summer 2017 Volume 12 • Issue 1

COLLEGE OF CHEMISTRY • UNIVERSITY OF CALIFORNIA, BERKELEY



The frontiers of research

- **OMAR YAGHI**
  Water for the 21st century
- **DAVID GRAVES**
  Cold atmospheric plasmas
- The Pitzer Center welcomes three theoretical chemists

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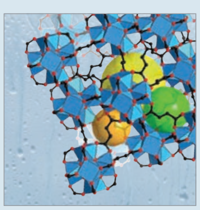

ON THE COVER

Illustrated here is a metal-organic framework, or MOF. The Yaghi group has recently developed a device that uses a MOF to adsorb water from the atmosphere and release it to provide drinking water.

ALL TEXT BY MICHAEL BARNES UNLESS OTHERWISE NOTED.

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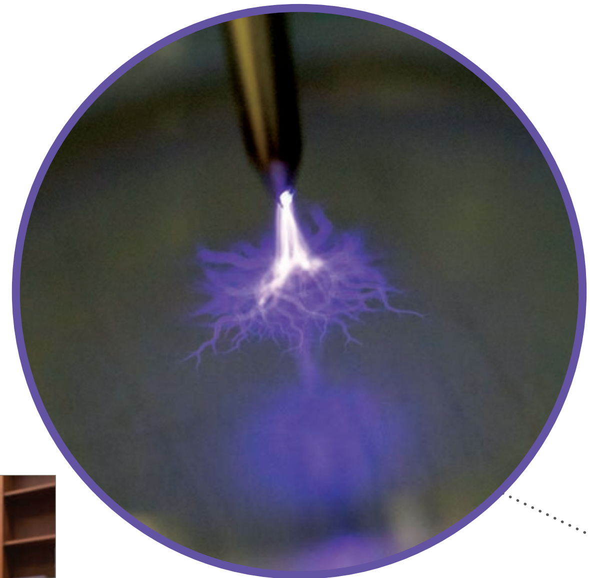

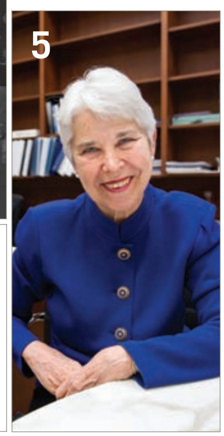

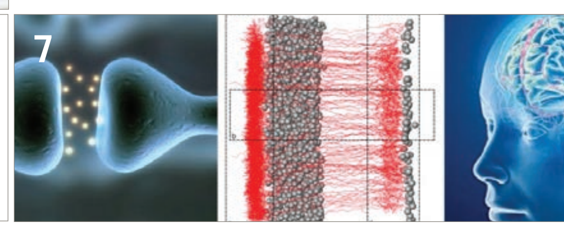

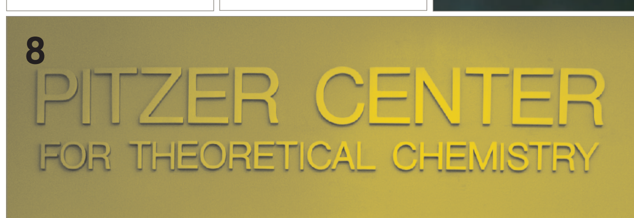

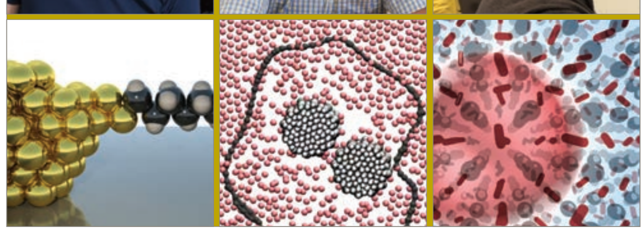

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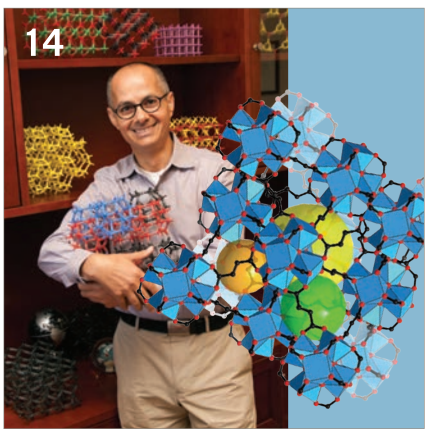
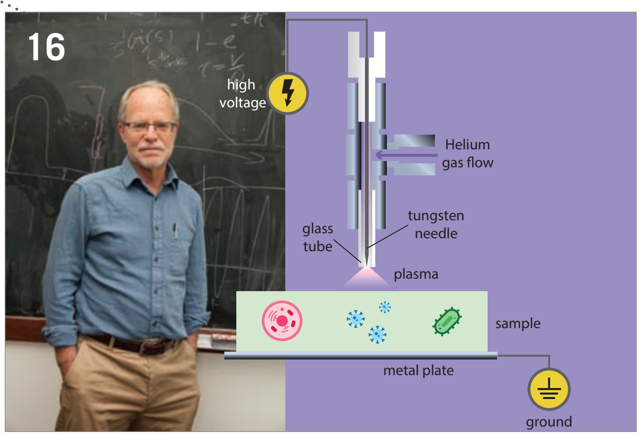
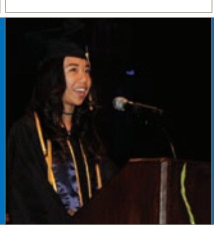
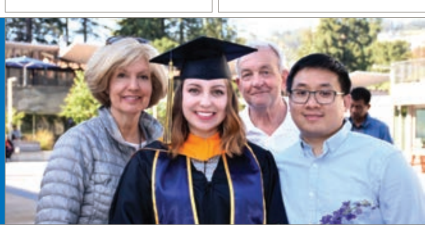
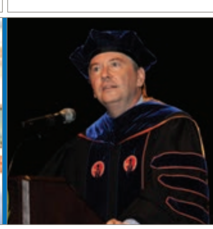
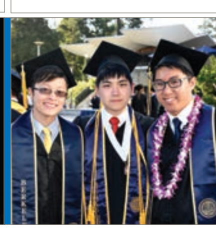












Building Upon Milestones

DOUGLAS S. CLARK
Dean, College of Chemistry
Gilbert N. Lewis Professor

It's been an eventful academic year as usual: our faculty have been recognized with numerous prestigious awards; we've also had retirements and new staff arrivals, celebrations, and memorials.

In the spring 2016 issue of *Catalyst,* you read about the plan to construct a joint chemistry and engineering building on the Donner Lab site. After consultation with campus administrators, we have now brought in another partner—the College of Natural Resources (CNR)—for a building in a new location.

The new COC/COE/CNR building, provisionally called the "Berkeley Science Hub," will be constructed on the site of the current Tolman Hall, situated in the northwest quadrant of campus. The Tolman Hall site will offer many advantages over the Donner location in terms of cost, benefits, and size of the footprint.

Also noteworthy is the first close of the Berkeley Catalyst Fund (see the alumni profile in the Spring 2016 *Catalyst*), which officially secured its first round of financing and is now up and running. This represents a major milestone and a new model for promoting entrepreneurism within the chemical sciences community, and I congratulate the many people whose combined vision, dedication, and determination made it possible.

This spring the American Chemical Society designated the Mars Infrared Spectrometer (IRS) as a National Historical Chemical Landmark; a plaque and mockup of the spectrometer were unveiled in the lobby of Pimentel Hall in May. In the late 1960s chemistry professor George Pimentel, along with Kenneth Herr, who worked in his lab, designed and built the Mars Infrared Spectrometer, two of which were carried aboard NASA spacecraft Mariner 6 and 7 to examine the red planet.

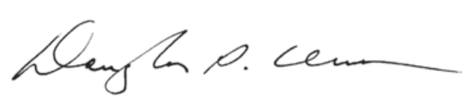
It is largely thanks to Pimentel and Herr that we know as much as we do today about Mars and its chemical make-up, including the fact that there was once water on its surface. This is the second National Historic Chemical Landmark in the College—Gilman Hall being the first—and exemplifies the far-reaching impact of chemistry at Berkeley.

Other distinguished faculty, among many recognized this year, include chemistry professor Robert Bergman, who was awarded the Wolf Prize, and Jennifer Doudna (Chemistry and Molecular & Cell Biology), who received the Japan Prize. (Jennifer also was our commencement speaker.) Bob Bergman retired in July of 2016 although he is still active in the Department.

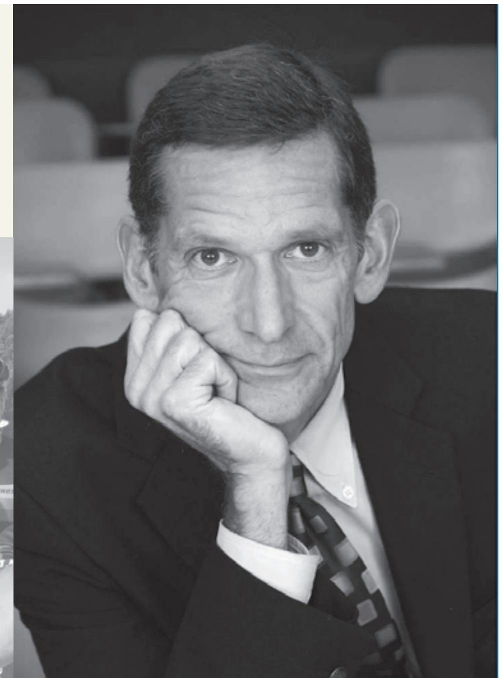
Also retiring this July are chemistry professors Alex Pines and Marcin Majda. Alex, like Bob, will still pursue his research interests and has agreed to teach Chem 1A this fall. Marcin served admirably as undergraduate dean for nine years. With Marcin stepping down as undergraduate dean, chemistry professor John Arnold has graciously agreed to step into this role. We also lost two colleagues, chemistry professors Ignacio "Nacho" Tinoco and David Chandler; you will read more about them in this issue.

Turning now to a new member of our ranks, I welcome our new assistant dean of College Relations and Development, Laurent "Lo" de Janvry, who joined the College a few months ago. I would also like to thank Mindy Rex, who has served in this position over the past several years and will now focus her attention on major fund raising.

I also bid farewell to the editor of *Catalyst,* Michael Barnes, who retired in July. Michael has been a distinguished science writer, a skilled photographer, a gifted editor, and always a wonderful conversationalist—thank you for your contributions to the College—we will miss you.



Catalyst magazine's editor, writer and photographer retires



We are very sorry to announce that, after eleven years roving the corridors of the College of Chemistry—and 20 years serving in the UC system—Michael Barnes, the principal editor, science writer and photographer for *Catalyst* magazine, is retiring. Michael has fulfilled his various roles with a singular blend of protean intellect, keen aesthetic sensibility, wide-ranging curiosity and delight in the unusual. We will miss him very much.

Michael is an alum of Cal. A Ph.D. student in economics at the time of his wife's untimely death in 1993, he left graduate school in order to raise his baby son. After a stint at UCOP as a research analyst, he arrived at the College of Chemistry in 2006, just in time to give our alumni magazine a 21st-Century overhaul.

One of his most important initial tasks was to find a designer with whom he could partner to create outstanding layouts for our magazine. His search identified Alissar Rayes—an equally talented, independent designer with not only a B.F.A. from the Academy of Art University in San Francisco but also a B.S. in chemistry from the American University of Beirut, Lebanon. Michael's decision to bring Alissar onto the team has borne fruit many times over. Theirs has been a brilliant collaboration, producing 20 memorable covers since Spring 2006, distributed each year to more than 15,000 alumni and friends world-wide.

As an editor and writer, Michael has purposefully chosen to create his in-depth science features with an emphasis on the human side of things, always remaining scientifically accurate and intellectually cogent. His ability to understand and translate into lay language the widely varying research endeavors of our faculty, feature after feature, year after year, while simultaneously bringing their personalities to life and illustrating them with first-rate photographs, has been remarkable.

Many people here have benefitted from his careful, creative and sensitive approach.

In and out of the office, Michael is all eyes and ears. He watches, he listens, he is constantly alert to the possibility of a diverting anecdote, a great photo, a significant story. He gathers material wherever he goes. The result is a vast reservoir of knowledge. For those of us who remember the multi-volume sets of our youth, Michael is a walking *World Book Encyclopedia*.

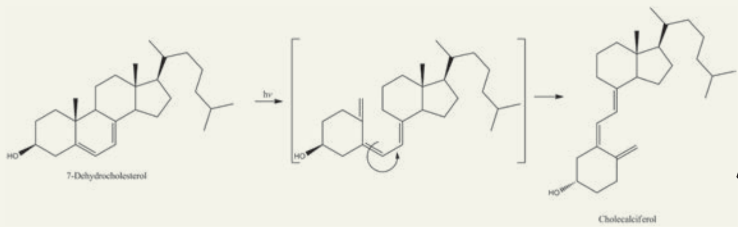
And away from work, Michael also covers ground. He is an energy conservationist, a public servant and an athlete. He is—no surprise here—a firm believer in fighting global climate change. With solar panels installed on his roof and clothes drying on a line, he sells energy back to PG&E. His familiarity with economic and scientific issues makes him a valuable public servant. He is now in his second term as a council member for the City of Albany, CA, where he focuses on evidence-based decision-making and writes a public service blog on issues before the council.

Moreover, Michael is an ardent bicyclist: he bikes to work; he bikes for pleasure; he participates in cycling events throughout California on weekends and vacations. He has twice won jerseys for finishing the Mt. Diablo Challenge (an 11-mile event that climbs in elevation from 600' to 3,850' at the summit) in fewer minutes than his age in years.

Recalls chemistry professor and fellow bicyclist John Hartwig, "One day, at the bottom of the back side of the Berkeley Hills, I encountered Michael. Meeting him while bicycling is one of my nightmares. It meant I had to ride up the backside of the hills with him, after having ridden 30 miles (actually more like 25, but 30 sounds a bit better) of hills already. On this trip up, to keep his pace I was breathing so hard I could barely talk, but Michael calmly pedaled and told me about his future plans and, sadly, his decision to retire. As always, that day, it was a pleasure and memorable to spend time talking with Michael, even if it involved an uphill battle and sad news."

We regret Michael's departure from the College and wish him the very best as he continues to cycle through life.

NEW & NOTABLE



Leone lab develops ultrafast devices to explore vitamin D3, other molecules

On a sunny day, energetic UVB photons hit a certain type of organic molecule, 7-dehydrocholesterol, in your skin. These molecules absorb the photons, causing a ring-opening reaction that leads to the creation of vitamin D3. Thanks to recent research in the Leone lab, we are gaining new insights into how the ring-opening reaction takes place.

In order to better understand such reactions in real time, the Leone lab's Andrew Attar and colleagues are developing ultrafast spectroscopic devices that not only fit on a table top, but also produce the hard-to-generate UVB photons that allow your skin to make vitamin D3.

SPECTROSCOPY

UC BERKELEY

Carol Christ appointed Berkeley Chancellor

Carol Christ, who joined the UC Berkeley faculty in 1970 as an assistant professor of Victorian literature, has been confirmed by the UC Board of Regents as the campus's 11th chancellor. Her tenure as chancellor was effective July 1.

A popular, highly regarded administrator and scholar, she will be the first female chancellor in Berkeley's 149-year history. During her first three decades at Berkeley, Christ (rhymes with "list") served in a wide range of leadership roles, rising from English department chair to executive vice chancellor and provost, the campus's No. 2 administrative position.

She headed east to lead Smith College as president from 2002 to 2013, then returned to Berkeley in 2015 to direct the Center for Studies in Higher Education. She reassumed her former role as second in command last May on an interim basis.

Since resuming her former duties as executive vice chancellor and provost, Christ has been instrumental in tackling what had been a $150 million budget deficit, working tirelessly with constituencies across the campus to identify efficiencies and new income streams.

EBI

ENERGY BIOSCIENCES INSTITUTE.org

EBI, Shell sign $25 million partnership to fund new energy tech research

UC Berkeley's Energy Biosciences Institute has entered into a five-year research agreement with Shell International Exploration and Production to fund research that meets the growing demand for energy in ways that are economically, environmentally and socially responsible.

The agreement is to spend up to $25 million over five years on fundamental research in the areas of global energy transition and new energy technology.

Lisa Yang and Stan Reeder serve up attitude and cupcakes at a tabling event for the Class of ’17 Campaign.

VICTORIA JASCHOB PHOTO

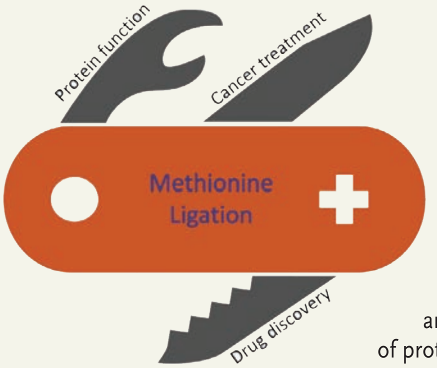
Class of ’17 Campaign

This year’s College of Chemistry Class Campaign raised funds to purchase umbrella tables for the Chemistry Plaza, increasing the area of the college where students can gather to study, eat and relax.

The Class Campaign committee, Stan Reeder, Maureen Morla and Lisa Yang, were leaders from the college’s two main student groups: co-ed fraternity Alpha Chi Sigma (AXE), and the student chapter of the American Institute of Chemical Engineers (AIChE). The committee selected the focus for the campaign and set a goal of $4,000, which they easily passed, raising $4,600.

The Class Campaign was started in 2009 as a way for students to give back to the college before graduating and to leave something of lasting value for classes to come. Previous campaigns have focused on renovating the undergraduate labs in Latimer Hall and updating the undergraduate curriculum to include greener lab practices.

GIVING BACK



Chang and Toste invent a new type of chemical Swiss army knife for proteins

Berkeley chemistry professors Chris Chang and Dean Toste have developed a new method of protein ligation, the joining of molecules with proteins.

The technique, called Redox Activated Chemical Tagging (ReACT), involves the modification of proteins by attaching chemical cargos to the amino acid methionine. ReACT functions as a new type of chemical Swiss army knife that supports a wide variety of fields, spanning fundamental studies of protein function to applications in cancer treatment and drug discovery.

INNOVATION

Klinman wins Gibbs Medal

Chemistry emerita professor Judith Klinman has received the 2017 Willard Gibbs Medal Award of the Chicago Section of the American Chemical Society.

Klinman was cited for her groundbreaking discoveries in enzyme catalysis, including the application of kinetic isotope effects and the discovery that protein structures have evolved to catalyze effective quantum mechanical tunneling.

The Willard Gibbs Medal Award was founded by William A. Converse, a former Chicago Section Chair, in 1910 and first awarded in 1911. Gibbs was chosen to be the model for the award as an outstanding example of creativity in scientific investigation.

CHEMISTRY AWARD

Arnold appointed new undergraduate dean

The College of Chemistry welcomes chemistry professor John Arnold as the new Undergraduate Dean, effective July 1. Arnold, who brings to this position a strong record of teaching and mentoring and a proven dedication to students, will build upon the tradition of personalized advising within the college.

UNDERGRADUATE ADVISING

STARTUP

Raymond receives DOE grant to study lanthanide luminescence

Chemistry's Ken Raymond has just received a three-year, $450,000 grant from the Department of Energy to continue his research on energy transfer in lanthanide luminescent complexes.

The grant-funded research aims at investigating the energy transfer process in lanthanide complexes with organic ligands through a unique combination of experimental techniques, time-resolved UV-visible light spectroscopy and X-ray emission spectroscopy.

Raymond's startup, Lumiphore, has licensed its lanthanide fluorescence technology to several biomedical companies.

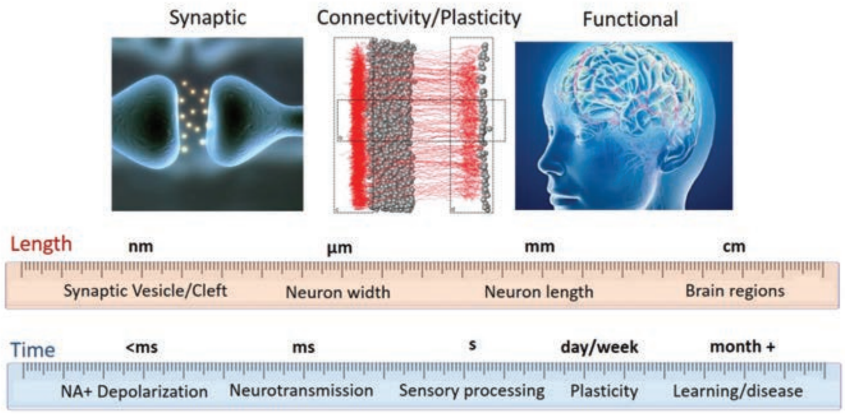
INTERNATIONAL AWARD

Doudna wins Japan Prize

Berkeley's Jennifer Doudna and Emmanuelle Charpentier of Germany's Max Planck Institute have been awarded the 2017 Japan Prize for their invention of the revolutionary gene-editing technology known as CRISPR-Cas9, which has swept into research labs around the world and is already yielding new therapies for cancer and hereditary diseases.

Doudna and Charpentier each will receive a certificate of recognition, a commemorative gold medal and 50 million Japanese yen (approximately $420,000). The honors were presented at an award ceremony on April 19 in Tokyo.

BIOMEDICAL RESEARCH



College faculty win CZ Biohub grants

Thirteen UC Berkeley faculty, including the college's Markita Landry, Ke Xu and Wenjun Zhang, are among 47 new investigators chosen by the Chan Zuckerberg Biohub to receive up to $1.5 million each over the next five years to conduct cutting-edge biomedical research—with no strings attached.

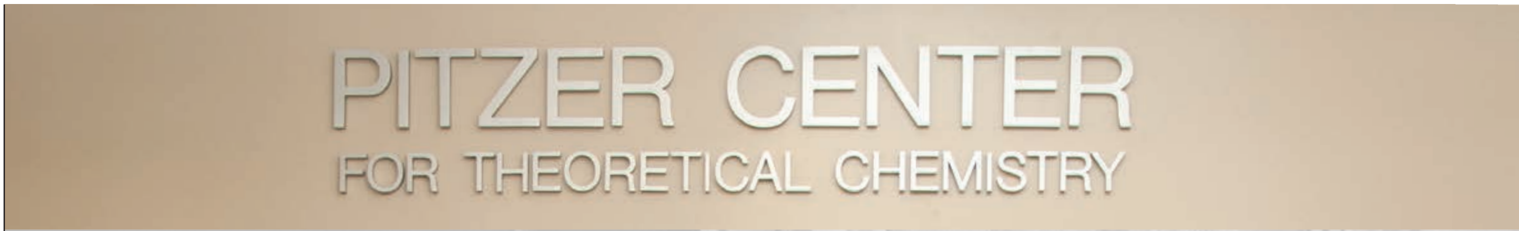
The CZ Biohub was established in September 2016 with $600 million over 10 years from Facebook founder and CEO Mark Zuckerberg and his wife, pediatrician Priscilla Chan, and operates as an independent nonprofit medical research organization collaborating with UC Berkeley, Stanford University and UC San Francisco to fund research.

LANDMARK

College earns ACS historical designation for Pimentel spectrometer

On May 15, the Mars/Mariner infrared spectrometer was officially designated an American Chemical Society National Historic Chemical Landmark.

The honor was bestowed 50 years after the first model of the instrument was assembled at the College of Chemistry by a team led by chemistry professor George Pimentel and his former Ph.D. student Ken Herr. Two identical versions of the Pimentel/Herr spectrometer flew past Mars in late 1969, one on board the Mariner 6 and the other on board the Mariner 7 spacecraft.



Thanks to the very generous support of the Pitzer Family Foundation, the Kenneth S. Pitzer Center for Theoretical Chemistry was created in 1999 as both a facility and a program.

Bringing together the research groups of a remarkable core of faculty of theoretical chemists and chemical engineers who were previously scattered throughout the college, the Pitzer Center has fulfilled its promise as one of the world's preeminent centers for research in theoretical chemistry.

Gilman Hall was built in 1917 and, although a beautiful old building—a National Historic Chemistry Landmark, the site of Glenn Seaborg's discovery of plutonium—its infrastructure cannot be modified sufficiently to support modern wet labs.

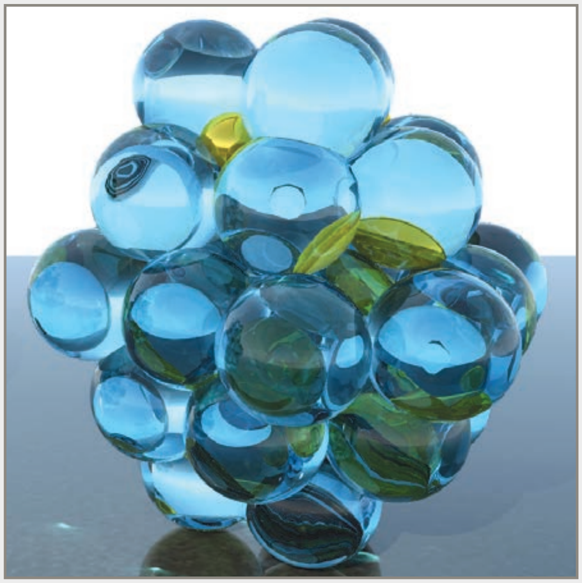
The renovation of 2,300 square feet for expanded theoretical chemistry facilities is an ideal use of Gilman Hall. The Pitzer Center Annex on the third floor of Gilman Hall accommodates 26 new student workstations as well as a conference room.

The new workspace for the different theoretical groups, the seminar rooms and the common space are providing exactly the kind of rich, interactive research environment that was originally envisioned and that has been made possible by the Pitzer Family Foundation.

Three new theorists—Eran Rabani, Kranthi Mandadapu and David Limmer—call the Pitzer Center home. You can read about them and their work on the following pages.

Faculty, students and staff celebrated the opening of the new Pitzer Center Annex on the third floor of Gilman Hall in November, 2016.

Below right: **This image portrays a colloidal nanocrystal that has been doped with impurity atoms. Doping of semiconductors enables their widespread application in micro- and opto-electronics. The Rabani group is applying these principles to colloidal semiconductor nanocrystals.**



Eran Rabani finds a scientific home in the Pitzer Center

Theoretical chemists can be like the quantum realms they study. Each is unique and difficult to categorize. The College of Chemistry's theorists can be loosely divided into three groups—those who use and develop statistical mechanics, those who study and develop quantum dynamics, and those who develop and apply electronic structure theory. Says chemistry professor Eran Rabani, "I work in all three subdisciplines, so in that sense I hope to be a bridge between different research groups."

Born in Jerusalem in 1967, Eran Rabani's childhood was punctuated by travels abroad as his father, a scientist, paid extended visits to Berlin, Copenhagen and the Argonne National Laboratory near Chicago. Rabani graduated from high school back home in Jerusalem, served for three years in the IDF, and returned to Jerusalem to earn his B.Sc. *summa cum laude* at the Hebrew University of Jerusalem in 1991. He remained at the Hebrew University for grad school and completed his Ph.D. in theoretical chemistry in 1996.

In 1996 Rabani moved to Columbia University for a three-year postdoctoral appointment. He had barely set foot in New York City when Louis Brus arrived at Columbia from Bell Labs. While at the labs, Brus had invented colloidal quantum dots and had also been the post-doctoral mentor of Paul Alivisatos, Berkeley Executive Vice Chancellor. "After I arrived at Columbia," says Rabani, "I knocked on Brus' door and ask him to 'teach me about nanocrystals.' We talked every day."

In 1999, Rabani joined the faculty at Tel Aviv University, Israel. He came to Berkeley first as a Visiting Miller Research Professor in 2010–11 and was permanently lured to the College of Chemistry in 2014. He returns to Tel Aviv often where he maintains his position as the director of the Sackler Center for Computational Molecular and Materials Science.

Rabani's research spans theoretical chemistry and physics, and he sees an important distinction between them. "The way you think is important," he explains. "Physics cares about how the world works. It seeks finite universality, or explaining the most observations with the simplest and most general theories. Chemistry is more about finding exceptions. It is often the details that matter more. I enjoy both worlds."

Research in the Rabani group involves the development of theoretical and computational tools to investigate fundamental properties of nanostructures. This includes the structural, electronic and optical properties of semiconducting nanocrystals. The Rabani group has also been involved in the study of several aspects of the self-assembly of nanomaterials, a critical process in fabricating and controlling spontaneously organized nanoscale devices and one of the major challenges of nanotechnology.

Rabani has published several papers with departmental colleagues Alivisatos and Phill Geissler on the characteristics of quantum dots and nanocrystals. His group has also made fundamental breakthroughs in simulating the complex interactions of quantum mechanics's many-body problem.

Says Rabani, "The Pitzer Center is a unique environment. Being around so many other theorists helps create synergies—we feed off each other. Berkeley is the best science university in the world. If you are interested in basic science you cannot ask for more..."

Kranthi Mandadapu on continuum and fluctuations

Kranthi Mandadapu realized early in life that he was good at math. He was born in 1984 in a small town in Andhra Pradesh, a southeastern state in India that lies along the Bay of Bengal. Says Mandadapu, "My father was a clerk and my mother a school teacher. She was an inspirational biology teacher, but when I was young she was assigned to teach maths. It was hard for her at first, but I helped her—I enjoyed explaining things. In the end she enjoyed teaching maths, too."

At age 15 Mandadapu scored so highly in his secondary-school board exams—seventh out of 600,000 students—that he won a scholarship to attend a boarding school in the city of Hyderabad. Two years later, in 2001, he started his undergraduate studies at the Indian Institute of Technology at Madras (Chennai). There he studied civil engineering.

Civil engineers are responsible for understanding and modeling the forces that affect dams, buildings, and other massive permanent structures. Perhaps nothing revealed the impermanence of these solid objects like the earthquake and tsunami that struck Chennai early on Sunday morning, the day after Christmas, 2004.

Although his institute was far enough inland to escape the floodwaters, Mandadapu vividly recalls the earthquake and how ill-at-ease it made him feel that morning. But life continued, the city slowly recovered, and he earned his B.S. in civil engineering in 2005.

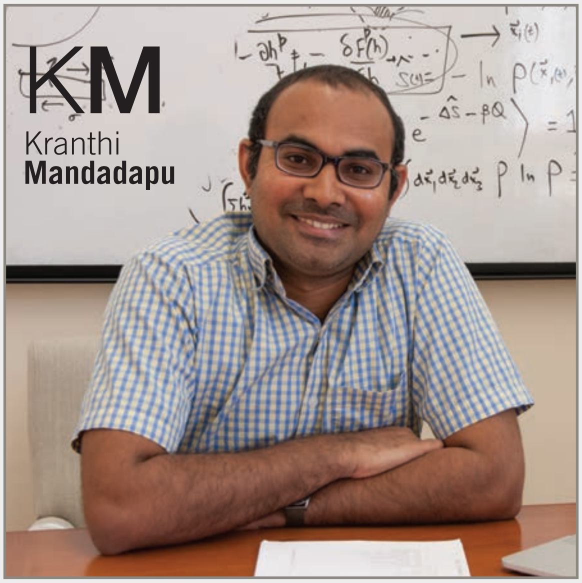
Mandadapu came to Berkeley's College of Engineering in the fall of that year. He earned his M.S. in civil engineering and switched to mechanical engineering for his Ph.D. studies at Berkeley. He worked with Panayiotis Papadopoulos and wrote his thesis on non-equilibrium molecular dynamics, graduating in 2011.

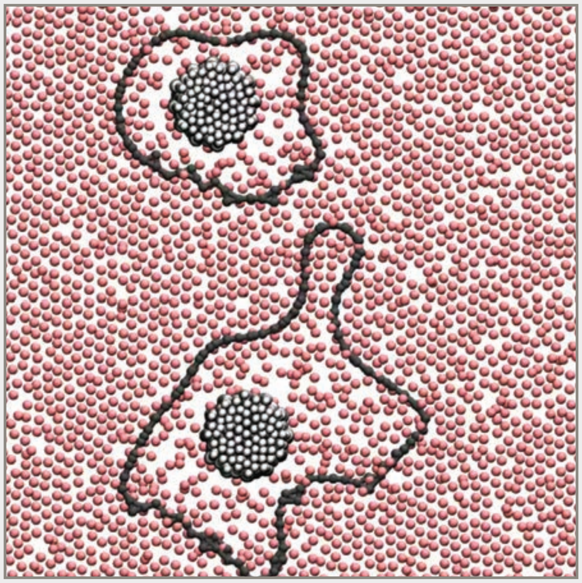
Classical, or Newtonian, mechanics—the science of describing the motion of objects under the influence of different forces—includes solid mechanics, fluid mechanics and statistical mechanics. Mandadapu has studied them all.

The statistical realm and the continuum realm require different approaches. Mandadapu explored continuum mechanics as a postdoctoral scholar at Sandia Labs in Livermore, then statistical mechanics, starting in 2013, during a second postdoc with the late David Chandler in the college. He also found a mentor in campus biophysicist George Oster.

As Chandler noted in his authoritative introductory textbook, statistical mechanics "is the theory with which we analyze the behavior of natural or spontaneous fluctuations." Mandadapu had started with civil engineering and the apparent solidity of large structures. Along the way, he grew interested in the realm of microscopic fluctuations, how bacteria move, and how proteins in biological membranes can assemble.

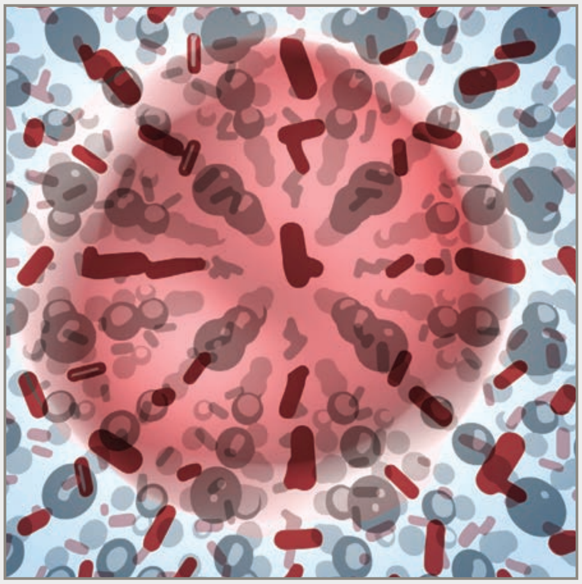
Mandadapu joined the CBE faculty as an assistant professor in 2016. He keeps one foot in the microscopic realm of statistical mechanics, and the other in the macroscopic realm of solid and fluid mechanics. "I am trying to solve problems that span a range of length and time scales," he notes. "Every problem takes a year to solve. As I get to know them, I cannot help but fall in love with these problems."





The clustering of proteins in biological membranes is necessary for critical life processes like cell signaling and immunological response. The Mandadapu group is exploring the mechanisms that generate powerful forces of assembly and mobility for transmembrane proteins in lipid bilayers.

David Limmer returns to Berkeley



Snapshot from a molecular dynamics simulation of an excess charge in a hybrid organic-inorganic perovskite lattice. The charge shown with a red tint in center forms a polaron in the hybrid perovskite lattice.

Theoretical chemist David Limmer was born in 1986 in Clovis, NM, a town of about 40,000 people in the far eastern part of the state, nine miles from the border with Texas.

"Clovis culture" refers to a Paleoamerican group that is credited with giving rise to many later Native American peoples. The opportunity to study Clovis culture at the Blackwater Draw site lured Limmer's father from New York to an archeology program at Eastern New Mexico University in nearby Portales. There he met Limmer's mother, who was from an old homestead family that had lived in the area for decades.

Limmer excelled in math and chemistry in high school, graduating in 2004. For college, he attended the New Mexico Institute of Mining and Technology in Socorro, about 80 miles south of Albuquerque. There he worked with John McCoy, who had earned his Ph.D. with the late theoretical chemist David Chandler at Berkeley.

Says Limmer, "In my third semester I needed some advanced classes that weren't going to be offered, so I spent nine months at Los Alamos National Laboratory where I measured gas flows through polymers. That's where I discovered I wasn't meant to be an experimentalist. I had much better luck applying statistical mechanics models to the problem."

Limmer graduated *summa cum laude* from New Mexico Tech in 2008 with a B.S. in chemical engineering. As the top graduating senior, he won the campus's Brown Award that year. In the fall he began his Ph.D. studies with Chandler in the College of Chemistry.

Limmer completed his thesis with Chandler in 2013. Following a brief transitional postdoc at LBNL, he moved to Princeton University for a second postdoc at the Center for Theoretical Studies. He returned to Berkeley and joined the faculty as an assistant professor in 2016.

Working with colleague Naomi Ginsberg, Limmer is currently exploring an interesting phenomenon of perovskite materials. Synthetic perovskites can be created with a mixture of the halides bromine and iodine that allow their properties to be "tuned," making them useful for photovoltaic cells and other optoelectronic devices.

Says Limmer, "Imagine you are sitting in a dimly lit restaurant where you notice the vinaigrette salad dressing seems to be very well mixed. To get a better view, you shine your cell phone flashlight on the bottle, which causes the oil and vinegar to completely separate. Surprised, you turn off the light, only to see the vinaigrette return to being well mixed.

"That is pretty strange behavior, yet that is what the Ginsberg lab observed in their perovskite materials. If you shine a light on them, the mixed halide ions shift around the lattice until they are separated. This is not useful behavior in a PV material, but might be very useful in constructing optical switches and other sensors."

The Ginsberg and Limmer groups have been working together to explore the basis for this odd perovskite behavior. "This work is an example of a nonequilibrium process with practical importance," says Limmer, "which more generally is what my group is exploring here at Berkeley."

Adventures frontier

BY MICHAEL BARNES

Explorations always seem more tidy in retrospect. Take, for example, the expedition of Lewis and Clark. From our perspective, they blazed a trail across the American West. But if you read their journals, a different picture emerges.

In their own writings they often seem to be lost. They were fortunate to find a competent guide and translator in Sacagawea. And in the end, they did find the Columbia River, which carried them all the way to the Pacific Ocean.

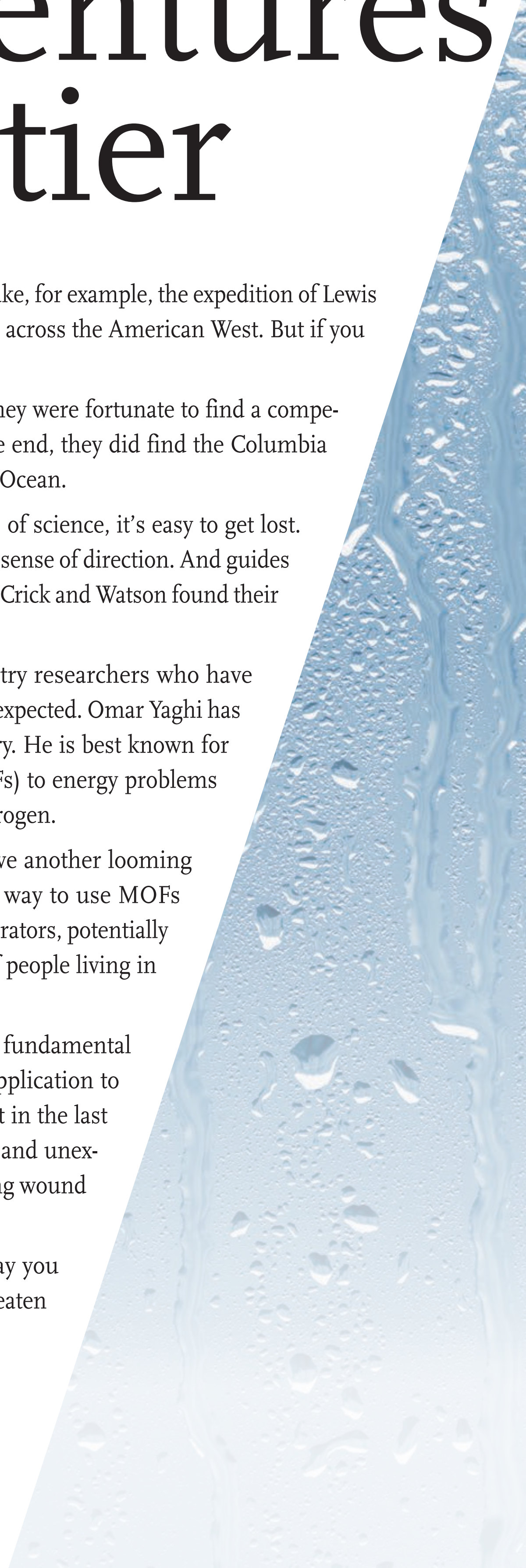
Scientific explorations are similar. On the frontiers of science, it's easy to get lost. Rigorous hypotheses, like compasses, can provide a sense of direction. And guides (sometimes unheralded) can help out along the way. Crick and Watson found their Sacagawea in Rosalind Franklin.

In this feature, we profile two College of Chemistry researchers who have trekked at the frontiers of science and found the unexpected. Omar Yaghi has created a new field in chemistry, reticular chemistry. He is best known for his application of metal organic frameworks (MOFs) to energy problems like the storage of clean-burning methane and hydrogen.

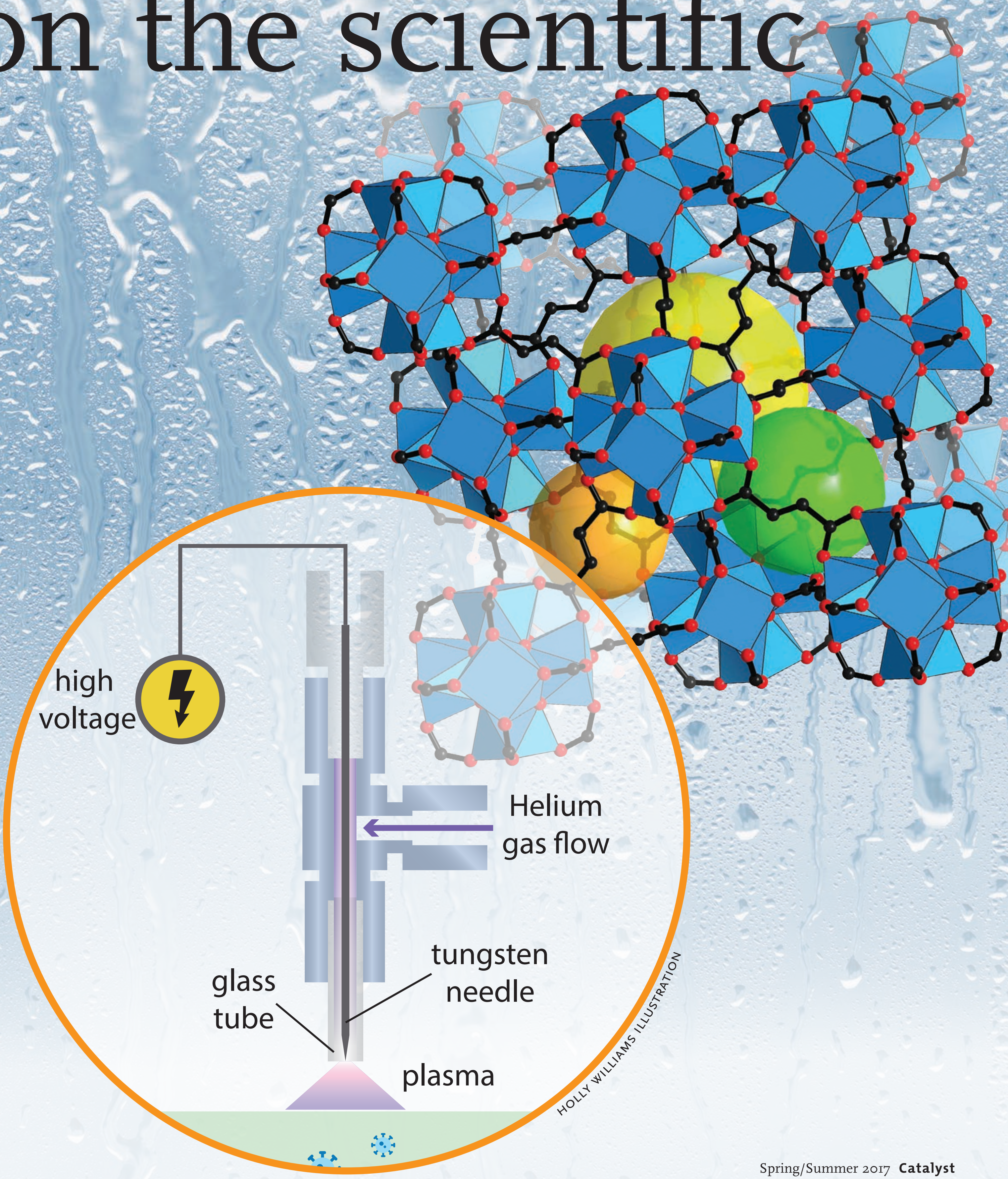
Along the way, Yaghi has found a way to help solve another looming problem—water shortages. He has discovered a way to use MOFs to enhance the efficiency of atmospheric water generators, potentially allowing them to provide clean water to millions of people living in arid climates.

David Graves has spent much of his career doing fundamental research on low-temperature plasmas and their application to semiconductor etching and surface treatments. But in the last decade he has turned his attention to the startling and unexpected biomedical applications of plasmas, including wound healing and cancer therapy.

Research, like life, doesn't always turn out the way you plan. For Yaghi and Graves the discoveries off the beaten path have been part of the adventure.



on the scientific



Wringing drinking water from dry air

The world is running out of clean water. By the end of the century more than 11 billion people are predicted to be sharing the planet. Climate change and sea-level rise will bring salinization of coastal aquifers, the disappearance of the glaciers and snowpack that provide water in dry summer months, and unpredictable shifts in rainfall that will result in both droughts and floods.

Currently, four billion people live with severe water scarcity at least one month of the year. Half a billion people face severe year-round water shortages. In many arid regions of the world, economic development and population growth will stress existing water supplies, leading to less water to drink and less water for crops.

Chemistry professor Omar Yaghi knows something about life in a dry climate. He grew up in Amman, Jordan, where fewer than 10 inches of rain falls in most years. To the east and south lie deserts so arid and austere that they served as a double for the planet Mars in the Ridley Scott movie, "The Martian."

One of the world's most highly cited chemists, Yaghi is using his skills to help provide water to arid regions of the globe. Along with his colleagues and students, Yaghi has developed a new field in chemistry, reticular chemistry. Researchers in this new field have created new materials—intricately structured nanoporous metal-organic frameworks (MOFs), covalent-organic frameworks (COFs) and zeolitic imidazolate frameworks (ZIFs).

These molecular frameworks can be tuned to create materials with specific pore sizes and unique chemical activity. Yaghi has developed MOFs with numerous applications, including capturing carbon dioxide from smokestacks and storing methane for clean-burning trucks. He is now turning his attention to trapping yet another gas, water vapor.

Capturing water from air is nothing new. The Incas were capturing water from fog high in the Andes centuries ago. Both air conditioners and dehumidifiers condense water vapor by passing humid air around a refrigerated coil. Atmospheric water generators, devices that pull drinking water out of the air, use similar techniques, but then purify and store the condensed water. Like refrigerators, all these modern devices require a big share of the electricity used by households.

A new generation of atmospheric water generators, produced by several companies (including Ecoloblue in the Bay Area), have brought down energy requirements. But producing a gallon of water for home use still requires more than one kilowatt hour of electricity. The units typically cost more than a thousand dollars and require expensive filters that must be replaced regularly.

Atmospheric water generators range in size from household units to industrial-scale models that fit on a large truck. These machines work fine in places like the Bay Area where the relative humidity is often 60 percent or greater. Home versions can even be powered by solar panels. However, they are not practical for arid regions where the relative humidity is less than 20 percent.

Yaghi is working to overcome these limitations with a powdered MOF material that will selectively adsorb water from air at low relative humidity and release it when heated. At 30 °C. (86 °F.) and 20 percent relative humidity, there are only six grams of water vapor per cubic meter of air. In those conditions, you would have to wring out every water molecule in a cube of air 5.5 meters (18 feet) on a side to collect just one liter of liquid water. Yaghi's MOF can act as a water vapor concentrator to raise the relative humidity of the air before it is processed to extract drinking water.

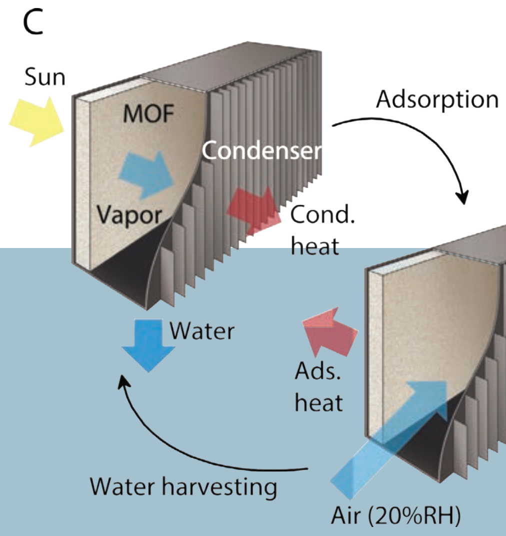
To build a proof-of-concept device, Yaghi enlisted the help of MIT mechanical engineering professor Evelyn Wang. The device contained a five-centimeter square layer of powdered MOF. Left on a rooftop at MIT, the device adsorbed water overnight that was released the next morning by the warmth of the sun and then condensed to liquid water.

Says Yaghi group member Eugene Kapustin, co-author of a recent *Science* magazine paper on the topic, "For now our proof-of-concept device is small and creates a few milliliters of water every cycle. It does not require a condenser—simple air cooling is enough.

"Because of its nanoscale pore size, the MOF may be able to keep out bacteria and other contaminants. These contaminants must be filtered out of the water produced by conventional atmospheric water generators. Further testing of our MOF is ongoing."

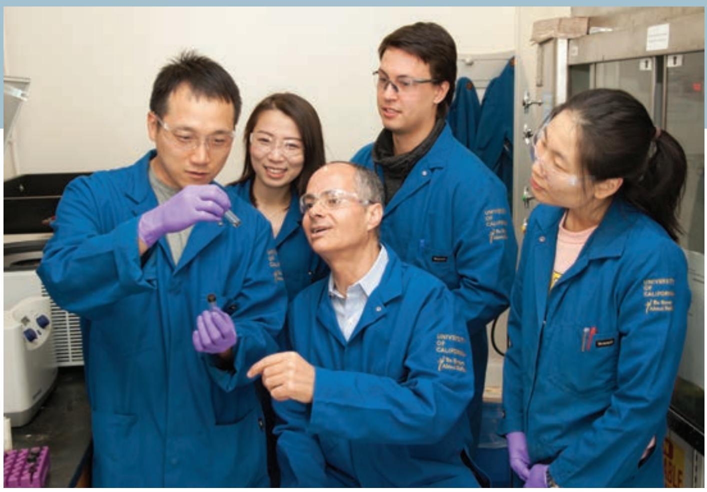
Notes Yaghi, "My group does basic research to discover new materials and develop their interesting properties. Our MOFs can increase the efficiency of atmospheric water generators for use where clean water is scarce. So far the results are encouraging. Perhaps in the next few years we'll see bolt-on MOF-based vapor concentrators that will allow us to push atmospheric water generators further out into the desert."

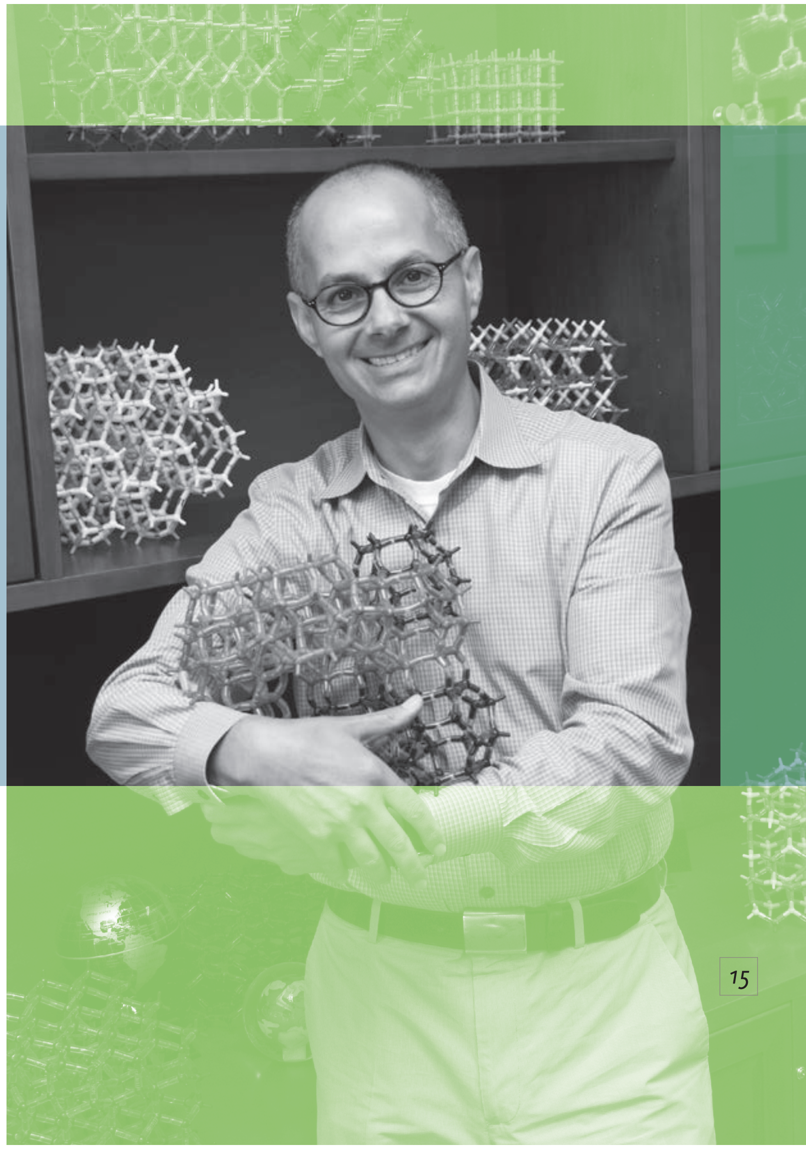
The world has taken interest in Yaghi's work. In Jordan, Princess Sumaya bint El Hassan, a science advocate and the president of Jordan's Royal Scientific Society (RSS), is keen on developing this technology. In a recent visit to UC Berkeley, she was awarded a Chancellor's Citation by Chancellor Nicholas Dirks. This citation is awarded to distinguished visitors, alumni and friends whose great achievements the university salutes and whose presence honors and benefits the campus.



Above: **In this diagram, at the lower right, air enters the water-harvesting device and water vapor is adsorbed by the layer of MOF. In the upper left, sunlight warms the saturated MOF, releasing the concentrated water vapor which condenses to liquid water and is collected.**

Below: **Members of the Yaghi lab examine a new MOF material that can confine and stabilize proteins for crystallography measurements.**





Yaghi, who is the founding director of the Berkeley Global Science Institute, has worked closely with Princess Sumaya over the past five years to re-engage the Jordanian diaspora community in scientific research to address global problems. A delegation from the institute has met with the Princess to discuss plans for building a reticular foundry, a joint UC Berkeley-Royal Scientific Society research institute that will serve as a hub of scientific research attracting top talent from throughout Jordan and the Middle East region. Says Yaghi, "It is my hope that this joint partnership will train the next generation of problem-solvers, innovators and scientific leaders."

Princess Sumaya also serves as chair of the World Science Forum (WSF), which will be hosted by Jordan in November 2017. The WSF is a leading forum for science and policymaking, and this will be the first time it is held in the Middle East. The theme for the 2017 WSF is "Science for Peace," and she hopes that the event will inspire young people and give policymakers renewed appreciation for science and the scientific method.

In the Spring of 2017, Yaghi also met with Jordan's King Abdullah II bin Al-Hussein to discuss plans for the Global Science Reticular Foundry. Says Yaghi, "The King enthusiastically accepted the proposal for the new building in Amman."

Adds Yaghi, "The scientific focus will be on the basic science of new materials with an emphasis on applications in food, food security, energy and water. A third goal is popularizing science and creating research opportunities for emerging scholars."

As the director of the Berkeley Global Science Institute, Yaghi has helped create Centers of Global Science in Japan, Vietnam, Korea and Saudi Arabia. Their mission is to partner with institutions of learning, foundations, government and industry, in the United States and abroad, to create centers of research in foundational sciences to address global problems and build a culture of science.

Says Yaghi, "I am extremely encouraged by the potential of the international science centers the Berkeley institute has helped create in solving global problems such as water scarcity."

Treating disease with cold atmospheric plasmas

David Graves still remembers the first time he saw the Bay Area. "I had just graduated with a B.S. in ChemE," he recalls. "It was 1978 and the petrochemical industry was booming. I had 13 offers for plant visits, including one with Chevron Research in Richmond. They put me up in the St. Francis Hotel in San Francisco. I fell in love with the Bay Area—it was so beautiful."

It would take Graves another eight years to make the Bay Area his home, but along with his plasma research, it has become an anchor in a life and career that have been peripatetic both geographically and intellectually.

Graves was born in 1955 in Daytona Beach, FL. His father co-owned a restaurant with his stepfather, but later joined the U.S. Air Force. By age seven, Graves was living in Homestead AFB, an hour's drive southwest of Miami, one of the handful of air force bases he would call home as he was growing up.

Graves started high school in North Bay, Ontario, the location of a joint U.S./Canadian base, but graduated in 1973 from Dysart High School in a western suburb of Phoenix near Luke AFB. He started at the University of Arizona in Tucson as a chemistry major. But he switched his major to chemical engineering as a second-semester junior because he had heard that "ChemE had lots of jobs."

With his newly minted B.S. he began working for Chevron Research in June 1978. "I joined the computer process control group where I was the youngest member of the computer control team," Graves says. "My first project was at the Chevron Chemical ammonia plant in Fort Madison, Iowa."

Chevron next assigned him to Pascagoula, MS, where he realized he didn't want to be a process engineer. In late 1979, Graves called his former professor James White, who had taught him computer process control at the University of Arizona. "He told me he could get me into the spring grad school courses, and he did."

Graves earned his M.S. in ChemE in 1981 for his research on pulverized coal combustion, working with Jost Wendt. He moved on to a ChemE Ph.D. program at the University of Minnesota. There he worked with Klavs Jensen on low-temperature plasmas.

At the time low-temperature plasmas were a new and risky area of research. "I was warned not to study them because their physics and chemistry were so little understood. But plasmas had potential and I was curious about them." Graves completed his Ph.D. in 1986, was married to his wife Sue, and joined the Berkeley faculty later that year. Their three children were born at Alta Bates Hospital in Berkeley.

He says, "The plasmas I study are not the variety found inside stars or fusion reactors. Those are superheated, completely ionized gases. I study low-temperature, partially ionized gases which are also known as cold atmospheric plasmas. Common examples are neon or fluorescent lights and, in the natural world, lightning."

Graves adds, "A main area of research for my group has been the fundamentals and applications of low-temperature plasmas to the microelectronics industry. There plasmas are used for etching the silicon wafers used to make computer chips and for thin-film deposition techniques. We typically combine various types of plasma modeling and simulation methods with well-controlled experiments to develop insights into mechanisms governing the processes."

Silicon Valley has been grateful for Graves's research, and his group started a long and fruitful relationship with Lam Research, headquartered in Fremont, CA, a leading supplier of wafer fabrication equipment. Lam endowed the Lam Research Distinguished Chair in Semiconductor Processing, a chair held by Graves from 2011–16.

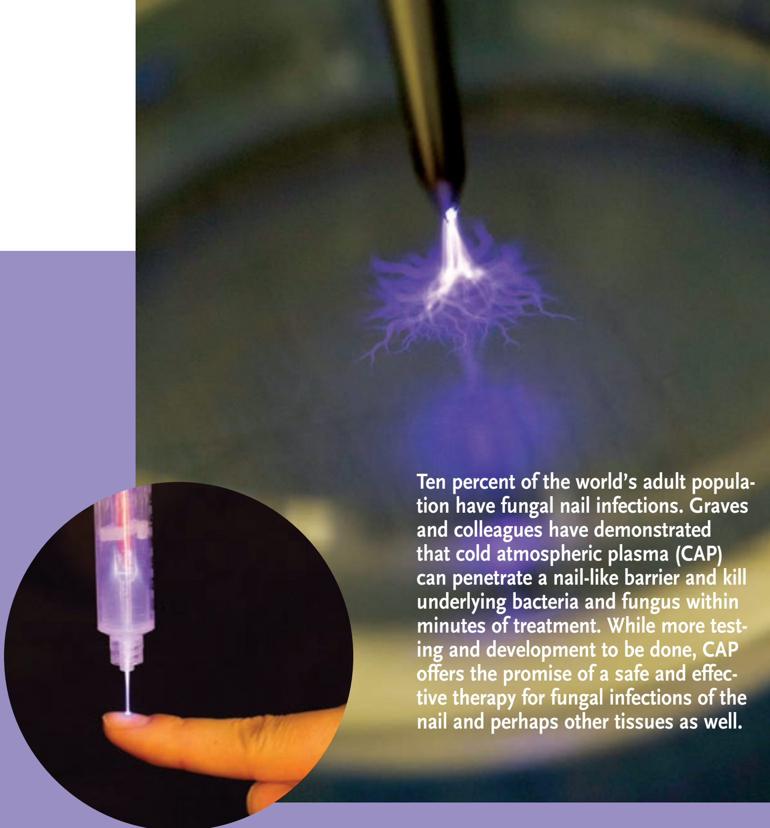
After more than 30 years at Berkeley, Graves could be content to wind down his career. Instead, like that young man who lived on many different air force bases while growing up, he is still moving. He is now exploring another expanding area for plasma research, one that has tremendous potential but is also poorly understood.

"Plasma biomedicine started in the mid-1990s with studies of plasma decontamination of surfaces. By the early 2000s, Eva Stoffels and colleagues at the Eindhoven University showed that atmospheric pressure low-temperature plasmas alter mammalian cells without causing necrosis and under some conditions even leading to apoptosis, programmed cell death," says Graves. "From that starting point the medical applications have grown. I began to hear about plasmas being used in Europe for wound sterilization and wound healing. More research showed that plasmas could shrink tumors."

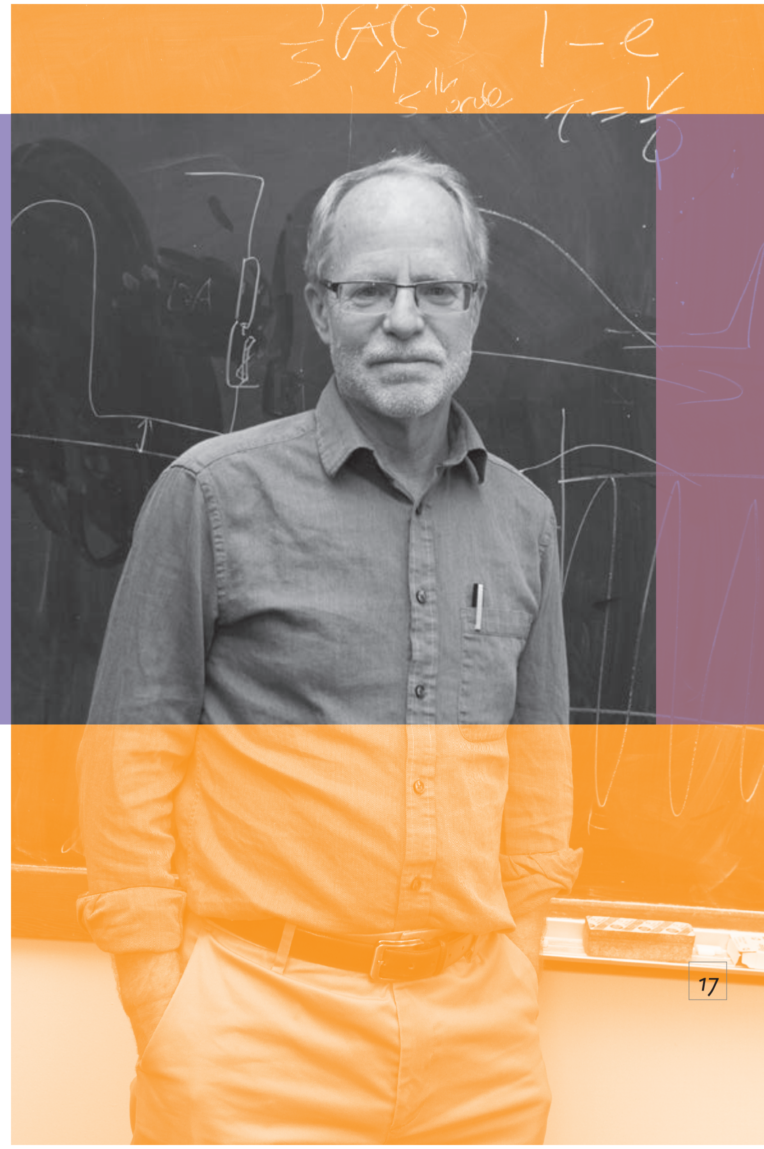
There was a whole new area being explored on the biological effects of plasmas. Graves and others suspected it had something to do with the reactive oxygen and nitrogen species (RONS) created when the plasmas reacted with the Earth's atmosphere.

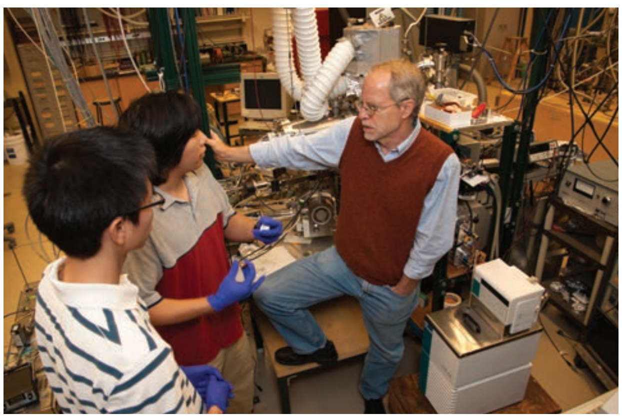
Says Graves, "We used to think that RONS were just 'bad guys,' damaging by-products of cellular metabolism. But now we know they are often 'good guys' that play important roles in immune response, tissue repair and cell signaling. I documented this by spending hundreds of hours researching the biology and medical literature for a 2012 review article in the *Journal of Physics D.*"

Berkeley chemistry professors Judith Klinman, Michael Marletta and Chris Chang have also made fundamental discoveries about RONS—Klinman on how enzymes control the formation of radical



Ten percent of the world's adult population have fungal nail infections. Graves and colleagues have demonstrated that cold atmospheric plasma (CAP) can penetrate a nail-like barrier and kill underlying bacteria and fungus within minutes of treatment. While more testing and development to be done, CAP offers the promise of a safe and effective therapy for fungal infections of the nail and perhaps other tissues as well.





Graves with students in the section of his lab where research is conducted on plasma applications for semiconductor etching and thin-film deposition.

oxygen species, Marletta on the role of nitric oxide in immune response, and Chang on the cellular signaling role of hydrogen peroxide.

Although the therapeutic benefits of plasmas may seem far-fetched, the possibilities are taken more seriously in Europe and in Asia. This emerging field has several journals, including *Clinical Plasma Medicine,* published by Elsevier. Graves is now senior editor of a new journal in the field—*Transactions on Radiation and Plasma Medical Science*, published by IEEE. In Germany, several commercial plasma medical devices, including the kINPen MED, have been approved for clinical use, primarily for wound healing.

Notes Graves, "Plasma is a well-established treatment for wound healing and tissue decontamination. There is also growing evidence that in the treatment of cancer, tumors respond to external applications of RONS in a manner similar to how they respond to interior exposures from radiation and chemotherapies. Recently, we worked with a Bay Area startup to investigate using plasma to treat toenail fungus. The preliminary results look pretty good."

But Graves cautions, "What has not been shown is that plasmas are consistently better than existing drugs or medical devices, or that they can work synergistically with them. A tremendous amount of research still needs to be done both on exactly which RONS are generated by plasma devices, and on the specific therapeutic benefits of each of them."

Unfortunately, research funding budgets are shrinking in the United States, so Graves finds himself once again on the move. The French language he begrudgingly studied while attending high school in Canada has come in handy. He has polished his language skills and after several trips to confer with European researchers, he can now give scientific talks in his "near-fluent" French.

"I cut my teeth early in my career doing process control," Graves concludes. "When I apply that perspective to biology, I'm amazed at how sophisticated the process control mechanisms are even in single cells.

"It turns out my new research interest is more complicated than I thought, but I'm far from the first researcher to make that observation. Humans have a tendency to overestimate scientific progress in the short run, but to underestimate it in the long run. Science tends to work that way. I wish I could live 300 years just to see how this all turns out."

Class of 2017

What will they be doing after commencement?

In the spring, some of the students who planned to walk in the May 2017 commencement ceremony shared their plans with us:

"For now, I'll be starting at a pharmaceutical company in Nevada and then getting married pretty soon after that!"
—**Yassin Barakat** *(B.A. Chem)*

"Noelle will be working as a postdoctoral researcher in the Energy Nanomaterials Department at Sandia National Laboratories in Livermore, CA. She plans to apply the experience in porous materials chemistry she gained in the Yaghi Lab to her new position."
—**Noelle Catarineu** *(B.S. Chem)*

"I will be attending graduate school in the fall to study polymers in a renewable energy context, such as solar cells, polyelectrolytes for batteries, depolymerization, or biodegradable polymers."
—**Sophia Y. Chan** *(B.S. ChemE)*

"I am currently a staff research associate at UCSF, I plan to spend one year gaining research experience in lab before continuing to graduate school for a Ph.D. in biology or biochemistry."
—**Man Kwan Kirsten Chui** *(B.S. ChemBio)*

"I plan to work for two years, then spend a year between South and Central America, then go to graduate school."
—**John P. Connor** *(B.S. Chem)*

"I will be travelling Southeast Asia in the months after graduation and then begin working full-time!"
—**Sushant P. Gadgil** *(B.S. ChemE & Mat Sci Eng)*

"Bernardo will be pursuing a Ph.D. in chemical engineering at (either MIT/ Caltech/Princeton), and will be supported by the National Science Foundation and the Paul and Daisy Fellowship for New Americans."
—**Bernardo Gouveia** *(B.S. ChemE)*

"I will be teaching secondary school chemistry in Mozambique for the Peace Corps for two years before I plan to go to graduate school."
—**Jessica Granger-Jones** *(B.S. Chem)*

"Go back to Greece, start new ventures department in our businesses while building warehousing infrastructure to

EXCERPT FROM COMMENCEMENT ADDRESS BY JENNIFER DOUDNA

We are living through a time of deep distrust in science and scientists, a time in which facts are intertwined with alternative facts, a time where public support of scientific research and the scientific method itself are being questioned. And I feel that at least some of the responsibility for this state of affairs lies with all of us scientists. For too long we have focused our attention single-mindedly on our lab work and sharing the results of our research with like-minded colleagues. I urge each of you to step outside of this narrow definition of a scientist and get involved in the broader national and international discourse about science. We must re-build public trust in our work, and we must explain to our fellow citizens why our work matters, not just to publish the next paper but to advance human knowledge and to improve the human condition.

JENNIFER DOUDNA
Professor of Chemistry
Professor of Biochemistry & Molecular Biology
Li Ka Shing Chancellor's Professor in Biomedical and Health Sciences

create supply chain surplus in the trade between Europe and Middle East."
—Ioannis E. Haloulos *(M.S. ChemE)*

"I traveled through Europe for three months between thesis submission (December) and starting my next job (April). Next up, scientific consulting."
—David M. Herlihy *(Ph.D. Chem)*

"Moving to Florida to serve in the United States Air Force as a project engineer. Planning to spend time working with cutting-edge military technology and spending my off-time exploring the East Coast as well as travelling abroad to Europe/Asia."
—Frank Hoang *(B.S. ChemE)*

"Postdoc at the German Synchrotron, BESSY II."
—Robert W. Johns *(Ph.D. Chem)*

"I will be staying at Berkeley to get a Ph.D. in nuclear engineering."
—Kelly N. Kmak *(B.S. Chem)*

"I was so busy starting a new company that I failed to attend commencement in 2007. It's great to come back and enjoy Berkeley!"
—Thomas J. Lowery *(Ph.D. Chem)*

"I am currently working at UCSD as a research associate in the Xiong lab, and I will be starting my Ph.D. in chemistry in Fall 2017. "
—Dannielle McCarthy *(B.S. Chem)*

"I intend to enroll in a Ph.D. program to conduct research (thank you, Berkeley, for the wonderful research opportunities and world-class faculty)."
—Aditya Nandy *(B.S. ChemE)*

"I will be attempting to complete the Pacific Crest Trail starting the week following graduation."
—Washington S. Reeder *(B.S. ChemE)*

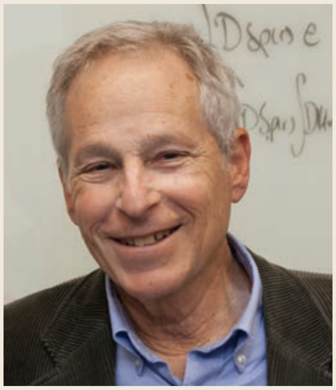
"After such rigorous coursework the last 4 years, I will be taking the summer to study Spanish language and culture in Madrid, Spain, before returning to the U.S. to embark on the next chapter of my life."
—Stephanie M. Scribner *(B.S. ChemE)*

"I will do research in food chemistry at the USDA before going to graduate school, either a Ph.D. in food science or a J.D. (to pursue the intersection of science and the law)."
—Amanda J. G. Sinrod *(B.S. Chem)*

"Graduate school in the Czech Republic for environmental engineering, later a career in wastewater treatment there or in Southern California."
—Kristina Slezacek *(B.S. ChemE)*

"Going to Japan over the summer to teach English."
—Shehan M. Thangaratnam *(B.S. ChemBio)*

Faculty



Emeritus professor **DAVID CHANDLER,** pillar of the physical chemistry scientific community, died April 18, 2017, at the age of 72 at his home in Berkeley, CA, after a 20-year battle with prostate cancer.

Born in New York, NY, on October 15, 1944, Chandler blossomed scientifically after high school despite significant learning disabilities and, following a year at Stevens Institute of Technology, transferred to MIT. Earning a B.S. in chemistry from MIT and a Ph.D. in chemistry from Harvard University, he then held professorships at the University of Illinois at Urbana-Champaign and at the University of Pennsylvania before joining our faculty in 1986.

Chandler is credited with crafting the modern language and concepts for describing structure and dynamics of condensed matter, especially complex systems with disorder and heterogeneity, such as liquids, glasses and biological assemblies. His career several times changed the course of the field of physical chemistry. His influence in his field of science carries forward through the more than 100 graduate students and postdocs he mentored, and through the thousands of scientists influenced by his numerous research articles and the symposia he founded or contributed to.

He is survived by his wife, Elaine, a retired physicist and his scientific collaborator, and by their extended family. For a more detailed obituary, see chemistry.berkeley.edu/news/david-chandler-dies-at-age-72.

Emeritus professor **IGNACIO "NACHO" TINOCO, JR.,** was a biophysical chemist who devoted his life to the study of nucleic acids. In particular, he pioneered the field of RNA folding and made fundamental contributions to the understanding of RNA structure and function. He died November 15, 2016, at the age of 85.

Tinoco earned his Ph.D. in chemistry from the University of Wisconsin-Madison. In his more than 60 years as a faculty member in the College of Chemistry, he authored over 300 publications and mentored nearly five dozen Ph.D. students, as well as dozens of postdocs who have gone on to prestigious positions in academia and industry around the world. He also wrote two textbooks, *Physical Chemistry, Principles and Applications in Biological Sciences* (in five editions) and *Physical Chemistry of Nucleic Acids,* and several chapters of a book on single-molecule studies.

Tinoco's first wife, Joan *(B.S. '58, Chem; Ph.D. '62, CNR),* died of cancer in 2002. He is survived by his second wife, Bibiana Onoa *(Postdoc '02, Chem),* a research scientist in QB3 in the Bustamante lab. In lieu of a formal obituary, Bibiana has created two videos that can be viewed at https://youtu.be/BLhcZajlNGc and https://youtu.be/VJsnp4UDBUY—visual tributes to the breadth and depth of Tinoco's life and work and to the enormous influence he had on his fellow scientists. He is survived by Bibiana and his extended family.

Friends of the college

SUSAN DINKELSPIEL CERNY *(B.A. '62, Art History & Archit),* wife of emeritus chemistry professor Joseph Cerny *(Ph.D. '62, Chem),* passed away December 1, 2016, at the age of 76. An artist and potter, she found an additional vocation in architectural preservation and was recognized in 2015 by the California Preservation Foundation for her "immeasurable contributions to protect the architectural heritage of Berkeley." Susan and Joe together established a graduate student support fund in the College.

MARY ELLA JOHNSTON, widow of the late emeritus chemistry professor, Harold S. "Hal" Johnston, has died. The couple were generous supporters of the College, regular attendees of College events and donors of an endowed graduate student fellowship.

Alumni

'51 **Frank G. Delfino** *(B.S. ChemE),* a generous supporter of undergraduate education in CBE, passed away this winter. Long retired from a career at BestFoods, he was a regular attendee at College alumni events.

'55 **Robert E. "Bob" Lundin** *(Ph.D. Chem with Gerhard Rollefson)* died March 14, 2017, in Richmond, CA. He had a career as a nuclear magnetic resonance spectroscopist at the U.S. Department of Agriculture Western Regional Laboratory.

'62 **Charalambos "Harry" Chiladakis** *(B.S. '51, ChemE; M.S. '62, ChemE),* former COC engineer who worked in the Giauque Low-Temperature Lab with professors David Lyons and Norman Phillips, died April 1, 2017. He was the first to construct a helium liquifier in the College.

For a complete list, please visit:
berkeley.box.com/v/chem-memoriam-summer2017

COMPILED BY KAREN ELLIOTT

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Upcoming Fall 2017 events

Reunion and Parents Weekend at HOMECOMING

October 21 **Coffee with the Deans - for Parents of Undergraduate Students**
8:30 a.m. – 10:00 a.m.
Chemistry Plaza & 120 Latimer Hall

Join us for coffee and pastries on the Chemistry Plaza, followed by a panel discussion and Q&A with College of Chemistry Dean Douglas S. Clark and Undergraduate Dean John Arnold.

No registration required for this complimentary event (capacity 150)

Faculty Presentation
10:30 a.m. – 11:30 a.m.
120 Latimer Hall

James and Neeltje Tretter Professor of Chemistry Omar Yaghi presents:
"Using the Sun's Power to Pull Water from the Desert Air"

More than two-thirds of the world population lives in water-stressed regions. We recently demonstrated that water in the atmosphere can be harvested to deliver fresh water using metal-organic frameworks (MOFs)—a class of materials we discovered twenty years ago that are currently being further developed at UC Berkeley's College of Chemistry and the Berkeley Global Science Institute.

No registration required for this complimentary event (capacity 150)

Alumni, Parents & Friends Lunch
11:30 a.m. – 1:00 p.m.
Chemistry Plaza

Mingle with fellow alumni, parents and friends for an informal lunch on Chemistry Plaza.

Please Note: Registration and fee required for this event.

Alumni Reception at the 2017 AIChE National Meeting

October 31 **7:00 a.m. – 8:30 p.m.**
Minneapolis, MN
Location TBD

Please check our website at chemistry.berkeley.edu/events for details closer to the date.

+ For more information on events, visit **chemistry.berkeley.edu/events,** or email **coc_events@berkeley.edu.**

The new Pitzer Center Annex under construction. The annex, on the third floor of Gilman Hall, opened in November, 2016.

DON'T MISS OUT!

The College of Chemistry has moved to electronic invitations for our events.

To make sure you hear about upcoming events and news, please submit your email address to: **chemistry.berkeley.edu/email.**

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