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Catalyst

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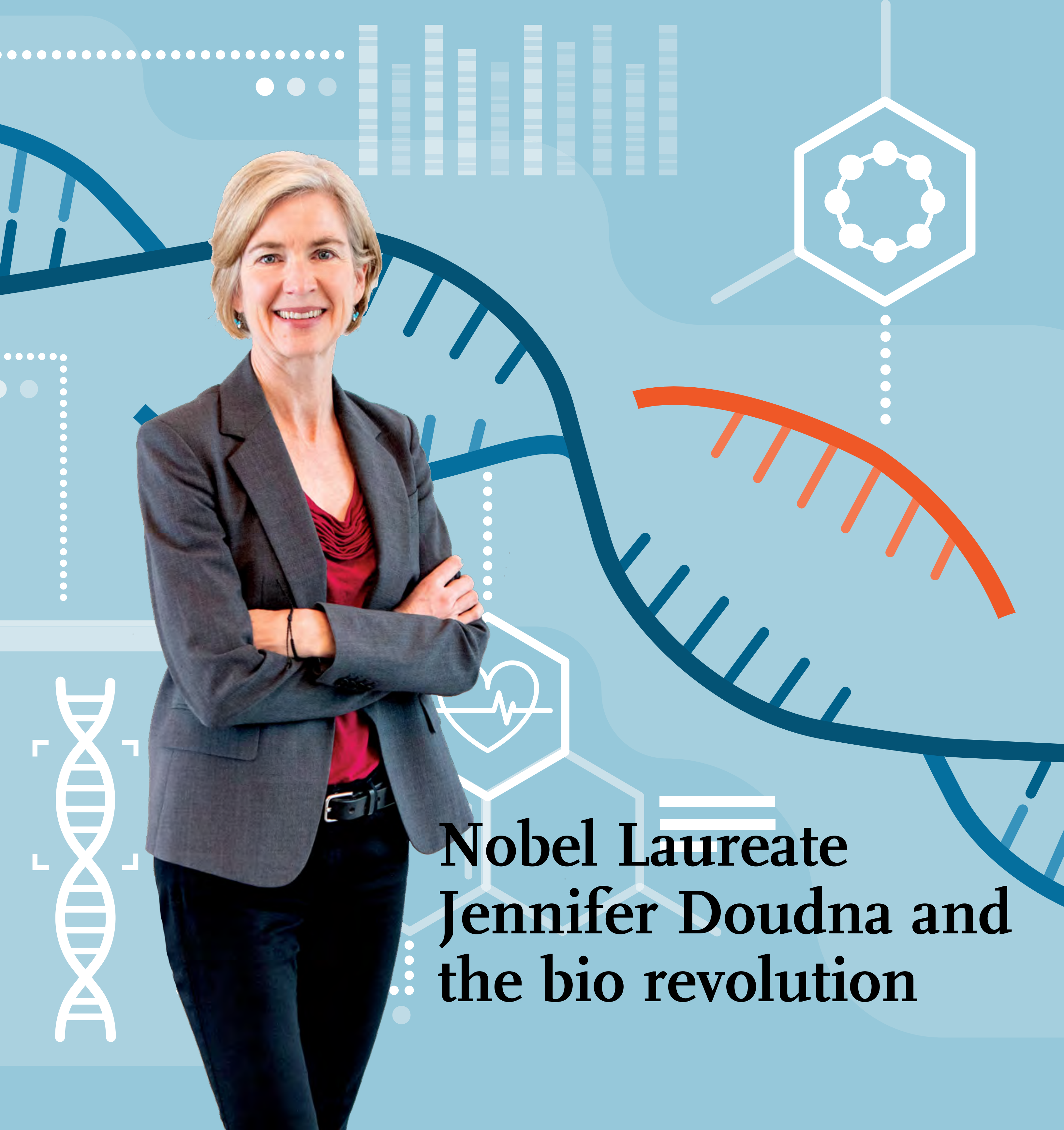
COLLEGE OF CHEMISTRY • UNIVERSITY OF CALIFORNIA, BERKELEY



Nobel Laureate Jennifer Doudna and the bio revolution

Catalyst

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ON THE COVER

In this issue, we celebrate Professor Jennifer Doudna's Nobel Prize and the bio revolution she has helped create.

COVER PHOTO: KEEGAN HOUSER

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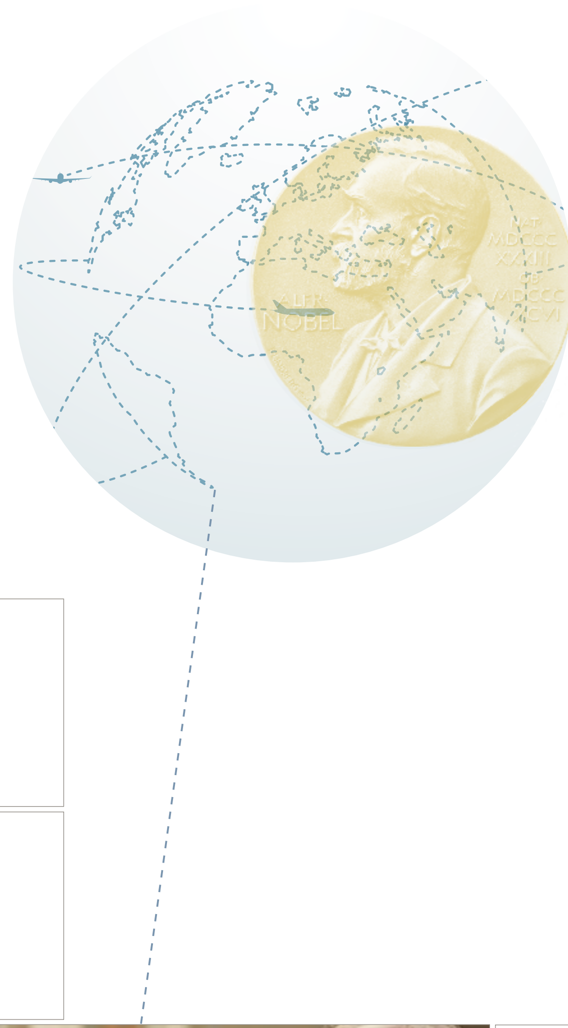

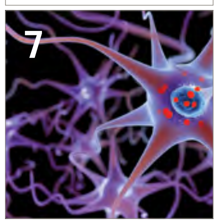

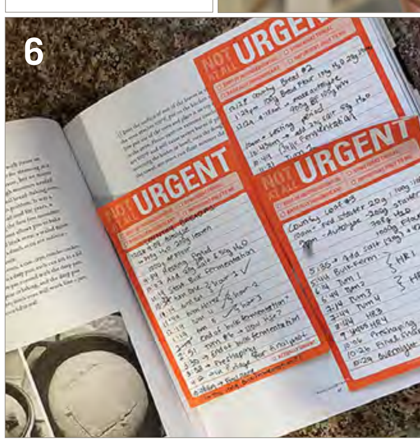

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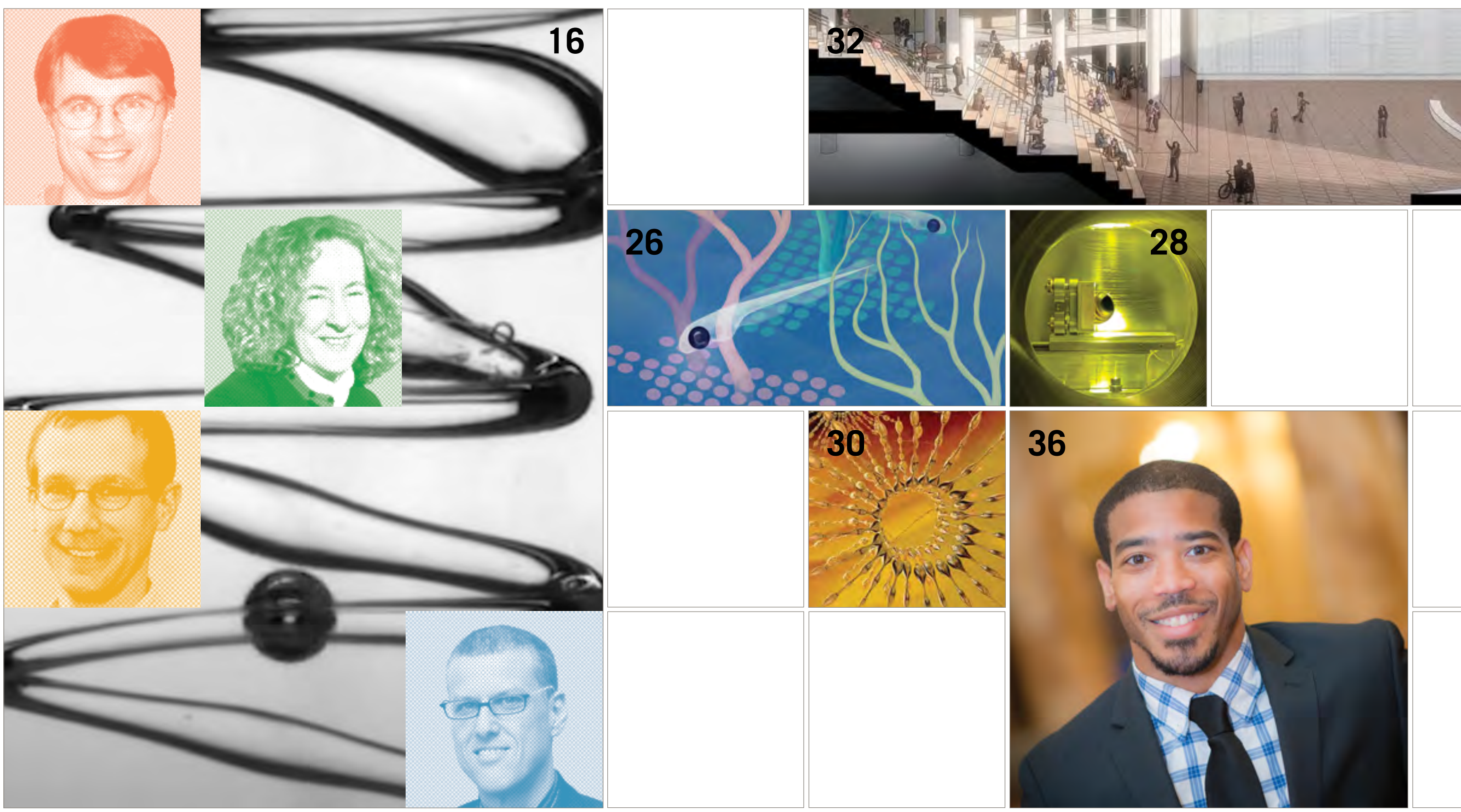


Strength and hope during adversity

If the last year has taught us anything, it is that living through an unthinkable situation can become second nature, and that by working together we can adapt to make the best of the most demanding conditions. I have come to realize that the study of phase transitions goes beyond the boundaries of our College of Chemistry labs. In March 2020, we were all forced to ask ourselves, "How do we go from a state of constant physical interaction to a state of constant isolation, all the while maintaining the same level of productivity and effectiveness?" Countless hours were spent by faculty, staff, students, and researchers trying to identify the best methods to make this transition palatable and sustainable. I remain extremely proud and grateful for the hard work committed by everyone to keep the college running smoothly.

We are still euphoric from the excitement surrounding Jennifer Doudna receiving the 2020 Nobel Prize in Chemistry, sharing it with collaborator Emmanuelle Charpentier for the co-development of CRISPR-Cas9. What an incredible achievement and inspiring message. It was a pleasure to co-host, with our graduate students, an online discussion with Jennifer in November to hear about the history of her remarkable journey and her vision for the future of gene-editing. Also, last fall, the college was honored to virtually host Birgitta Whaley as the 67th Gilbert Newton Lewis Memorial Lecturer. In her lecture, she took us on a journey of "finding the quantum in biology," and you can read more about this fascinating work in the main science feature in this issue. I very much look forward to the days when these celebratory events can happen in front of a packed auditorium again.

One of our greatest examples of triumph in the face of adversity over the last year is in our faculty recruitment efforts. Last July, assistant professor Ashok Ajoy joined us in the Department of Chemistry. This July, Joelle Frechette, from Johns Hopkins University, will join the CBE faculty as a full professor. Both departments have recently completed virtual interviews — never before done and flawlessly executed — for the next round of faculty hires, and both departments have identified amazing, diverse candidates whom we are actively pursuing. I hope to be announcing those successful efforts this time next year.

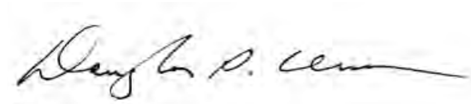
Since my last message, we have made significant strides in strengthening our ability to address diversity, equity, inclusion, and belonging (DEIB) matters in the college. Anne Baranger has been appointed as our inaugural associate dean for DEIB, and Brice Yates has joined the College as chief DEIB officer. Together they lead the newly created College Advisory Committee for Diversity, Equity, Inclusion, and Belonging, and they have established several goals for advancing DEIB in the College, including developing a five-year strategic plan. They have recently collected proposals for our graduate diversity fellows' projects, which is a reminder of just how inspiring and driven our graduate students are.

In early May we welcomed our first William A. Lester Lecturer. This new lectureship, named for our distinguished colleague, was established in 2020. It will bring to Berkeley eminent scholars from diverse personal and professional backgrounds to present their research and engage in discourse about their experiences and challenges of becoming scientists. I am thrilled to engage in this long overdue focus in our named lectureships.

In other College news, I would like to acknowledge Ron Silva, who has served as our Advisory Board Chair for the last three years. Ron's leadership was crucial in helping the College meet several challenges, and I am grateful for his exemplary service. Ron is succeeded in this role by our alumnus John Markels, currently the President of Vaccines at Merck and a longstanding member of the board. I look forward to working with John to advance our goals for the future, including construction of

the new state-of-the-art Heathcock Hall, for which we recently received a $10 million commitment from PMP Tech. My excitement and gratitude continue to grow with each step we take towards realizing this goal.

Reflecting on these and so many other highlights from the last year, I am truly impressed, but not at all surprised, by the capacity of our College to make the successful transition to a new way of life while raising the bar of excellence even higher. Together or apart, faculty, students, and staff in the College of Chemistry will always find solutions to the toughest problems facing us today. We continue to celebrate our shared passion for and achievement in producing the best chemistry and chemical engineering research in the world.



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

NEW & NOTABLE

RESEARCH • VIEWS
DISCOVERIES • AWARDS

Nobel gold medals delivered by diplomatic courier around the world

Because of the pandemic, the award ceremony for the Nobel Prize in Stockholm was postponed in December 2020. Nevertheless, the Nobel committee sent the Laureates their medals and beautiful hand painted diplomas. Eleven of the medals, including Professor Jennifer Doudna's, traveled with diplomatic immunity via diplomatic pouch across the world.

Have you ever wondered what the Nobel Prize medal is made of? Before 1980 the medal was made from 23 carat gold. Newer Nobel Prize medals are 18 carat green gold plated with 24 carat gold. Green gold (known as electrum) is an alloy of gold and silver, with trace amounts of copper. The diameter of the Nobel Prize medal is 66 mm but the weight and thickness vary with the price of gold. The average Nobel Prize medal is 175 g with a thickness ranging from 2.4-5.2 mm.

CHRIS POLYDOROFF

Chemistry professor and alumnus Paul Alivisatos *(Ph.D. '86, Chem)*, who directed the Lawrence Berkeley National Laboratory for seven years and served the UC Berkeley campus as vice chancellor for research and currently as executive vice chancellor and provost, all while continuing his pioneering work in nanocrystals, has been appointed president of the University of Chicago, his undergraduate alma mater.

"I can think of no one better suited for this extraordinary opportunity, and no one who will be harder for us to replace," said Chancellor Carol Christ. "Paul has been an extraordinary partner; a tireless, visionary leader; a friend; and a true champion for Berkeley's mission, values and academic excellence."

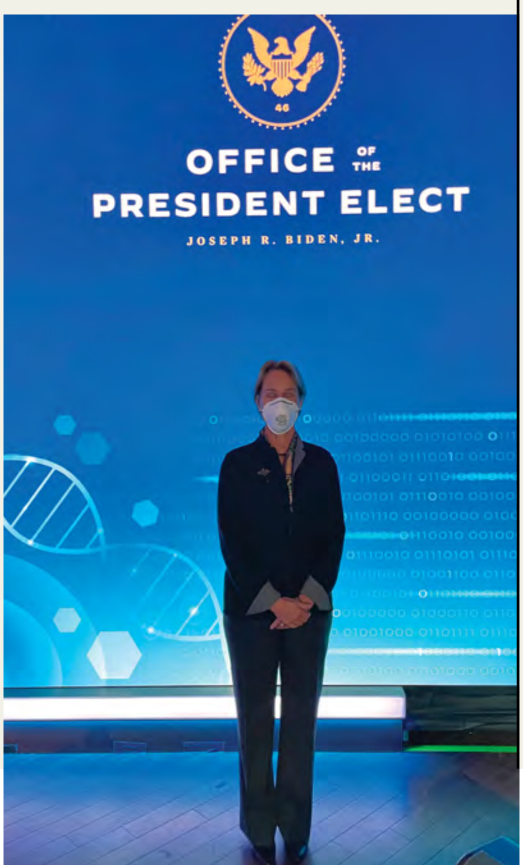
We will miss you at the College of Chemistry but know that many students at Berkeley received excellent educations under your tutelage. Students at the University of Chicago will benefit from your guidance of the institution. Best of luck from all of us.

Frances Arnold named co-chair to President Biden's Council of Advisers on Science and Technology

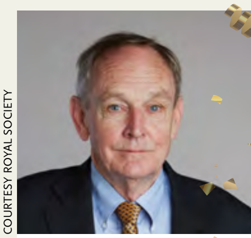
In a move to strengthen the position of science in the government, President Biden has selected geneticist Eric Lander to be science advisor for his new administration. President Biden also elevated the position to Cabinet rank. He has also chosen Maria Zuber (MIT) and alumna and Nobel Laureate Frances Arnold (CalTech) to serve as co-chairs of the President's Council of Advisers on Science and Technology. Arnold, winner of the 2018 Nobel Prize in Chemistry and the recipient of numerous other honors, is a respected pioneer in the fields of protein and chemical engineering.

The council will advise the president on matters involving science, technology, education, and innovation policy. The council will also provide the president with scientific and technical information that is needed to inform public policy relating to the American economy, the American worker, national and homeland security, and other topics.

Arnold said of the appointment, "I want to work to preserve our fragile planet, build our economy and workforce for the future, and pass a better world to all Americans. I feel I can do this by supporting science and science-based decision-making in the Biden administration. I have great hope that we can put science back to work for the benefit of all."



COURTESY FRANCES ARNOLD


COURTESY ROYAL SOCIETY

Theoretical Chemist William Miller turns 80

Professor Emeritus William (Bill) Miller's daughters and coworkers organized a zoom 80th birthday party for him in March. The party included lots of reminisces from Bill, his colleagues, and many of his former coworkers.

During his career, Bill made many profound and diverse contributions to theoretical physical chemistry of molecular motion, from semiclassical mechanics to reactive scattering, and from chemical kinetics to path integrals. Bill literally shaped the way theoretical dynamicists think. His enthusiasm and deep insight set a model for students and colleagues and will continue to provide a source of inspiration for future generations of theoretical chemists.

Happy Birthday!

David Grossman (BS '78, Chem) to co-lead community health at Kaiser Permanente

Kaiser Permanente, the nation's largest integrated, nonprofit health system has announced that David Grossman, MD, MPH, and Stephanie Ledesma, MS, will co-lead the organization's Office of Community Health. The team will partner closely to identify and address social health needs among Kaiser Permanente's members, and — at the same time — to improve overall conditions for health and equity in the communities the organization serves.

In the last year, Kaiser Permanente established a social health practice to design and build new and innovative ways to connect members to social health services while bolstering the organization's grant-making strategy to build and sustain communities' capacity to meet growing needs. These efforts were previously led by Bechara Choucair, MD, who joined the Biden administration as the White House COVID-19 vaccinations coordinator in January.

Dr. Grossman will work in partnership with the Permanente Medical Groups to lead Kaiser Permanente's social health strategy as well as the organization's public health advocacy and response to the COVID-19 pandemic. Ledesma will lead all community health operations and functions that support the organization's community health portfolio.

"At this point in our pandemic response, it is critical that we accelerate our efforts to integrate how we address our members' social health with our broader care delivery system," Dr. Grossman said.


COURTESY KAISER PERMANENTE

TALIA PATT

Seniors Brendan Huang and Carolyn Hong, who both have received the COVID-19 vaccine and are in the same social bubble, met in an organic chemistry lab as sophomores, became fast friends and wound up baking sourdough bread together. It's an adventure that Hong calls "our sourdough journey."

Donating from the heart

Friends Carolyn Hong and Brendan Huang had a delicious dilemma. Last semester, the UC Berkeley seniors' freezers were overstuffed with sourdough bread. They'd taught themselves to bake it — increasingly, to perfection — during the COVID-19 pandemic, which set off a nationwide bread baking craze, and, initially, a shortage of flour and yeast.

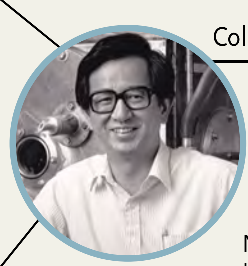
Friends suggested they sell their bread, which is visually and gastronomically appealing. "But I wasn't comfortable with selling for a profit," said Hong. Neither was Huang.

"So, we decided to charge $10 a loaf and subtract the price of flour and donate whatever is remaining to Feeding America," said Hong. "We've donated close to $300, which Feeding America says translates to 3,000 meals for families in need, which is pretty amazing."

Huang said he and Hong "love attaching notes to our deliveries, reminding people of their impact" on fighting hunger.

New Lectureships announced for 2021

College establishes two new chemistry lectureships in honor of Yuan Tseh Lee and William Lester



A newly endowed lectureship has been established in honor of Nobel Laureate and Professor Emeritus Yuan Tseh Lee. The lectureship is intended to invite distinguished scholars in the field of chemistry to present their research at an annual presentation at the College. The first lecture will be given by Prof. Lee in the fall of 2021.

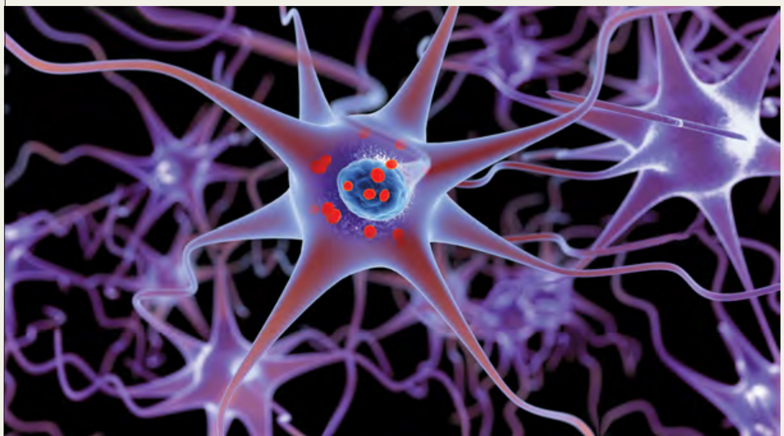
The lectureship was established by gifts from College alumnus and Professor of Chemistry Daniel M. Neumark *(Ph.D. '84, Chem)*, and Ellen B. Neumark, in memory of Prof. Neumark's parents George and Miriam Neumark. Additional gifts were made by Ted Hou *(Ph.D. '95, Chem)* and Sophie Wang *(Ph.D. '96, Chem);* Laura Smoliar *(Ph.D. '95, Chem)* and Mark Arbore; and College Advisory Board member Ron Silva *(B.S.'76, Chem; J.D. '79, JFK University)* and Lauren Silva.

The College has also established a lectureship to honor Professor of the Graduate School William Lester. The lectureship is intended to welcome distinguished underrepresented minority (URM) scholars to present their research and engage in discourse about their experiences and challenges of becoming scientists. The first lecture will be presented by Professor Joe Francisco of UPenn. Professor Lester said of the lectureship, "The thrust of this lecture is that it will add to the positive direction in diversity programming underway in various sectors nationally."

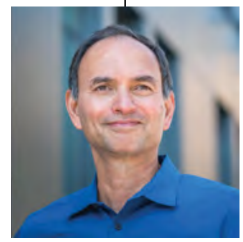
Douglas Clark, Dean of the College remarked, "Bill Lester is a great scientist and wonderful colleague who has made important contributions to the College and our profession on many levels, including his tireless efforts to promote diversity within chemical education and professional practice."

DENNIS GALLOWAY, UC BERKELEY ARCHIVE PHOTOS

PTEN-induced kinase 1 (PINK1) therapy moving to next phase



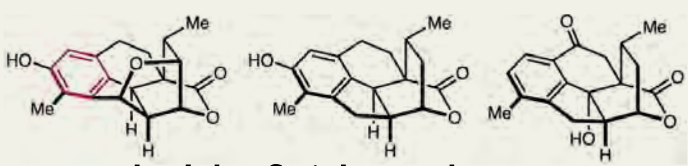
Mitokinin, Inc., a biotechnology company developing PINK1-targeted therapeutics for the treatment of neurodegenerative diseases, announced today that AbbVie, a leading global biopharmaceutical company, has purchased an exclusive right to acquire Mitokinin following completion of IND enabling studies on Mitokinin's lead PINK1 compound. Based on technology discovered at UCSF by Mitokinin co-founders Nicholas Hertz *(Ph.D. '13, Chem and ChemBio UCSF)* and Kevan Shokat (Prof. of Chemistry UCB and Professor of Chemistry and Prof. and Co-Chair, Dept. of Cellular and Molecular Pharmacology, UCSF). By increasing PINK1 activity, Mitokinin aims to address the mitochondrial dysfunction contributing to Parkinson's disease pathogenesis and progression.



Fourth Edition of Electrochemical Systems is now available

The long-anticipated fourth edition of Electrochemical Systems by Chemical and Biomolecular Engineering Professors John Newman and Nitash P. Balsara is now available. The new edition updates all of the chapters, adds content on lithium battery electrolyte characterization and polymer electrolytes, and includes a new chapter on impedance spectroscopy. Topics include electrochemical theories as they relate to the understanding of electrochemical systems, the foundations of thermodynamics, chemical kinetics, transport phenomena, and how to apply electrochemical principles to systems analysis and mathematical modeling.

The book can be used to model and understand a variety of electrochemical systems including batteries, hydrogen- and oxygen-based fuel cells, corrosion, production of aluminum and chlorine (electrochemical synthesis), biological systems, electroplating and electro-finishing, and renewable energy.

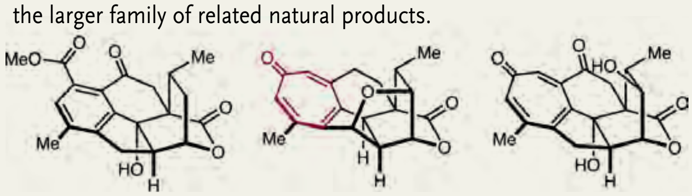


From the lab of Richmond Sarpong

In new research, Professor Richmond Sarpong and his co-researchers (DOI: 10.1021/jacs.1c00293), have developed concise total syntheses of the natural products cephanolides A-D utilizing retrosynthesis guided by chemical network analysis which successfully identified important and strategic bonds.

The chemical synthesis approach constructs the cephanolide skeletal framework by employing a simple cross-coupling followed by an intramolecular inverse-demand Diels-Alder cycloaddition. The researchers employed late-stage oxygenation to achieve structural diversification, setting the stage for the preparation of other structurally similar natural products.

The cephanolides are related to another natural product called harringtonolide, which shows nanomolar activity against cancer cell lines (KB cells). As such, they have the potential to serve as tools to better understand the underlying mechanisms for the anticancer activity of the larger family of related natural products.



OREGON STATE UNIVERSITY

Alumna Geraldine Richmond joins the Department of Energy

Geraldine Richmond *(Ph.D. '80, Chem)*, University of Oregon's Presidential Chair in Science, has been nominated to serve in the Biden administration as undersecretary for science in the Department of Energy.

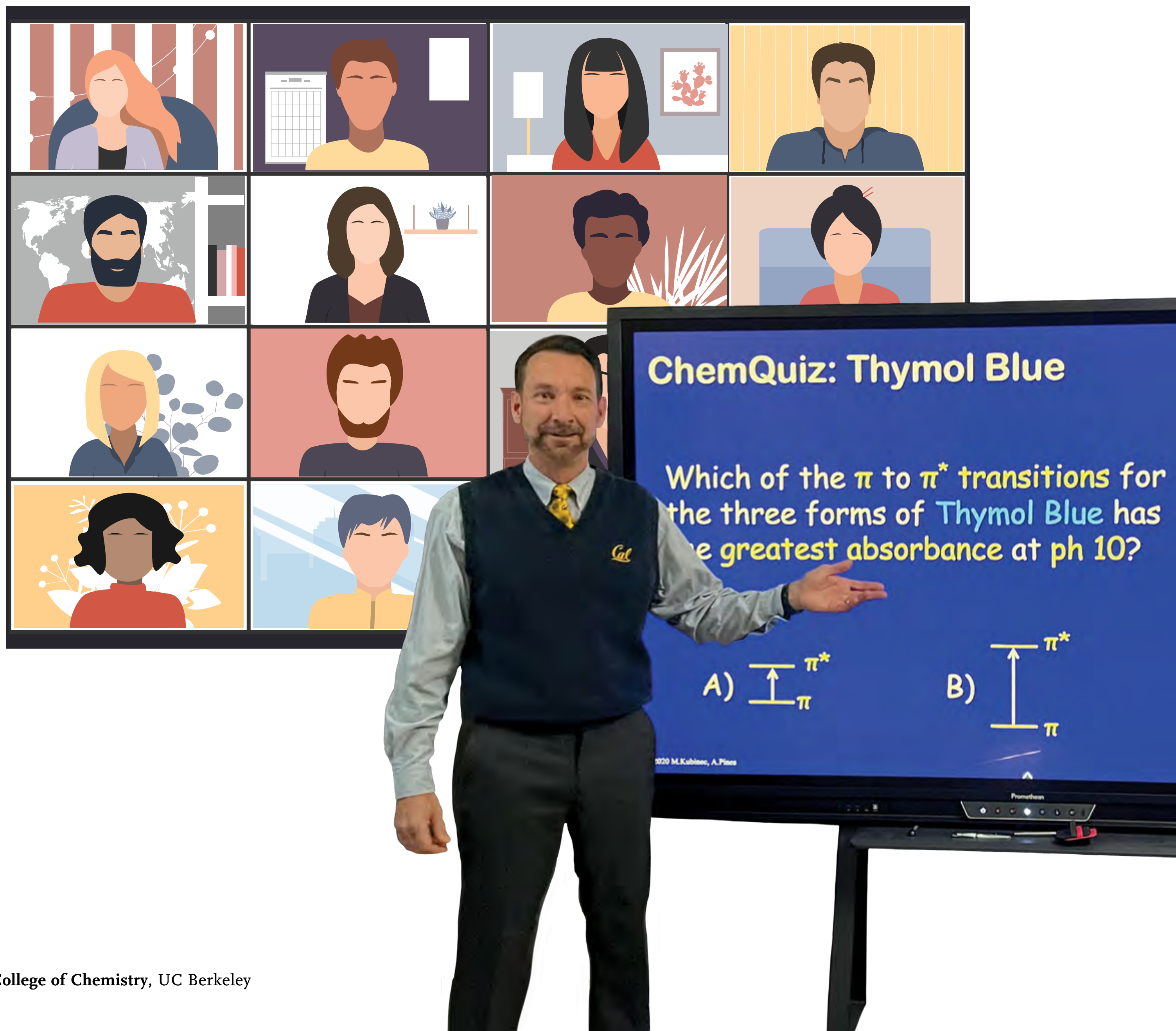
The undersecretary for science oversees the Energy Department's Office of Science, advises the secretary of energy on energy and technology issues, monitors the department's research and development programs, and advises the secretary on management of the DOE's national laboratories, among other duties.

Richmond has carved out a groundbreaking career studying the molecular characteristics of water surfaces, studies that have relevance to environmental issues such as oil remediation, atmospheric chemistry and alternative energy sources. She has designed state-of-the-art laser systems, optics equipment and computers that work in tandem to understand molecular processes at liquid surfaces that have environmental importance.

Richmond also has been a pioneer in advocating for the advancement of women in science.

FUTURE TECH

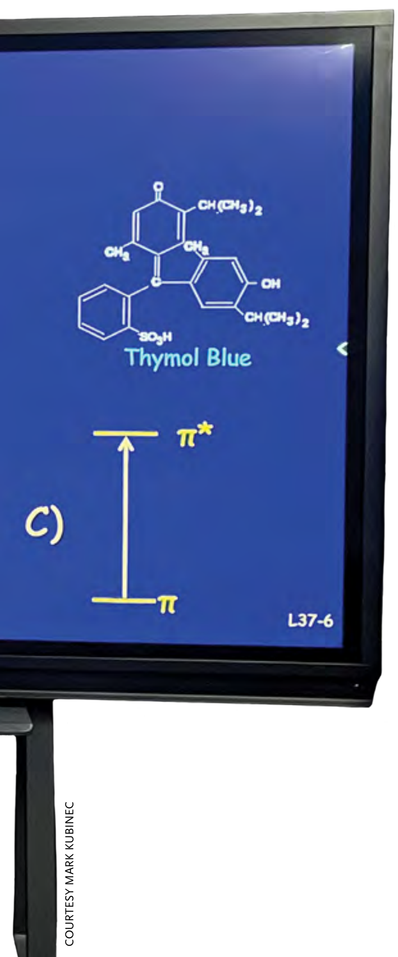
Advancing the use of technology in chemistry distance learning



BY MARK KUBINEC *(Ph.D. '94, Chem)*

Every fall semester, the 534-seat auditorium in Pimentel Hall swells to capacity three times daily to welcome the nearly 1,500 freshmen enrolled in Chemistry 1A. Multiple large video screens, one towering 20 feet above the main stage, help make every seat feel like the front row and enhance the learning experience. Nevertheless, college lectures are often described as the process of passing information from an instructor's notes to the students' notes without passing through the heads of either. My colleagues and I deliver chemistry lectures in this larger than life, potentially intimidating environment in a high production value and interactive experience to keep students thoroughly engaged. Demonstrations are flashy. Explosions are loud.

A vital part of our teaching strategy is peer-based, employing flipped-classroom learning techniques adapted to the large lecture hall setting. Students spend almost half their class time discussing and answering clicker quizzes' meticulously designed to prompt reflection and discussion with nearby students and graduate student instructors (GSIs). The combination of a few theatrical elements, and this interpersonal approach, makes Chem 1A a remarkably popular introduction to general chemistry.



COURTESY MARK KUBINEC

Then came the pandemic. Berkeley, like so many other institutions, was compelled to transition to 100 percent remote learning on very short notice. We faced the prospect of delivering the same high level of interactive, engaging learning entirely online for the 2020 summer session. A simple Zoom meeting wasn't going to suffice. Instead, we employed a blend of online, interactive technologies simultaneously. First, a YouTube livestream for the real-time lecture was combined with a live chat stream monitored by GSIs for questions and comments. Second, students watched the livestream in small-group Zoom breakout rooms where they used an iClicker system to respond to quizzes together. Finally, a custom and immediately available video review suite afforded an opportunity for asynchronous learning.

Students felt safe and welcome in small Zoom-bomb-proof breakout rooms – just like sitting with friends in lecture. The breakout rooms created the flipped classroom – guided by GSIs and myself, who used Zoom technology to randomly pop into individual rooms – as the full class watched and chatted on the livestreams.

It may sound complicated. It was, especially at first. But students quickly adapted to having the Zoom, Livestreams and iClicker applications all running simultaneously. We also settled on an 86", large-format touch screen as the focal point and command center for Livestream and interactive components. The panel is nearly the size of a Pimentel Hall chalkboard and the company (Promethean) and distributors worked closely with us to meet the aggressive timeline for launching the course. Because it's essentially a giant tablet, with the swipe of a finger, we could run and annotate the PowerPoint presentation, play video chemistry demonstrations, run full-screen interactive chemistry apps, and manage the interactive concept tests and zoom rooms, all from a single platform.

With the help of the GSIs, we converted a spare bedroom in my home to a make-shift studio to broadcast in real-time to students from a dozen different time zones starting 8:00 a.m. Pacific Daylight time! The Livestream and asynchronous video were (and still are) openly available, and we soon discovered viewership far exceeded enrollment, often exceeding 6000 views a week.

We pushed the boundaries of the technology and pedagogy in a fast-paced, eight-week course. In evaluations, students commented on how helpful (and cool) it was to really explain what was going on by pausing a video demonstration, zooming in, and adding annotations right on the screen. The overall learning experience felt similar to our live classroom. We commonly heard feedback that the online learning didn't feel like isolated learning and the course made up for some of the disappointment students initially felt over not being able to come to campus for their first semester at Berkeley.

At Berkeley and beyond, the number of instructors employing interactive educational applications and flipped classrooms is skyrocketing. Our summer course demonstrated that students could readily adapt and respond to a blend of technologies. Use of an interactive flat panel screen can amplify and enhance these and many other educational experiences in the classroom and online; they are a near-perfect marriage of pedagogy and technology.

CHEM 105 REMOTE LAB

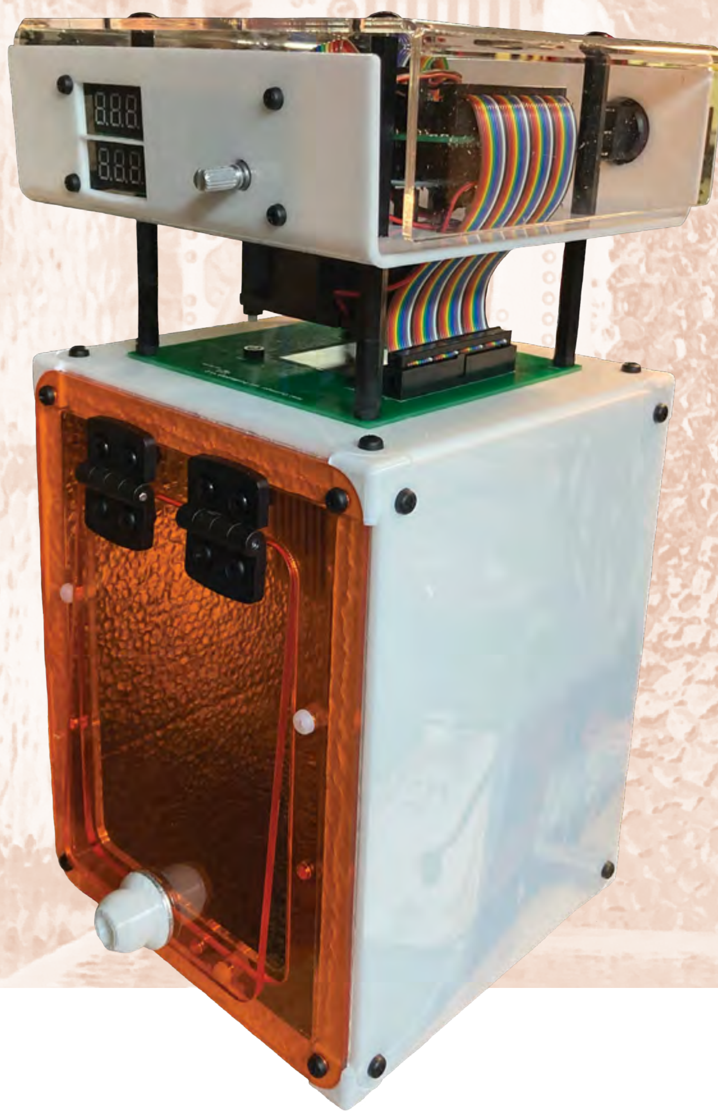
BY ASHOK AJOY *Asst. Professor of Chemistry*

We conceived of a "remote laboratory" experiment during the Fall 2020 semester as a means to give students in Chem 105, the upper division course in instrumental and analytical chemistry, hands-on experience with laboratory equipment amidst the COVID pandemic. The project leaders were research scientists Paul Reshetikhin and Emanuel Druga.

Our goal was to provide every student in the class a small device that we could ship to them and they could build and perform experiments with from the confines of their homes. This would allow them to engage with laboratory equipment while also giving them a flavor of the inner workings of instruments they would come across in future academic or industrial settings.

The lab "kit" shipped to every student and consisted of a 6in. cubical box, with a controllable resistive heater. The goal of the experiment was to stabilize the temperature of the box to within 0.2°C, and elevated 10deg above ambient. Students were meant to accomplish this by setting up a temperature feedback ("PID") loop. As a result, they were exposed to important concepts in feedback control in the context of temperature, that form a critical component in many laboratory instruments (e.g. gas chromatography). Moreover, through the experiment, the students learned how to interface and control an instrument with a computer through Labview and Python, a skill that is valuable in industry.

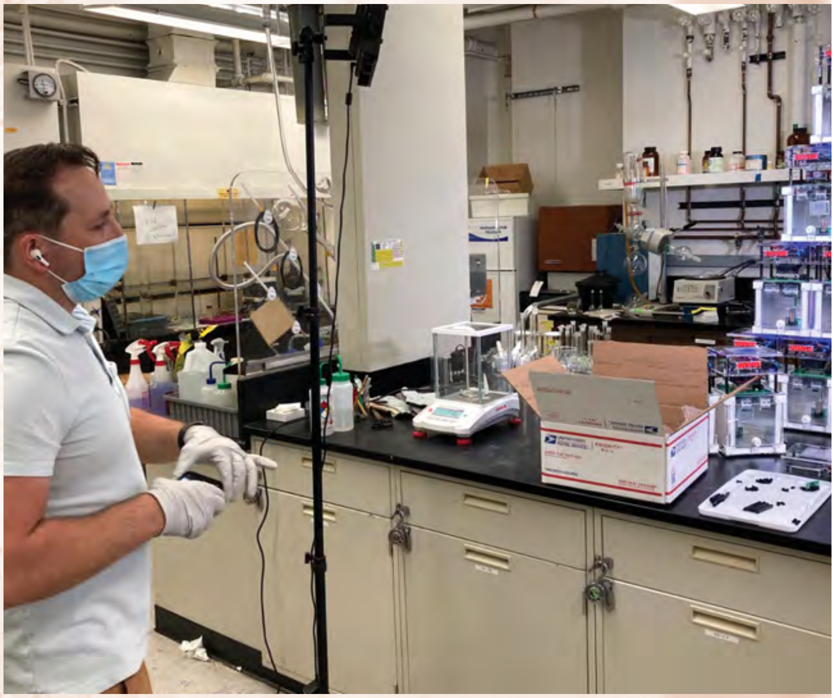
Perhaps the biggest draw of the experiment was that the students had to build the devices themselves. Our team designed, constructed, 3D printed and laser cut the components. The kits also shipped with an Arduino microprocessor and custom made printed circuit boards. These were provided to the students as a laboratory "kit", which they then had to assemble themselves. We were pleasantly surprised as to the extent the students enjoyed this; after spending several hours on



Zoom every day for their other classes, for many students this was there only source of hands-on activity. They even infused their own creativity into the experiment. For example, one student altered the 3D printed parts originally provided with thermoplastic material so that the device changed color as the temperature was altered.

Catering for a relatively large class size (26 students in Fall 2020 and 50 students in Spring 2021) meant that we had to design the devices to be low in cost and relatively easy to be produced en masse. Our final design employed low-cost electronics with custom made printed circuit boards (PCBs) that could be all snapped together with minimal soldering. The central heating component was also produced in a PCB, while the high-performance and low-cost sensors were employed to provide temperature values inside and outside the device. The devices cost ~$100 each and every student in the class had access to a device for several weeks to carry out their experiment from home.

Overall, the feedback from the students in this class was overwhelmingly positive. They enjoyed the chance to engage with an instrument at a deep level, and the experiment fostered a "builder" spirit in them. For many of them the experience was a highlight in an otherwise tumultuous semester.



Emanuel Druga works on the remote laboratories.

Upper photo: L-R: Paul Reshetikhin and graduate students Michelle Crook and Alex Prophet, do the box assembly.

ALL IMAGES COURTESY ASHOK AJOY LAB

NOBEL LAUREATE

Jennifer Doudna

& the bio revolution

BY MARGE D'WYLDE
PHOTOS BRITTANY HOSEA-SMALL

In a brief private ceremony on the morning of December 8, 2020, on her patio in California, Jennifer Doudna, the UC Berkeley Li Ka Shing Chancellor's Chair in Biomedical and Health Sciences, and Professor of Chemistry and Molecular and Cell Biology, was awarded the Nobel Prize in Chemistry.

Nothing was ordinary about this event, even by Nobel standards. The annual Stockholm ceremony, replete with pageantry and an amazing banquet, was postponed due to the ongoing COVID pandemic until at least the fall of 2021. Only immediate family including her husband and fellow scientist Jamie Cate, son Andrew Cate, and sister Ellen Doudna were in attendance. Her sister Sarah Doudna attended by phone from New York. Barbro Osher, Sweden's Honorary Consul General in San Francisco and a member of the UC Berkeley Board of Trustees, along with Anna Sjöström Douagi, Nobel Foundation VP of Science and Programs, drove from San Francisco to deliver the medal and hand painted diploma which had arrived from Sweden by diplomatic courier.

While the world was battling the COVID-19 pandemic, the Nobel Prize committee had quietly achieved a scientific milestone, awarding prizes in the physical sciences to three women. The recipients included UCLA's Andrea Ghez who shared the Nobel Prize in Physics "for the discovery of a supermassive compact object at the center of our galaxy." In addition, Doudna and Emmanuelle Charpentier, Founding and Managing Director, Max Planck Unit for the Science of Pathogens, shared the Nobel Prize in Chemistry for the "development of a method for genome editing". Their research had revealed how the Cas9 protein, part of the CRISPR system in bacteria, targets viruses, and allows for the process to edit the genomes of many organisms, including humans.

In another first, Doudna and Charpentier shared the coveted prize without a male counterpart. In 2018, Frances Arnold (Ph.D. '86, ChemE) was the first Cal alumna awarded the Chemistry Prize. Including the newest recipients, only seven women have won the Chemistry Prize since its inception in 1901.

According to the Nobel Foundation, "since Doudna and Charpentier's announcement of the CRISPR/Cas9 genetic scissors in 2012, their use has exploded. The tool has already contributed to many important discoveries in basic research in the human genome. Plant geneticists have used the technique to develop crops that withstand mold, pests, and drought. In medicine, clinical trials of new cancer therapies are underway, and the dream of being able to cure inherited diseases is about to come true. These genetic scissors have taken the life sciences into a new epoch already bringing breathtaking benefits to humankind."

CRISPR/Cas9 (CRISPR) has opened a portal to a whole new way of viewing biotechnology, creating possibilities for using the technology in biotherapy, plant breeding, disease modeling, disease diagnostics, and much more. The technology is also yielding great insight into the functions and roles of different types of genes in relation to climate change.

An example of the climate mitigation using CRISPR is taking place with coral reefs, the most biodiverse and climate-sensitive ecosystem in the world. Coral reefs sustain about 25% of all the ocean's fish and contribute to the livelihoods of over half a billion people. CRISPR has allowed researchers to identify which genes are involved in coral bleaching and to begin determining ways that can safeguard against this effect in the future.

The CRISPR discovery has also sparked the creation of innumerable startups, which have attracted hundreds of millions of dollars in investment worldwide in search of new cancer, hemophilia, and cystic-fibrosis treatments to name a few areas of experimentation. By 2019, over 15,000 research articles inspired by CRISPR research had been published.

According to Doudna, "It's a great tool for scientists because it gives all of us that are working with biological systems a way to manipulate the genetic material that tells cells what to do and tells organisms how to behave and how to act. And so, this has been amazing as a technology for fundamental discovery. But beyond that, it also provides a tool that allows real manipulation of disease-causing genes. And I think that's one of the ways that CRISPR is going to impact all of us in the coming years."

URGENT RESEARCH AND TECHNOLOGY NEEDED TO SOLVE COMPLEX BIOTECHNOLOGY CHALLENGES

In 2014, two years after the Nobel Prize-winning discovery was initially announced, Doudna thought the technology was mature enough to tackle a cure for the devastating hereditary disorder sickle cell disease that afflicts millions of people around the world. Some 100,000 Black people in the U.S. are afflicted with the disease. The Innovative Genomics Institute was formed as a partnership between the University of California, Berkeley and the University of California, San Francisco combining the fundamental research expertise and biomedical talent needed to work on the problem.

The new research team sought to repair the single mutation that makes red blood cells warp and clog arteries, causing excruciating pain and often death. Available treatments today typically involve regular transfusions, though bone marrow transplants can cure those who can find a matched donor.

After six years of work, the research team recently received approval for clinical trials by the U.S. Food and Drug Administration. This will enable the first trials in humans of a CRISPR-based therapy to directly correct the mutation in the beta-globin gene responsible for sickle cell disease.

The trials, which are expected to take four years, will be led by physicians at UCSF Benioff Children's Hospital Oakland and UCLA's Broad Stem Cell Research Center, who plan to begin this summer to enroll adult and adolescent patients with severe sickle cell disease.

The Innovative Genomics Institute's clinical diagnostics laboratory, which was built last year under Doudna's leadership to provide free COVID-19 testing to the Berkeley community, will play a key role in analytical support for the trial by developing diagnostics to monitor patient well-being and track the efficiency of the treatment.

"We are motivated to work toward a cure that can be accessible and affordable to patients worldwide," Doudna said of the trials.

In a 2019 Time article, Doudna stated, "There's a possible future where genetic disease is a thing of the past, where we routinely sequence DNA and treat harmful mutations as an outpatient procedure. But we must ensure that in this future, everyone will have access to these new technologies and there's a consensus on rules to regulate whether and how this technology is applied to the human germline."

DEVELOPMENT OF CASX AND TREATMENTS FOR GENETIC BASED DISEASES

Many companies developing CRISPR gene-editing therapies use variations of CRISPR-Cas9, the original gene-editing system described in 2012. Since then, Doudna's research group and others have looked for alternative Cas enzymes with better or different properties for gene editing beyond Cas9. One result of their search was finding a distinct family of RNA-guided genome editors dubbed CasX.

Discovered in 2016 by Jill Banfield and Doudna in some of the world's smallest bacteria, the protein is similar to Cas9, but significantly smaller: a big advantage if you're trying to deliver a gene editor into a cell.

In 2018, Doudna, Benjamin Oakes, UC Berkeley biochemist David Savage, and former Doudna postdoc Brett Staahl co-founded Scribe Therapeutics (Scribe) to create gene-editing therapies based on CasX.

"CasX has some features that could give it an upper hand over Cas9 as a gene-editing therapy," Oakes explains. "For one, CasX is a smaller protein than Cas9, which should make it easier to get into cells in the human body with gene-therapy delivery vessels like adeno-associated viruses."

Rather than "shoehorning" enzymes that evolved to work well in bacteria but not in humans into treatments for human disease, Scribe is engineering CRISPR molecules from scratch. This will allow the company to address problems seen in traditional CRISPR, such as safety, efficacy and off-target effects, where the treatment edits untargeted parts of the genome, causing harmful side effects.

Although Scribe continues to improve CasX, it has started working on gene-editing therapies for neurodegenerative disease with versions of the enzyme that it has already created. In October 2020, Scribe announced a partnership with Biogen to create CasX-based therapies for genetic forms of amyotrophic lateral sclerosis (ALS) and an option to work on another undisclosed neurological disease target.

CRISPR TESTING AND THE COVID-19 PANDEMIC

In 2020, at the height of the pandemic, Doudna, and other members of the Innovative Genomics Institute, convened to discuss what they could do to help battle COVID-19. During that meeting the group decided to pivot their projects and convert the research labs into an automated COVID testing facility expanding existing efforts to develop CRISPR-based diagnostics and genetic medicines that might help mitigate the pandemic.

Literally overnight the clinical diagnostics laboratory was turned into a lab that could test for COVID-19. Under Doudna's leadership, free COVID-19 testing was rolled out to the Berkeley community. Doudna commented, "In a typical year, if you tried to map the trajectories of all of the scientific projects in even one department at a large public institution like UC Berkeley, you'd find lines going in all directions at once. What happened last year was different. With a shared vision, a diverse team of professors, postdoctoral researchers, engineers, graduate students and volunteers all willingly put their personal and professional projects on hold to do something that had never been done before."

The science behind a PCR-based COVID-19 test was right in the team's comfort zone but spinning up a clinical laboratory was another matter entirely. Doudna continues, "Looking back, I'm still in disbelief at how quickly the team was able to safely overcome massive technical, logistical and physical barriers. In just three weeks, we secured lab certifications, developed new software and hardware with industry partners, ran the first of thousands of tests, received philanthropic funding to support lab operations, and started two dozen additional research projects, including a new rapid, point-of-need COVID test."

RIDING THE WAVE OF THE BIO REVOLUTION

Doudna's scientific research and startup endeavors are revolutionizing the biosciences. In addition to her innovative research work, she is co-founder of a number of companies including: Mammoth

JENNIFER DOUDNA is president of the Innovative Genomics Institute (a joint center of UC Berkeley and the University of California, San Francisco) which she co-founded with Jonathan Weissman in 2014. She is the Li Ka Shing Chancellor's Chair and Professor of Chemistry and Molecular and Cell Biology at UC Berkeley. She is an investigator with the Howard Hughes Medical Institute, and senior investigator at the Gladstone Institutes. She co-founded and serves on the advisory panel of several companies that are developing CRISPR technology.

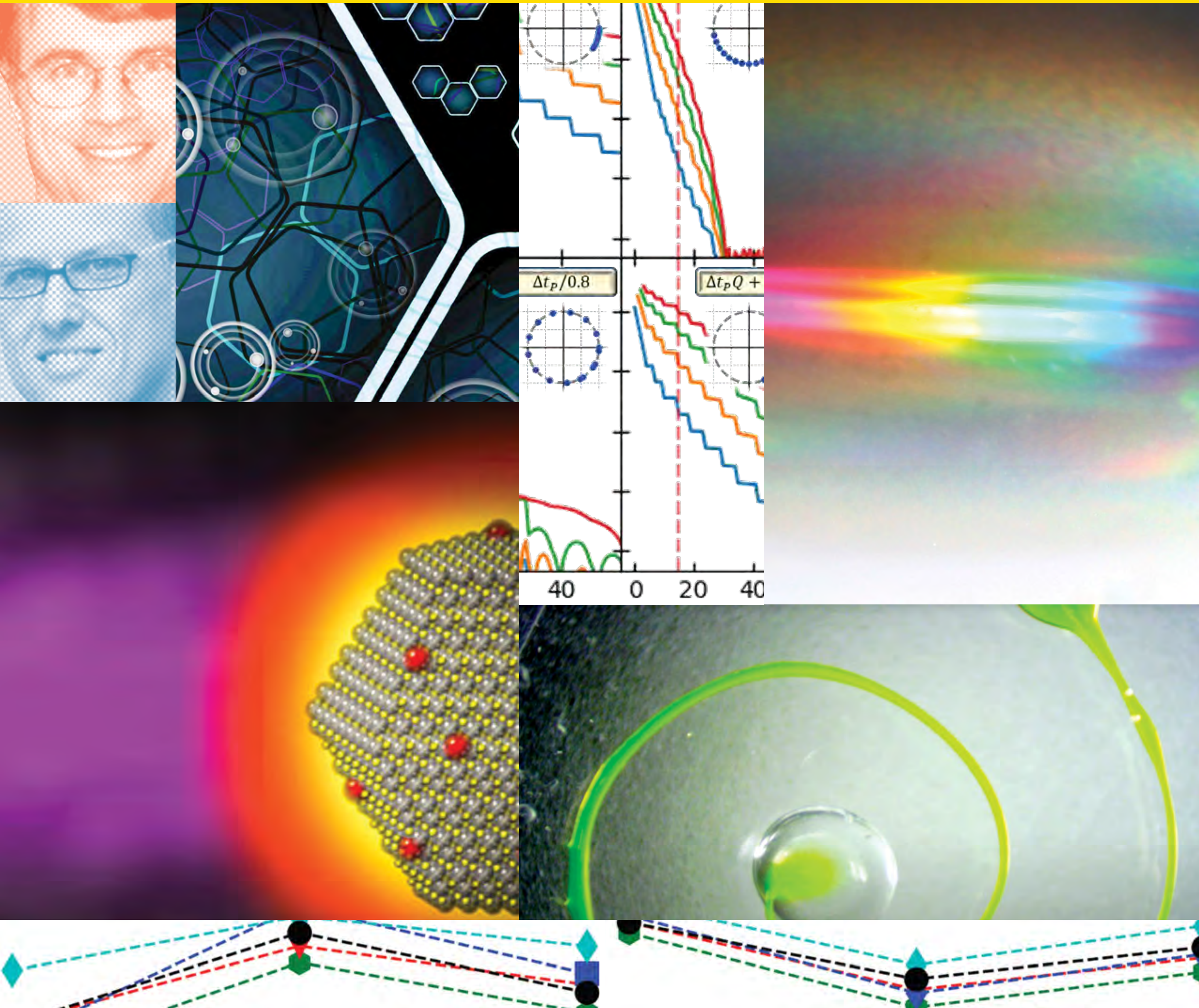
Biosciences, Caribou Biosciences, Intellia Therapeutics, Editas Medicine, and Scribe Therapeutics.

These companies are tackling some of the biggest challenges that the world is currently facing. Mammoth is working on a new type of COVID-19 test; Caribou is pursuing novel cancer therapies; publicly traded Editas is pursuing treatments for ocular, neurodegenerative, and blood diseases as well as cancer therapies; and Scribe Therapeutics is running trials for a CRISPR based approach to treat sickle cell disease.

Doudna is a biochemist, scientific leader, mentor, and entrepreneur. But most importantly, she is a scientist still focused on research and running her lab. In an article last year for C&EN magazine, Doudna commented, "I love the science. When I wake up in the morning, that's the first thing I'm thinking about, and when I go to bed at night, that's usually the last thing I'm thinking about."

> "CRISPR is a story of fundamental discovery science, collaboration, and the harnessing of a powerful engineering technology that gives new hope and possibility to our society."
>
> —**JENNIFER DOUDNA**, Nobel Laureate

The new era in theoretical



BY MARGE D'WYLDE

chemistry

Our understanding of quantum mechanics as we know it today was introduced about 100 years ago. Physicist Niels Bohr made foundational contributions to the insight of atomic structure and quantum theory in the 1920's.

Physicist Erwin Schrödinger published his famous "Schrödinger's cat" thought experiment highlighting the paradox of quantum superposition in 1935. Chemist G.N. Lewis, who was a renowned researcher and dean of the College of Chemistry between 1912 and 1941, did extensive experimentation on relativity and quantum physics, coining the term "photon" for the smallest unit of radiant energy, in 1926.

Early work in quantum chemistry was pioneered by physicists Walter Heitler and Fritz London, who published a study on the covalent bond of the hydrogen molecule in 1927. Quantum chemistry was subsequently developed by a large group of researchers that included theoretical chemist Linus Pauling at Caltech and physicist John C. Slater at Harvard who introduced various theories such as the Molecular Orbital Theory.

Today, many of our College of Chemistry scientists work across the disciplines of chemistry and physics. In fact, the College is renowned for its pioneering work in this area. Physicist and Nobel Laureate Ernest Lawrence arrived at the University of California's Berkeley campus having been wooed from a faculty position at Yale University by promises that included working with chemists in the College of Chemistry. His research relationship with G.N. Lewis, Glenn Seaborg, and, Melvin Calvin helped lead to ground-breaking discoveries in heavy water processing, the discovery of plutonium, and the discovery of the carbon dioxide assimilation in plants.

The first theoretical chemist at the College of Chemistry was the renowned Kenneth Pitzer who joined the faculty in 1937 after completing his Ph.D. in just two years. Pitzer was the founder of modern theoretical chemistry at Berkeley. He not only used quantum and statistical mechanics to explain the thermodynamic and conformational properties of molecules, but also pioneered quantum scattering theory for describing chemical reactions at the most fundamental level. He also made contributions to relativistic effects in chemical bonding and the theory of fluids and electrolyte solutions.

Robert Harris was next, arriving in 1963, followed by William Miller and Henry Schaefer in 1969. William Lester joined in 1981. Interestingly, Schaefer's story about becoming a theoretical chemist echoes tales from some of our current scientists in the theoretical chemistry group. Schaefer's true scientific calling was revealed during an organic chemistry course when he almost demolished a fume hood with a failed aniline experiment. According to his professor, "The damage here is far in excess of the lab fee you paid. Have you ever considered theoretical chemistry?

Today there are seven active faculty in the College's theoretical group. The members are working on some large scale problems. Quantum computers, quantum biology, and quantum dots are taking up some of the faculty's time. Others are working on theoretical questions about the structure of aqueous solutions and interfaces, nanostructures, cell signaling, and electronic structure.

Simulating chemical reactions is a complicated process. Today it takes powerful computing to model the increasingly complex molecular structures being researched. In tandem with the computers, theoretical chemists create more complex algorithms and mathematical analysis as chemistry research moves ever deeper into the quantum realm.

U.S. governmental agencies are also relying on theoretical chemists' research in groundbreaking efforts to build a fully realized quantum computer and network and hoping to be the first to eventually realize the establishment of the quantum internet. In a new "space race", other quantum network efforts are underway in Japan, the U.K., the Netherlands, and China. There is much to be gained from getting there first.

One possible future for theoretical chemistry is when chemists are able to discover new chemical reactions with a computer, and then verify them in the lab. In 2019, Google researchers announced they had used a quantum computer to simulate a chemical reaction for the first time. Although the simulation was of a simple reaction, this event marked a step towards verifying the use of quantum computers in chemistry.

According to Ryan Babbush who worked on the project at Google, "We're doing quantum computations of chemistry at a fundamentally different scale now. Years ago, quantum calculations were done with a pencil and paper by hand. While this reaction may be relatively basic, and it isn't necessary to have a quantum computer to simulate it, this work is still a big step forward for quantum computing. Scaling this algorithm up to simulate more complex reactions should be fairly easy."

Here, we catch up with four members of our theoretical group to see what they are working on including Martin Head-Gordon, Director of the Pitzer Center for Theoretical Chemistry, Birgitta Whaley, Phillip Geissler, and Eran Rabani.

Discovering the frontiers of electronic structure theory

MARTIN HEAD-GORDON

- KENNETH S. PITZER DISTINGUISHED PROFESSOR OF CHEMISTRY
- DIRECTOR OF THE PITZER CENTER FOR THEORETICAL CHEMISTRY AT UC BERKELEY
- FELLOW OF THE ROYAL SOCIETY
- MEMBER OF THE NATIONAL ACADEMY OF SCIENCES AND AMERICAN ACADEMY OF ARTS AND SCIENCES

Martin Head-Gordon's theoretical chemistry research is focused on the frontiers of electronic structure calculations through the development of novel theories and algorithms. His investigations center on the development and application of electronic structure theories, to analyze problems that are currently beyond the reach of standard methods. Since this information is crucial to understanding and controlling the chemistry of molecules, applications of electronic structure theory play an important and growing role in many areas of chemistry. Realization of this goal generally requires the coupling of fundamental quantum mechanics with large scale scientific computing.

Head-Gordon says of his research, "There is this concept that really began with Nobel Laureate John Pople about the fact that a good quantum chemical model should require no input other than what atoms are involved, where are the nuclei, and then the rest should be calculated by the model. You can then try and validate the model on some chemistry where you know the answers pretty well. If the results come out to your satisfaction, you can begin to computationally predict answers to other research questions with the model."

Head-Gordon is Director of the Pitzer Center for Theoretical Chemistry. The Center was established in 1999 to promote a home for excellence in theoretical chemistry by enhancing the education and research of students at Berkeley. The Center was established through an endowment from the Pitzer Family Foundation in honor of Professor Kenneth Pitzer *(Ph.D. '37, Chem)* and his wife Jean Mosher Pitzer. The Center is currently housed in sections of historic Gilman Hall, which was home to the labs of Nobel Laureates William Giauque and Glenn Seaborg and currently is home to seven active theoretical chemists and their labs.

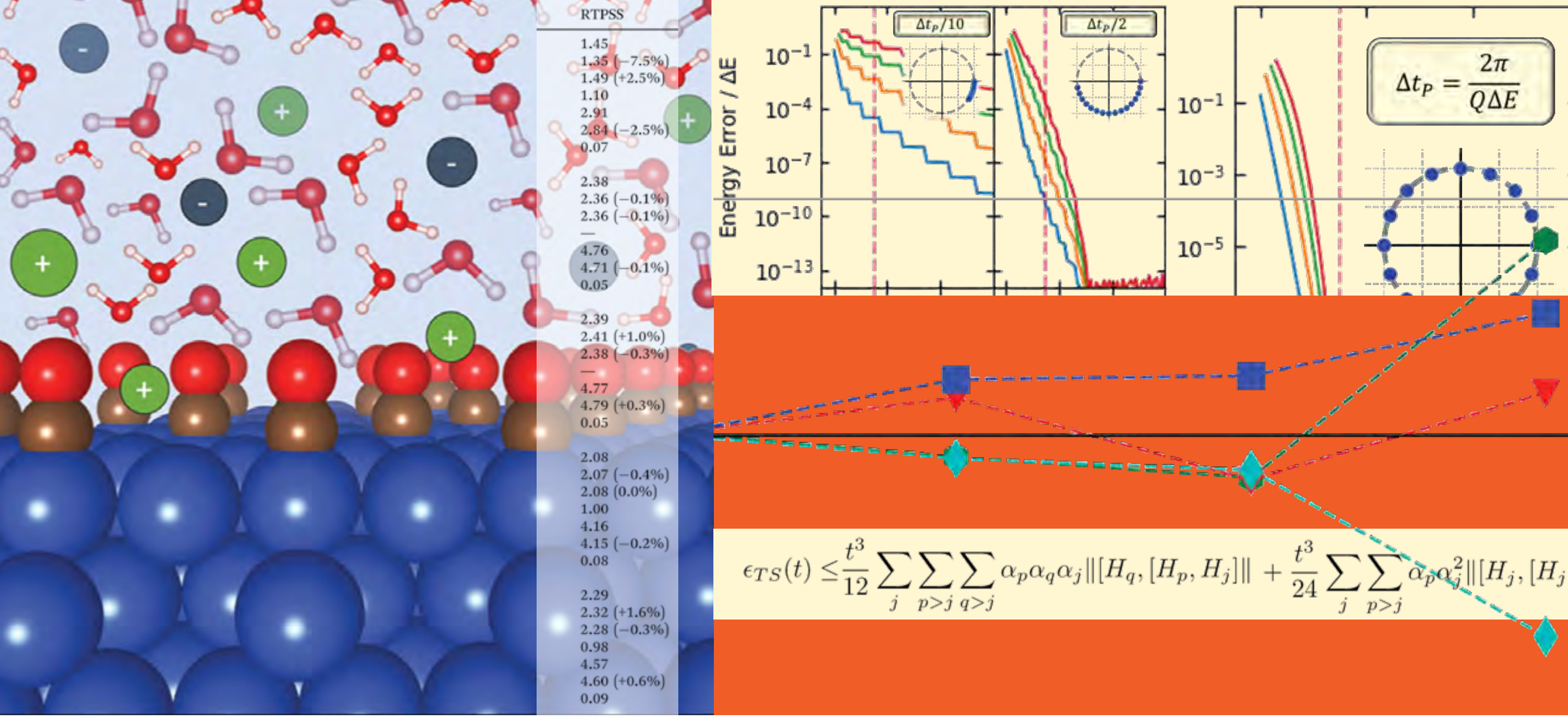
BUILDING BETTER THEORETICAL COMPUTATIONS

What kinds of problems are you currently working on?

MHG — In terms of my group's perspective, we are mostly about trying to exploit breakthroughs in computing hardware by making our own software, making new theories, and ultimately new algorithms. It is kind of like a food chain: from formal theory, to algorithms, to software, and then finally to groups that can use our software to solve problems.

Some members of the group are working on making better density functionals. Others are bridging between numerical experiments, which is what we do in quantum chemistry, and the research of experimental chemists. It is a form of energy decomposition analysis (EDA). For example, our EDAs are being used to understand the origin of hydrogen-bonding, to design better force fields (with Teresa Head-Gordon's group), and to understand the role of non-bonded interactions in catalysis (with John Hartwig's group).

Because our computational methods complement experiments, we often collaborate with experimental groups. One productive area of collaboration that I already briefly alluded to is catalyst design and function for areas such as new energy (converting photons to fuels), chemical transformations, and polymer up cycling.



What is Q-Chem software?

MHG — I have been involved in the Q-Chem project since the early 1990s. It was started by two members of John Pople's research group in 1992. He was my Ph.D. advisor at Carnegie Mellon. I joined as the third founder in 1993. We describe it as open team software because there are 100 to 200 active developers around the world who submit source code to the project. The software is licensed worldwide. We're lucky that we've been able to build up a significant community around Q-Chem with contributions to areas that include density functional theory, electron correlation, excited states, molecular interactions, and more. John Pople joined us as a director and code developer in 1999.

We think there are something like 50,000 copies of our code being used by chemists, material scientists, and others around the world. I think it's a way to have a larger impact in chemistry research. You can learn more about the Q-Chem project at https://www.q-chem.com/.

How are you solving chemistry problems using a simulated world?

MHG — There is the real world and then there's the simulated world, and they should match. Quantum mechanics is thought to be essentially exact for chemistry, just like Newton's equations are exact for predicting satellite orbitals around the earth. But while we can solve Newton's equations as accurately as we like and then build rockets and launch satellites on that basis, the equations of quantum mechanics are very difficult to solve. So, while Schrödinger's equation itself is exact, we can't solve it exactly. And so that's what keeps my research area busy. We are trying to improve our approximations and make them more accurate, so they can be more useful for predicting chemistry. That's what drives electronic structure theory.

What is your current interest in quantum computing?

MHG — Currently, I am collaborating with Birgitta Whaley on some research because quantum chemistry is thought to be one of the possible early applications for quantum computers. I published a paper in *Science* in 2005 which simulated quantum chemistry on a quantum computer. Quantum computing research is a focus of intense interest right now because of exciting advances in hardware, with the prospect of more to come.

Nothing can simulate a quantum system better than another quantum system. For that reason, quantum chemistry is a promising application on a quantum computer. It will be really fascinating to see where that goes.

SOLVING FUTURE PROBLEMS

What is a big problem that can benefit from a quantum chemistry focus?

MHG — The Haber-Bosch process (which takes nitrogen from the air and converts it into ammonia to make fertilizers) is one of the most energy intensive chemical processes in the world. If we could have a green alternative to that, it would be wonderful.

The ideal solution would be to use solar energy to produce ammonia. Imagine having a catalyst that could take atmospheric nitrogen and water, do a little bit of electro catalytic magic with the aid of some green energy to produce ammonia and oxygen. In fact, there are already some catalysts that will do this. But they are not yet active or efficient enough to be industrially useful.

Quantum chemistry can help by unraveling the mechanism of an existing catalyst that maybe has a too slow turnover frequency or too high energy cost. Once we understand the origin of its limitations, we might be able to improve it or gain inspiration for a better catalyst.

The quantum realm
BIRGITTA WHALEY

- PROFESSOR OF CHEMICAL PHYSICS
- DIRECTOR OF THE UC BERKELEY QUANTUM INFORMATION AND COMPUTATION CENTER
- CO-DIRECTOR OF THE NSF CHALLENGE INSTITUTE FOR QUANTUM COMPUTING
- EXECUTIVE BOARD MEMBER, CENTER FOR QUANTUM COHERENT SCIENCE
- FELLOW, AMERICAN PHYSICAL SOCIETY AND MEMBER, AMERICAN ACADEMY OF ARTS AND SCIENCES
- EMERITUS MEMBER, PRESIDENT'S COUNCIL OF ADVISORS ON SCIENCE AND TECHNOLOGY

Birgitta Whaley is a pioneer in the field of quantum mechanics. She is a foremost expert in the fields of quantum information, quantum physics, molecular quantum mechanics, and quantum biology. She is investigating the role of quantum mechanics in functional biological systems. Another research focus is on quantum control and quantum information. Her theoretical work in quantum computation is currently centered on creating algorithms, applications, and error correction for near-term noisy quantum computers.

Whaley states, "When it comes to really understanding the quantum world, we are still at an early stage. Quantum mechanics poses fundamental questions for our understanding of the world in which we live — from the behavior of the smallest particles to that of black holes, from the behavior of simple physical systems to complex chemical and biological phenomena that drive life."

In a recent talk, Whaley discussed new quantum biology insights, "Current research is showing mounting evidence for the existence of dynamical phenomena in biological systems that involve coherent quantum motion in unexpected situations, requiring us to revise our long-standing view of quantum effects in biology. New quantum research into plant and bacterial photosynthesis, bird navigation, and other biological processes is more than just cataloging the quantum chemical properties of the biological systems. What we are looking at, and what makes it very challenging, is that we want to understand the relationship of the biophysics/chemistry bridge to biological function. We are now looking at integrating microscopic, mesoscopic, and behavioral studies into our research and that is very challenging."

ON QUANTUM BIOLOGY

Why is the discovery of quantum mechanics in biology more recent than in chemistry?

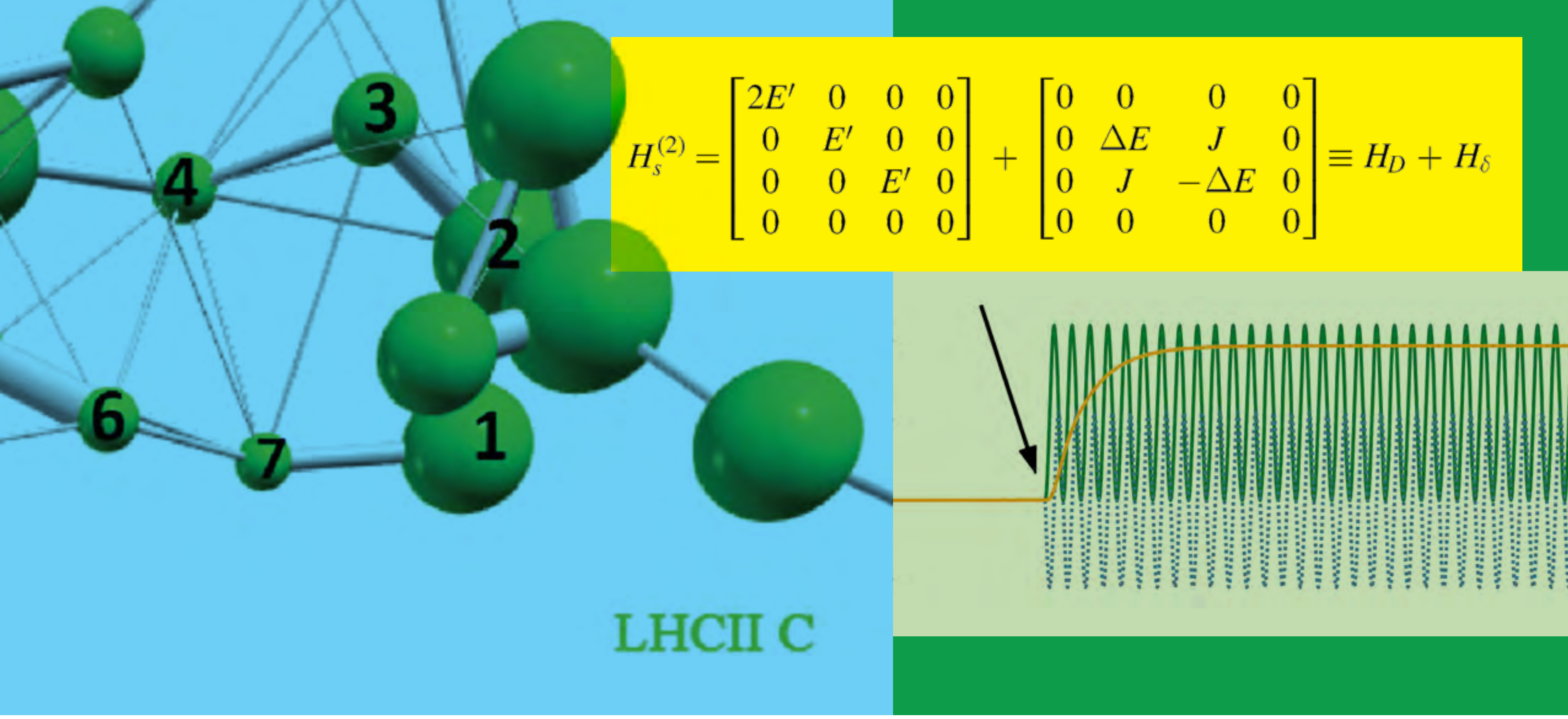
BW — The underlying influence of quantum mechanics in biology via its role in determining molecular energy levels and reaction barriers was acknowledged in the 1930s but things got more interesting for studying quantum biology after the advent of the laser in the 1960s. To get to the timescales where non-trivial dynamical quantum effects are relevant for biological systems, the timescale of electronic motions over femtoseconds had to be accessed. And that did not happen until methods of ultrafast spectroscopy were pioneered in the 1970s and 1980s. Previously, biologists realized that molecules had discrete energy levels but had no way to access the associated quantum dynamics of key molecular processes.

What are scientists looking for in quantum biology research?

BW — The line between the quantum and classical realms in physics and chemistry is porous. This is part of the reason why this is such an exciting area.

The overarching goal of research into quantum biology is to understand biological function across all time and size scales. This means two things. The first is to develop tools that can go all the way down from the macroscopic to sub-atomic particles to probe the structure and dynamics of biological systems. The second part is to travel from the smallest to the largest component in biology asking the question can "quantum coherence be relevant for a biological function"?

Function is like the jewel in the crown at the top of our understanding of biological systems. You shouldn't speculate about function before you actually know what the structure really is. And after structure, then you should start thinking about dynamics. How does this work? What



are the mechanisms? What are the timescales? And what are the quantum features that you might see in measurements? And only when all this is understood can you start to think about function.

What is next for quantum biology research?

BW — Recent research has shown mounting evidence for the existence of dynamical phenomena in biological systems that involve coherent quantum motion in unexpected situations, requiring scientists to revise their long-standing view of quantum effects in biology being restricted to understanding of molecular energetics, stability and kinetics.

These revelations have led to a new generation of studies bringing the tools of advanced quantum optics and quantum information science and technologies to probe complex biological phenomena such as photosynthesis and bird navigation, raising our understanding of the role of quantum mechanics in functional biological systems.

ON QUANTUM COMPUTERS

Are there commercial applications for quantum computers?

BW — In late 2018, Congress passed the National Quantum Initiative which directed the Office of the President to establish goals and priorities for a 10-year plan to accelerate the development of quantum information science and technology applications. I was invited to join the President's Council of Advisors on Science and Technology to create recommendations in the areas of Industries of the Future including artificial intelligence, quantum information science, and advanced manufacturing and biotech. The quantum recommendations included building infrastructure at scale utilizing Federal investment in quantum computing user facilities and a quantum internet and intranet. A number of federal programs have since been set up to explore scientific and information processing applications of quantum computers. Many of these will have commercial applications, e.g., in communications, chemicals and pharmaceutical industries, or in the financial sector.

What is currently happening in quantum computer research?

BW — Quantum computers are not going to be sitting on our desktops any time soon, but we are now building them. They have the potential to execute complex algorithms billions of times faster than classical computers. Currently we are at "stage one", with quantum machines having on order of 50-70 quantum bits (qubits). What is not clear is when and how we will go from stage one to stage two, with more than 100 qubits and some error correction. In the current iteration, we don't have enough qubits to explore the full power of quantum algorithms.

Performing the simulations that many people undertake in chemistry on classical computers is very time consuming when done at scale. For instance, when Phillip Geissler is simulating the chemical dynamics of multiple solutes in water, he needs to make a simulation that is as large as possible. But the time for that computation can scale exponentially with the number of particles, which puts a constraint on how much information it can yield.

However, if you can do the simulation on a quantum computer with an algorithm whose time scales only polynomially with the number of particles, there is a signification gain. It's a difference in the scaling of compute time as you go to larger numbers of particles or degrees of freedom.

So, the power of quantum computation lies in the way in which the required resources increase as you go to a large scale calculation. If you're doing calculations only on small scale systems, you never see this difference between the classical and the quantum.

Statistical mechanics of complex materials and biological systems

PHILLIP GEISSLER

- ALDO DE BENEDICTIS DISTINGUISHED PROFESSOR OF CHEMISTRY
- MEMBER, AMERICAN CHEMICAL SOCIETY
- AWARDED THE DONALD STERLING NOYCE PRIZE FOR EXCELLENCE IN UNDERGRADUATE TEACHING AND THE UC BERKELEY DISTINGUISHED TEACHING AWARD
- ALFRED P. SLOAN FELLOWSHIP AND A KAVLI FRONTIERS FELLOW

Phillip Geissler uses theory and computer simulations to study molecular phenomena at the frontiers of physical chemistry. His work spans a variety of systems ranging from aqueous solutions and interfaces to biomolecular assemblies, to nanoscale materials. These systems share essential motifs of disorder and heterogeneity that are amenable to the tools of modern statistical mechanics. Using those tools, he explores emergent physical principles which govern complex molecular systems.

"A characteristic feature of the microscopic world is that nothing stands still. For instance, if you look at a glass of water on a macroscopic scale, it will appear that nothing is happening," Geissler states. "It looks completely placid. But it is universally true that if you zoom in and focus on what's going on at the scale of nanometers or angstroms the molecules are in constant motion."

His work with longtime collaborator Richard Saykally, a physical chemist in the department, has clarified many aspects of these molecular motions in liquid water. For example, their combined experimental and theoretical approach resolved a forty year old question about how water molecules arrange themselves in a liquid drop. They demonstrated that nearby molecules in water adopt not just a few intermolecular structures, but instead a whole continuum of arrangements – from strong hydrogen bonds to highly distorted geometries. They later showed how dissolved salts can stick to the interface between liquid water and air, controlled in part by microscopic undulation of the liquid's surface.

ON CREATING THEORETICAL SOLUTIONS

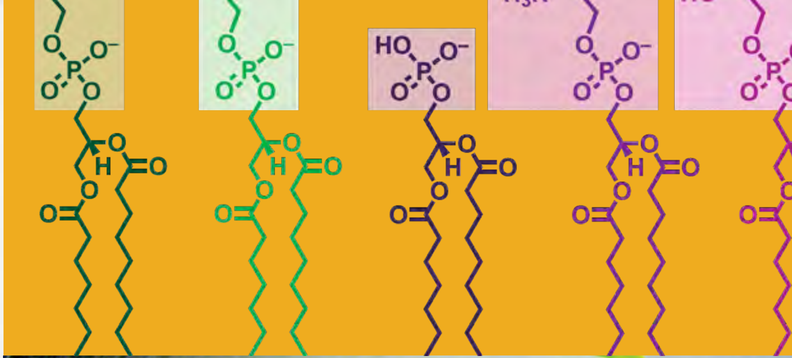
What are examples of your research in statistical mechanics?

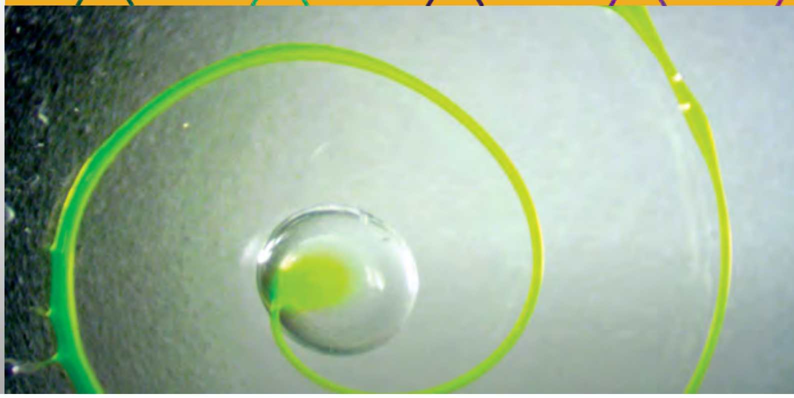
PG — In a very recent example, we showed that active particles – self-propelled particles that move in different ways than typical molecules – can crystallize much as common substances do. Like bacteria and flocks of birds, these particles consume energy to power their motion and thus do not follow familiar laws of equilibrium thermodynamics. And yet they can condense and crystallize in close analogy to water. This tantalizing result suggests that we can eventually understand living, nonequilibrium systems with principles and concepts similar to those we currently teach in undergraduate physical chemistry. My young theory colleagues David Limmer and Kranthi Mandadapu are doing important research to discover such new laws.

In another example, we worked with Berkeley Lab material scientist Thomas Russell to develop a way to print 3-D structures composed entirely of liquids. The approach uses a modified 3-D printer to inject threads of water into silicone oil, sculpting tubes made of one liquid into another liquid. The key is a special nanoparticle-derived surfactant that locks the water in place, in essence a special soap that prevents the tubes from breaking up into droplets. Our theoretical contribution helped establish a physical basis for the locking mechanism, which gives clues on how to improve these nanoparticles.

What kinds of theoretical problems interest you?

PG — What fascinates me is how the variability of microscopic structure can dictate the way things work. The kinds of problems that appeal to me are problems where the answer is not a single structure, or not just an average, but the answer really lies in understanding what underpins those variations and what combinations of molecular motions are important to how a particular phenomenon works..





For over a hundred years, we have known that macroscopic properties of materials (their conductivities and heat capacities and catalytic behaviors) are controlled by fluctuating arrangements of atoms and molecules. But in many areas of chemistry, experimental tools have emerged only in the last couple of decades to witness in vivid ways the existence and the importance of those variations. The growing, detailed recognition that microscopic variability is essential to how proteins function and assemble, how nanocrystals form and react provides a wealth of exciting problems for us to work on.

Nano-science has been a revolution in that regard, both in developing the ability to image what goes on at microscopic scales, but also in synthesizing miniature materials that demand an accounting of fluctuations. So now systems of interest have moved from things that look placid to things that are fundamentally variable. I like to say this is the age of statistical mechanics.

How do theorists and experimentalists work together?

PG — Historically, there was not a clear separation between experiment and theory. That has been a product of the last 50 years or so. I think it is important to recognize how the scientific process plays out in chemistry. When we say we understand something, it's because we have a theoretical model for how the world works and we can compare that model with what happens in reality. Traditionally, those two things were inseparable parts of the research being done by chemists. They developed the model descriptions, mathematical descriptions of how the universe might work at the molecular scale and performed measurements in the laboratory to hold up against those models.

Science is much more specialized today. Laboratory skills and innovations have become technical in a way that really occupies most of one's expertise. The same thing has happened on the theoretical side. The kinds of mathematical analysis and computing skills required to build complex molecular models have become a specialized endeavor. But the process of discovery still requires combining these capabilities. It also benefits profoundly from combining experimental and theoretical perspectives. I have come to realize how strongly the way you think about a problem is shaped by the tools that you have.

ON CREATIVE TEACHING

You are a highly regarded teacher at the College. One of your known specialties is you play the guitar and sing in Chem 1A classes. How did you get started with that?

PG — My father and mother are accomplished musicians. I grew up in a very musical household and from a young age music really appealed to me. It took a while for me to find my instrument the same way it took a while for me to find theoretical chemistry as my discipline. After several years of failed piano lessons, I found the guitar and fell in love. (Finding theory as my love required several years of growing bacteria and breaking glassware.)

The songs I use in the course were introduced to me by my high school biology teacher. She and I even performed one at a high school talent show. The songs were written by Michael Offutt, who is still composing and performing today. They involve very basic chemistry and turned out to be perfect for Chem 1A.

I was surprised to see how often my musical performances were mentioned in students' course evaluations. Many students wrote that the songs helped them study and remember important concepts. And for some of them, it was just entertaining. I think any time someone who is passionate about teaching tries a new way of communicating, something good comes out of it. Some students learn in ways that you never really thought about. The songs really resonated with many of them.

Theoretical and computational nanoscience

ERAN RABANI

- GLENN T. SEABORG CHAIR IN PHYSICAL CHEMISTRY, UC BERKELEY
- PROFESSOR OF CHEMISTRY, TEL AVIV UNIVERSITY
- FOUNDER AND DIRECTOR OF THE SACKLER CENTER FOR COMPUTATIONAL MOLECULAR AND MATERIALS SCIENCE, TEL AVIV UNIVERSITY
- SOME OF HIS MANY AWARDS INCLUDE VISITING MILLER PROFESSORSHIP, THE BRUNO MEMORIAL AWARD, AND THE ISRAEL CHEMICAL SOCIETY AWARD

Eran Rabani is a pioneer in developing theoretical and computational tools to investigate fundamental properties of nanostructures. He currently investigates the structural, electronic, and optical properties of nanocrystals, doping of nanoparticles, exciton and multiexciton dynamics at the nanoscale, and transport in correlated nano-junctions. Much of this relies on the development of stochastic electronic structure techniques to describe the ground and excited state properties in large-scale nanostructures.

He is also a pioneer in describing real-time dynamics of many-body interacting systems. In 2011, he was inspired by a challenge from Nobel Laureate Philip W. Anderson, who wrote that the understanding of classical glasses was one of the biggest unsolved problems in condensed matter physics. Rabani and his colleagues at Columbia University were intrigued and asked the question, "If we looked at the material at the quantum level, would we still see the hallmarks of a classical glass?"

The researchers demonstrated that under very special conditions, namely a few degrees above absolute zero, glass could melt. "It all has to do with how molecules in materials are ordered," Rabani explained. "At some point in the cooling phase, a material can become glass and then liquid if the right conditions exist."

ON RECENT THEORETICAL FINDINGS IN QUANTUM DOT RESEARCH

You are part of a research team who recently announced exciting new findings about the behavior of quantum dots.

ER — Bright semiconductor nanocrystals known as quantum dots give QLED TV screens their vibrant colors. But attempts to increase the intensity of that light generate heat instead, reducing the dots' light-producing efficiency. Results from our recent study have broad implications for developing future quantum and photonics technologies.

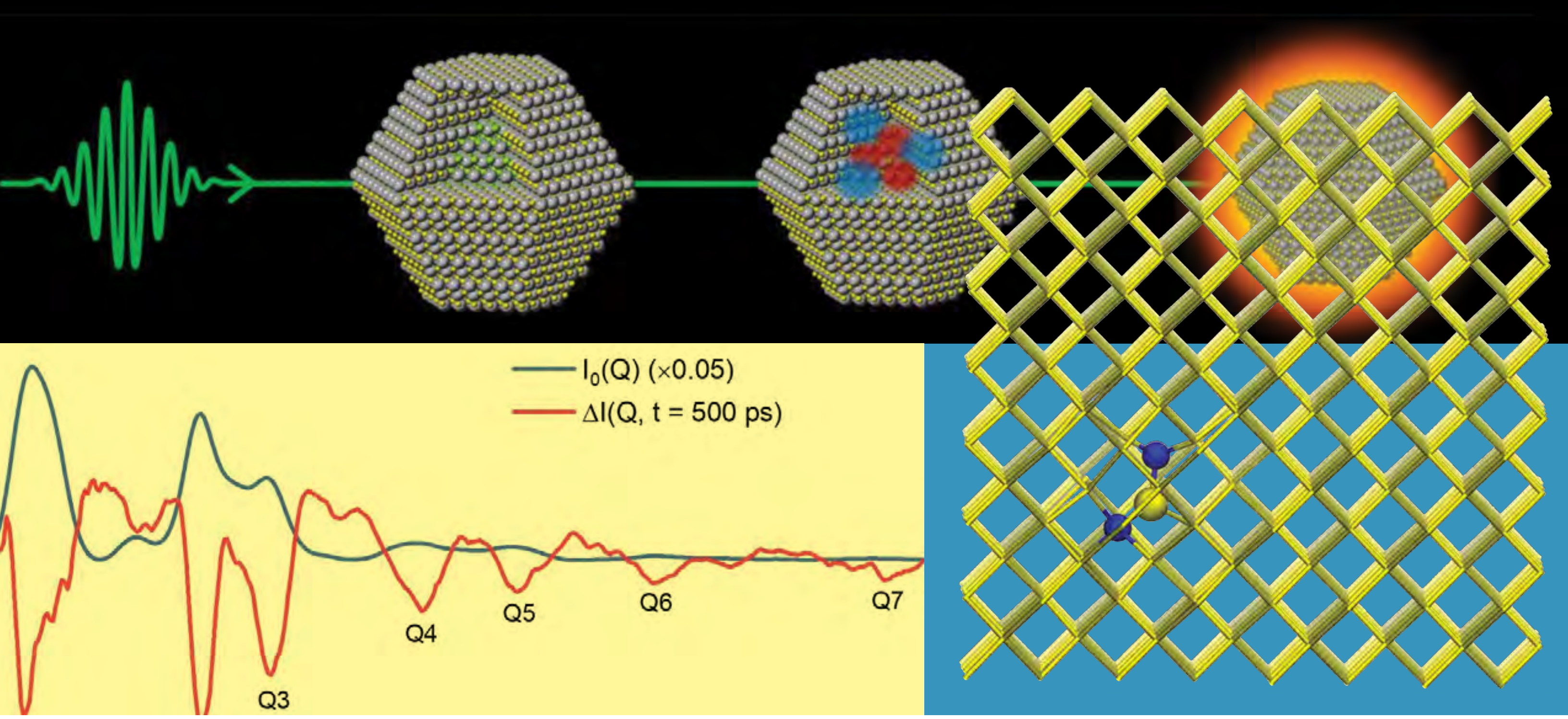
Members of my lab worked with other labs at Stanford and Berkeley to study the behavior of quantum dots as they were hit with various wavelengths and intensities of laser light. The scientists used a high-speed "electron camera" to watch dots turn incoming high-energy laser light into their own glowing light emissions. Several members of my lab, including graduate students Dipti Jasrasaria and John Philbin, worked to calculate and understand the resulting interplay of electronic and atomic motions from a theoretical standpoint.

We met with the experimenters regularly. Ideas were flowing back and forth between the team members, but it was all seeded from the experiments, which were a big breakthrough in being able to measure what happens to the quantum dots' atomic lattice when it's intensely excited.

The theoretical question we looked at specifically was the mechanism for this outcome. That is what my group explained. Through atomistic simulations and coupling many different ideas together, we ended up with a core picture which we were able to synch with the observable outcomes from the experiments. I thought that was impressive.

How does this research enhance our understanding of photonics?

ER — This research is part of an ongoing DOE Energy Frontier Research Center grant on photonics at thermodynamic limits,



managed by Jennifer Dionne who is the Senior Associate Vice Provost for Research Platforms at Stanford. The center includes four principal investigators from Berkeley including myself, Paul Alivisatos, Naomi Ginsberg, and Eli Yablonovitch who is from Electrical Engineering and Computer Science.

The center's research goal is to demonstrate photonic processes, such as light absorption and emission, at the limits of what thermodynamics allows. This could bring about new technologies including refrigeration, heating, and cooling as well as quantum computers and new engines for space exploration, which would be powered entirely by light.

In this project, using femtosecond electron diffraction measurements corroborated by atomistic simulations, we uncovered transient lattice deformations accompanying radiationless electronic processes in colloidal semiconductor nanocrystals. Investigation of the excitation energy dependence in the core/shell system showed that hot carriers created by a photon energy considerably larger than the bandgap induced structural distortions at nanocrystal surfaces on few picosecond timescales, were associated with the localization of trapped holes. Elucidation of the structural deformations associated with the surface trapping of the hot holes provided atomicscale insights into the mechanisms deteriorating optoelectronic performance and a pathway towards minimizing losses in nanocrystal-based devices.

ON THE FUTURE OF THEORETICAL CHEMISTRY AT UC BERKELEY

If you could predict the future of theoretical chemistry, what would it look like?

ER — I think it's very hard to predict the future, even though I'm a theorist and that's my job. I know how to do it for molecules, but to predict what human beings are going to discover is harder to do. What's unique about our department's members is that their approach is broad so there is a chance of discovering things in many different directions, not just in one. All of them are equally important.

What is significant about the theoretical chemistry research at Berkeley?

ER — What is unique about Berkeley, and different from the other places I have visited, is the very collaborative nature of the organization. I collaborate with many experimentalist from our department (Paul Alivisatos, Peidong Yang) and from other departments and also interact very closely with other theorists, like David Limmer and Phill Geissler.

This is very important because it allows our students to be exposed to many different ideas and ways of working theoretically. The department offers a unique environment in that regard. The faculty are all working on distinctive, exciting research. Also, we have a big theory group here at Berkeley with tremendous quality in the research.

Where do you think the Pitzer Center theoretical chemistry group is headed?

ER — Theoretical chemistry is a modern discipline within the field of chemistry. Historically, a department would only hire one or two theoretical chemists. In recent years, the need for theoretical and computational support and the complexity of questions asked in chemistry, physics, and materials science, requires closer collaborations between theory and experiments. Today, we have seven theoretical chemists in the department working in diverse fields.

I have seen significant progress in the last decade in our understanding of the behavior of more complex chemical systems, being able to describe complex phenomena on more diverse length- and timescales. A lot of progress has been made in our understanding of various fields including information, biology, and materials sciences. Berkeley's theoretical group has been central in many of these recent developments.

We also have an exceptionally talented younger generation of faculty working on extremely challenging problems. Together with the more senior scientists I see a brilliant future for theoretical chemistry at Berkeley.

IN CONVERSATION WITH

CBE's Karthik Shekhar

BY DENISE KLARQUIST

In the fall of 2020, the Department of Chemical and Biomolecular Engineering (CBE) welcomed Karthik Shekhar as an assistant professor. Shekhar currently leads a research group (www.shekharlab.net) in the College of Chemistry and is also a member of QB3, the Helen Wills Neuroscience Institute, Cellular and Computational Biology, and the Biophysics graduate program. Combining his background in chemical engineering, computational biology, and neuroscience, Shekhar's work is guided by fundamental questions: What more can we understand about the general principles behind neural diversity in the brain? What are the molecular mechanisms that regulate its development? And how did it evolve?

Using experimental techniques of single-cell genomics and computational approaches based in machine learning, Shekhar and his team are generating insights into the developmental and evolutionary origins of cellular diversity, and exploring its biological consequences.

We recently spoke with Karthik to learn about the origins of his interests and his work.

DENISE KLARQUIST — You grew up in Mumbai, India. Tell me about your early background and what inspired your interest in science and technology.

KARTHIK SHEKHAR — My father was a chemical engineer, and, in my youth, he was definitely an inspiration although he was not a scientist; he became a successful entrepreneur. During high school, I enjoyed math and physics, but unlike in the U.S., where you have the option of entering in your first year of college and then later choosing to major, in India you had to decide in advance. So, I chose engineering because it was a more common option and it naturally made sense.

I attended the Indian Institute of Technology, Bombay (IIT), where I received my B.Tech. and M.Tech. in 2008. I did an internship at Purdue University during my third year and realized that research was something I enjoyed. I applied to a few Ph.D. programs and ultimately decided on MIT's chemical engineering program.

DK — How did you transition from chemical engineering in Mumbai and Boston to what you do now, which is at the intersection of cellular biology, chemical engineering and machine learning?

KS — During high school, modern molecular biology was simply not part of the curriculum in India the way it is now. And as an engineer, it was just not part of my thinking.

At MIT, the chemical engineering Ph.D. degree program has a biology requirement. You have to either demonstrate a sufficient number of credits in biology as an undergraduate, which I didn't have, or you have to supplement that with an MIT course. I ended up taking an undergraduate freshman biology class, which I wasn't very happy about at the time. But the nice thing about MIT is that all the basic undergraduate classes are taught by some remarkable scientists, giants in their field. And that's when I became excited and decided to bring these two aspects together; the quantitative thinking of physics, math, and biology.

In 2009, I joined Arup K. Chakraborty's group at MIT, who previously had been at Berkeley. I worked on applying statistical physical models to the area of immunology, particularly focusing on how the adaptive immune system works. Most of my focus was on understanding the evolutionary landscape of HIV, the Human Immunodeficiency Virus. This was when I began using machine learning methods to analyze large-scale biological measurements using technologies that were just being developed.

For my postdoc, I joined the Broad Institute, in the laboratory of Aviv Regev, where she was contributing to the emerging area of single-cell genomics. At the time, most genomic measurements were classically done by averaging many cells together. We began working on ideas to combine various engineering approaches with molecular biology tools to conduct measurements at the single-cell level where you treat each entity as separate. In consequence, the data that you end up measuring is large-scale and highly dimensional, so we needed statistical, inference, and machine learning techniques to make sense of it.

DK — A lot of what you're doing now has to do with studying vision and the retina. Can you explain why?

KS — Two reasons, really. The nice thing is that the retina has a very well-defined input, which is light, and a very well-defined output, which is the optic nerve. So, it's almost like a self-contained microcosm of the brain. The other reason is while it's been studied for more than 100 years, a lot remains that we don't fully understand.

During my postdoc, we focused on diversity of neurons in the retina in adulthood. Now, we're studying how this diversity arises during the early years of development. What molecular changes are

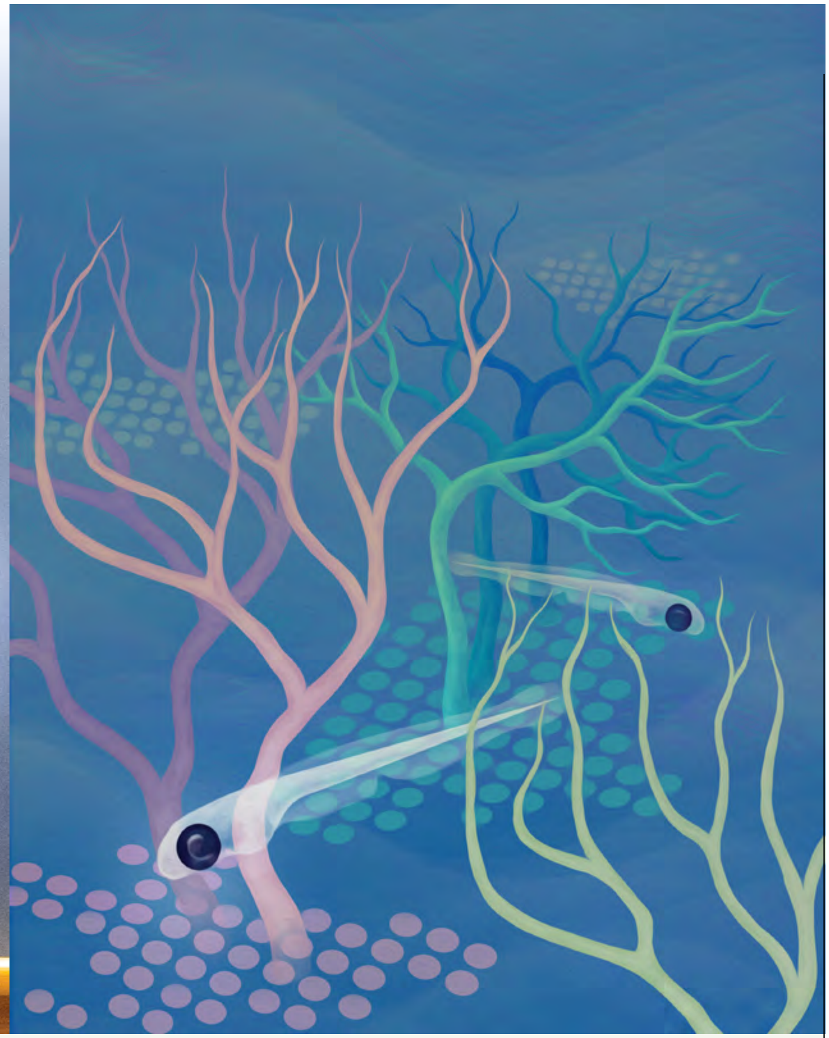


ILLUSTRATION JULIA KUHL AND YVONNE KÖLSCH (MAX PLANCK INSTITUTE OF NEUROBIOLOGY, GERMANY)

important and what's associated with that? We're also looking across evolutionary timescales. There is this nice dichotomy in that the basic fundamental architecture of the retina has been conserved for about 500 million years, however one level deeper, there is a lot of divergence we don't fully understand associated with the unique visual needs of different species.

Going beyond the retina, we have a project now in collaboration with Professor Larry Zipursky at UCLA to understand how diverse neurons develop in the visual cortex, and the interplay of genetic predisposition as well as visual experience. This is a new breed of research for me, and it was initiated during the pandemic!

DK — Tell us a little bit about what attracted you to Berkeley and what you enjoy most?

KS — At Berkeley, in particular the Department of Chemistry and Biomolecular Engineering, I felt at home intellectually. I've definitely felt like an outsider wherever I've been because you're either an engineer among biologists, or you're a biologist among engineers. But the assistant professors here are people who have a focus on energy, analytical chemical systems, some who are doing more condensed matter theory and so on. The intellectual diversity is almost an article of faith. Also, the fact that we have a great undergraduate student body, and for a chemical engineering department, we are one of the best in the country.

DK — Having come on board only a month before the pandemic forced the lockdown of campus facilities, your teaching experience at Berkeley has certainly been unique. What have you found most rewarding?

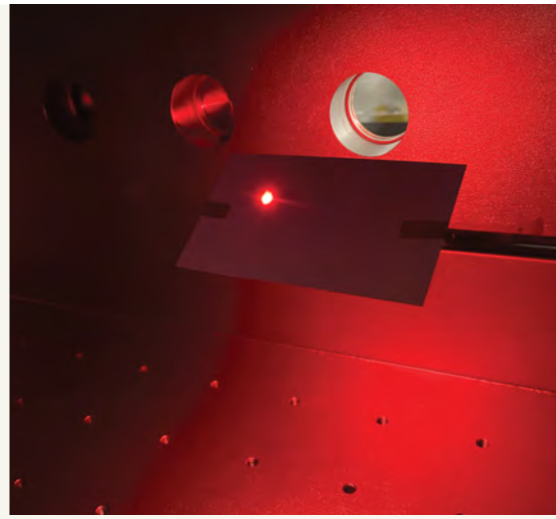
KS — I think if you enjoy teaching, and I really do, seeing 100 students write on their end-of-the-year evaluations that they enjoyed it, and they appreciated that it was taught well, that's a real kick. The way I see it, that's the greatest and most sustainable contribution scientists can make in their life because you're educating individuals who possibly will go on to make breakthroughs that you couldn't.

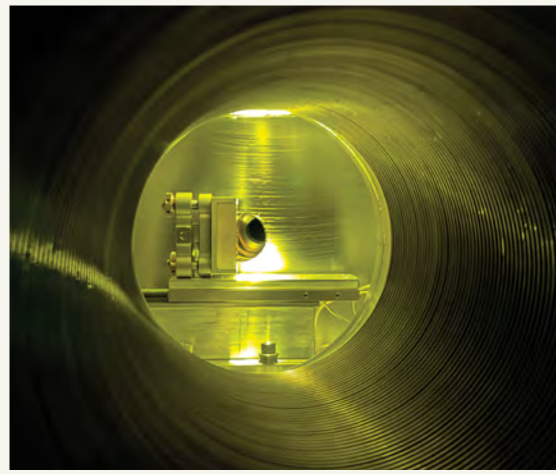
DK — Thinking about the future, what's next?

KS — Specific questions about how cell types evolve and how do you go from molecules to structure in the visual system were not things I was thinking of working on in 2020. I have also initiated a collaboration with my colleague Prof. Kranthi Mandadapu to explore new areas at the interface of neuroscience and physics, which I am really excited about. I hope a year from now there will be something related but completely different which I also could not have predicted. This is one of the joys of science. I'm reminded of a quote from Alice in Wonderland that says, "if you don't know where you're going, any road will take you there."

MICHAEL ZUERCH

Shining a light on solid matter energy dynamics





BY DENISE KLARQUIST

Comparing the complex materials science research that is the focus of Assistant Professor of Chemistry Michael Zuerch's work to a roller coaster ride may seem like an odd analogy. Yet, it is a remarkably effective means to explain how he is using light to understand and manipulate energy states in solid matter, which could ultimately lead to new mechanisms for solar energy conversion, information storage or even computation at the speed of light.

"It revolves around understanding the electron dynamics in a solid material once you photoexcite it," Zuerch explains. "Think of the electrons taking a ride in a roller coaster. When we shine in a light pulse, we kind of kick the electron up a hill, and then it comes back to the equilibrium state. However, when the electrons return to this relaxed state, they often change along with the atoms around them. What we want to know is how this happens."

Zuerch is one of the newest faculty members to join the Department of Chemistry. He and his multi-disciplinary research team are using ultrafast X-ray spectroscopy and nanoimaging to investigate electron dynamics, the roller coaster journey so to speak, in novel quantum materials and heterostructures. He uses sophisticated instrumentation to produce femtosecond laser pulses and attosecond X-ray pulses for high-resolution imaging of these ultrafast phenomena. Through this research, Zuerch seeks to potentially manipulate and stop the process at an intermediate state, hoping to answer vital questions in materials science and physical chemistry.

Born in a remote region of East Germany, just prior to the country's reunification, Zuerch attributes his open-mindedness and curiosity to his upbringing during this era. "My family strongly encouraged me to take advantage of the new opportunities to study and explore in the reunified and opened country; opportunities my parents did not have," he explained.

As a teenager, Zuerch initially hoped to study informatics and computer science. Constantly having to fix and rebuild the unstable computers he was using, he realized one of the limitations to computer speed had to do with the technology of semiconductors; it was the materials that limited upscaling. As his studies progressed, he noted the same limitations could also apply to energy storage and energy transfer.

An engaging high school teacher who was also an active research physicist opened his eyes to the practical aspects of experimental physics, influencing his decision to enroll at Friedrich Schiller University Jena where he obtained his diploma and subsequent Ph.D. in physics in 2014. Both the university and the city, home to companies like Carl Zeiss, are renowned for innovation in optics and lasers.

"Ultimately, going into physics was a very good decision; it combines a lot of those aspects I was originally interested in. My work still involves programming, and the one-of-a-kind optical and laser instrumentation we use, we need to build ourselves. A lot of those things relate to my past."

In 2015, Zuerch chose the College of Chemistry at Berkeley for his postdoc. While it may seem unusual for a trained physicist to land in the Department of Chemistry, Zuerch explained that given his expertise in non-linear optics and his interests, it was the best place he could find himself. "As a Ph.D. student, I became an expert in making X-ray laser light out of optical laser light, using X-ray flashes to take images of materials. But it was static; you need to watch the matter in motion to understand it. And so that's what attracted me to Stephen Leone and Daniel Neumark's work at Berkeley who became my postdoc advisors and are now my colleagues."

The question Zuerch sought to answer was how to add the time dimension to these spatial observations. "Berkeley is world-leading in that area, so it was really the best possible place for me to come and explore."

In the Department of Chemistry, Zuerch found a focus on the applications for his work. "In the chemistry department, there are people asking questions like how can

we use that for solar energy conversion? How can we use that to make solar fuels? Even though I am trained as a physicist, that's much closer to where I want to be."

When an offer came to return to the College of Chemistry as an assistant professor, he naturally jumped on the opportunity, joining the faculty in 2019.

This spring semester, Zuerch has been teaching a physical chemistry lab, which is one of the courses that has been particularly impacted by the pandemic. Like many instructors, he has faced the challenge of bringing the lab virtually to students, relying heavily on the ingenuity of his GSIs to create video based experiments.

Zuerch sees the diversity of expertise represented in the college as an enormous benefit. "My lab currently hosts chemistry students and two physics postdocs. I, myself, am a trained physicist, but now am mostly thinking about the chemistry applications of my research. It's really a melting pot of clever people with very different backgrounds coming together to resolve some big challenges. And that is the spirit of Berkeley I appreciate so much and another reason why I wanted to come back to this place. It's truly unique."

Moreover, Zuerch appreciates the collaborative and open environment that is a hallmark of the college. "People care about your success and your progress. It's extraordinary how researchers pool their ideas, creating joint proposals to attract funding which ultimately enables you to do the research. There is a lot of bouncing of ideas among colleagues which is fantastic."

Today, Zuerch finds himself at the interface between materials science, physics, and chemistry, seeking to unlock the means toward developing novel material processes that may enable better solar energy harvesting or efficient and faster computation.

Recently, Zuerch and his interdisciplinary team received a generous grant to fund the California Interfacial Science Initiative (CISI). The program is one of 15 research projects funded by the University of California's 2021 Multicampus Research Programs and Initiatives (MRPI) competition to support research and discoveries in fields important to UC and the people, environment, and economy of California.

The CISI project leverages the combined theoretical and experimental physical chemistry expertise of members from six UC campuses. With Zuerch at the helm, the collaborative effort seeks to address challenges arising from climate change and mitigate human impacts on the environment through the advancement of interfacial chemistry and interfacial molecular structure. Investigations in this area could lead to breakthroughs in clean water production, carbon dioxide capture, removal of plastics from water, clean energy production, and energy storage in next-generation solid-state batteries.

"As an advocate for public education, the fact that my first large grant is coming from the State and a public institution is very exciting," said Zuerch.

As to the future, Zuerch, like the vast majority of the UC Berkeley community, is looking forward to the day when he can return to campus and his lab. "Being in the lab with the students I work with is awesome. It's exciting to interact with these bright people and learn from them. And I hope they learn a few things from me."

In terms of his field, he sees opportunities to harness the vast dispersed expertise of the global research community to study the abundance of new materials that are being synthesized daily. In fact, the pool of materials is much larger than the capacity to study them.

"What I hope for the future would be an international collaborative framework, a database that brings all the small innovations together in a bigger picture. We have the tools and materials available, but we haven't quite yet found which opportunities are most promising. Finding those and encouraging researchers to contribute to this effort would be enormously valuable to society."

Introducing Professor Joelle Frechette

BY MARGE D'WYLDE

"I am looking forward to joining the CBE department at the College of Chemistry. Berkeley has some amazing scientists and facilities. It will be interesting to see what new research projects grow out of my relocating to the West Coast."

We are delighted to introduce Professor of Chemical and Biomolecular Engineering (CBE) Joelle Frechette who will be joining us this summer from John Hopkins Whiting School of Engineering. Frechette graduated from Princeton with a Ph.D. in Chemical Engineering and Materials Science in 2005. After postdoctoral work at UC Berkeley in the lab of CBE Professor Roya Maboudian, she joined the Johns Hopkins faculty in 2006. She was awarded the NSF CAREER award in 2008, the 3M untenured faculty award in 2008, and the ONR Young Investigator Award in 2011. In addition, she was elected as a Fellow of the American Chemical Society in 2017. She is a faculty fellow of the Hopkins Extreme Materials Institute. Currently she is vice president of the Adhesion Society.

A native of Montreal, Canada, her interest in science began late in high school. Frechette comments, "I liked how science taught me how the world works. It helped me understand my environment."

She discovered geology before college. "There was a lot of chemistry and physics involved in my first geology class. But I really appreciated the connection to the world around me, for example seeing rock formations while driving in a car and understanding their origins. It really struck a nerve, and something clicked. I went on and took a second geology class and that's what lead me to materials engineering in college afterwards."

She went on to undergraduate study at the École Polytechnique de Montréal which included a year abroad at the University of Arizona. It was there she discovered her passion for research. She was encouraged to apply to the Chemical Engineering Department at Princeton and went on to receive her masters and Ph.D. at that institution. While at Princeton her interest shifted to the measurement of surface forces.

After graduate school, Frechette investigated unwanted adhesion in microelectromechanical systems in a postdoctoral project at UC Berkeley in the lab of Roya Maboudian. Frechette comments, "I was a big fan of Roya's work. I had followed her research in grad school. The connection between surface phenomena to micro & nanotech was really neat. It was a super rewarding but short postdoc. Too short actually."

From there, she joined the chemical and biomolecular engineering faculty at Johns Hopkins. Once settled into her lab, she began publishing research on adhesion in fluid environments, particles at interfaces, and electrowetting. Frechette brings a broad engineering and chemical perspective to her research projects. She has repeatedly found solutions that are creative in their planning and execution.

In a novel experiment, Frechette and a chemical engineering colleague utilized off-the-shelf equipment, including Legos, to develop a way to visualize how nano particles travel through an array of obstacles. The design was a human scale version of a "lab on a chip" which scientists were using to determine how to separate single molecules. The ability to change the configuration of the Lego pieces, which stood in for obstacles designed to sift the particles on the chip, mimicked several sorting scenarios allowing the researchers to easily make multiple observations. Frechette said. "It's interesting that you can spend so much time devising elaborate research projects for investigations. And here,

Polymeria3 (digital print on aluminum) explores what happens to sticky polymers, at a molecular level, when two adhered surfaces are separated

PHOTO COURTESY CHRISTOPHER P. SLOAN.

we came up with a very simple idea that worked really well."

Currently her lab is looking at how things stick, or do not stick together in soft materials. Some of the lab's output is in the area of adhesion under extreme conditions. Adhesives are a huge industry. Frechette is drawn by the interdisciplinary aspects of adhesion science as it brings together chemists, engineers, and physicists. Frechette enjoys the engineering process and industry impact.

Frechette collaborated with the 3M company to investigate how surface properties affect wet adhesion (when Band-Aids are exposed to water and sweat for example). "This was a very interesting research problem," Frechette stated. "A member of the lab wound up designing and building a new instrument for the project. It was dubbed the 'multimode force microscope'. It is basically a fluorescent inverted microscope coupled with normal and lateral force measurement. The imaging capabilities allow us to monitor the deformation profile during adhesion measurements."

Other aspects of her research program are in the area of colloids and nanoparticles at fluid interfaces. Her group is also researching how to use particles at interfaces towards the development of optical materials. In a 2019 publication, a research team she led announced they had created a liquid manufacturing process to make compound lenses with most of the features of the mosquito eye as a potential miniaturized vision system for robots and drones. To create the microlens, the researchers used a capillary microfluidic device to produce oil droplets surrounded by silica nanoparticles. They organized multiple microlenses into a closely packed array around a larger oil droplet then polymerized the structure with ultraviolet light to yield a compound lens with a viewing angle of 149 degrees. They used a novel strategy to test the lens by printing numbers on a flexible, transparent sheet that was flexed above the lens.

Conceptual artist Christopher Sloan recently showcased Frechette's research in an interdisciplinary art project exhibited at Hopkins Extreme Materials Institute. Sloan, a former art director at National Geographic, was inspired by the molecular, atomic, and subatomic level projects that members of Frechette's lab and several of her colleagues were working on. The outcome was stunning 3D rendered models and printed works on aluminum.

Frechette commented, "The students in my group were stimulated by their discussions with Chris. The artwork that came out of the project was beautiful."

Jeffrey Reimer, Chair of CBE, commented on Frechette's arrival, "Professor Joelle Frechette brings to the chemical engineering discipline experimental rigor, insightful analyses, a proven track record of undergraduate teaching and research mentorship, administrative experience as a program leader, and an ability to articulate complex notions to a broad community. CBE believes her addition to the Berkeley campus will bring us further distinction and we look forward to seeing her in person in Gilman Hall!"

JOELLE FRECHETTE'S RESEARCH aims to understand and control solid-fluid interactions in soft materials. Her research interests in the area of colloid and interfacial science include: adhesion in fluid environments, particles at fluid interfaces and surface force measurements. Her group designs materials by harnessing the properties of solid and fluid interfaces for application in the areas of adhesion, separation, sensors, wetting, and optics. Her experimental approach includes the development of novel tools and instrumentation, modeling and simulations, and surface characterization.

COLLEGE ADVISORY BOARD

Alumni & Industry Leadership

BY MARGE D'WYLDE & LAURENT DE JANVRY

COLLEGE FACULTY AND ALUMNI AT A 2019 BOARD MEETING: (l to r) John Arnold, Andre Argenton, Ted Hou, Richmond Sarpong, Drew Lanza, Harmeet Singh, Alan Mendelson, Georgieanna Scheuerman (partially obscured), Ann Pease, Douglas Clark, Andrew Ramelmeier, C.H. Chan, Gary Masada, John Markels, Matthew Francis, Alexis Bell, Ron Silva, Margaret Chu-Moyer, Cynthia Murphy and Ellie Yieh.

When Professor Gilbert Newton Lewis was Dean of the College of Chemistry (1912 – 1941), interactions with industry were highly discouraged as this was seen as potentially disrupting the freedom of the faculty's research interests with undue corporate influences.

After World War II, with the growth of chemical engineering and organic chemistry came more interest in industry interactions with the College. Thus, the way was opened for the first new source of private funding to come from industry. Professor C. Judson King, when he became Chair of the Department of Chemical Engineering in 1972, initiated the first industrial Advisory Board for the department.

Members of the initial Board represented typical employing industries at the time and included Board Chair, Richard Emmert of DuPont; Walter Benzing of Applied Materials; Thibaut Brian of Air Products; David Brown of Halcon International; W. Kenneth Davis of Bechtel; H. D. Doan of Dow Chemical; Bryce MacDonald of Kennecott Corp.; John W. Scott of Chevron; and Frank B. Sprow of Exxon.

The departmental Advisory Board functioned for many years in a very helpful fashion. One of the first recommendations they made was for the development of graduate level instruction in process economics. Another was for further instruction in written and oral communication.

During his deanship of the College of Chemistry (1994 - 1999), chemical engineering professor Alexis Bell created an Advisory Board for the College of Chemistry at large, at which point the separate departmental Advisory Board was discontinued.

Bell commented, "I decided as dean that the College could benefit from having an Advisory Board. Since this concept had worked so well for the department, I asked my colleagues whether they saw any problem with terminating the departmental board and rolling it over into a college board. Since there was no objection, and the Department of Chemistry also supported the idea, we started a College-wide Board."

Since its start, the Advisory Board has served the College in a number of critical capacities. Up until Tan Kah Kee Hall became a capital project for the College, all buildings in the College had been funded by the State of California. With the State's changing fortunes, the University had to start raising funds for new buildings. The Board was essential to funding a large segment of the $40M project which was opened in 1997. Nobel Laureate and Professor Emeritus Yuan T. Lee *(Ph.D. '65, Chem)*, and alumnus John Heil *(Ph.D. '65, ChemE)*, who were both on the Advisory Board at the time, were integral to raising funds for the building which today hosts a number of active faculty research labs and the College's computing center.

In 2016, when former UC Berkeley Chancellor Dirks threatened to break up the College for campus budgetary reasons, the Advisory Board went into action to help activate the greater College of Chemistry community to band together and push back on the University's plans. In a letter to Dirks identifying the shortcomings of disbanding the College, the Board said, "We are very fortunate to have the history and brand power of the UC Berkeley College of Chemistry at this pivotal period, where developing new revenue sources is vital. We are also quite fortunate to have in place the leadership of Dean Douglas Clark, who has had the foresight to guide the College of Chemistry in a new direction to develop these crucial revenue sources."

The Advisory Board has also played a pivotal role in helping the University and College develop a venture capital fund. The Berkeley Catalyst Fund (BCF), founded in 2016, was started by alumni Laura Smoliar *(Ph.D. '95, Chem)* and Ted Hou *(Ph.D. '95, Chem)*. The BCF is responsible for investing in science based start-ups, with some earnings benefiting the College. Many of the startups the BFC invests in are direct outcomes of research by our faculty and graduate students.

The Berkeley Catalyst Philanthropic Fund (BCPF) was established to allow alumni to donate to the College of Chemistry, receiving tax deductible credit for their donations, which are then invested by the UC Berkeley Foundation into the BCF on behalf of the College of Chemistry. All potential proceeds benefit the College of Chemistry. The BCF and BCPF program has become the model for other University of California venture capital funds.

The Advisory Board continues to provide supportive leadership to develop and implement the College's strategic objectives

"As a former student and current Advisory Board member, I could not be prouder to be part of Berkeley Chemistry, especially with the recent awarding of the Nobel Prize in Chemistry to Professors Frances Arnold and Jennifer Doudna, two spectacularly talented teacher-researcher-scientists, both who have deep roots to our College and are great women role models. My own experience at UC Berkeley as an undergraduate chemistry major, an undergraduate research trainee, and chemistry stock room assistant formed the foundation for my career in chemistry – so being on the College of Chemistry Advisory Board is a way to give back to the College that has given so much to me."

—**MARGARET CHU-MOYER,** *B.S. '83 Chem, Ph.D. '93 OChem (Yale), Vice President of Research, Amgen Inc.*

"I decided to join the College's Advisory Board because for me, the experience of pursuing a Ph.D. in Chemical Engineering in the CoC was incredibly rich. The opportunity to collaborate and live with the best students and faculty anywhere in the pursuit of learning and the creation of new understanding was profound, and the relationships formed have been deep and lasting. The opportunity to extend those relationships and at the same time give back and contribute to the bright future of the College was an obvious choice."

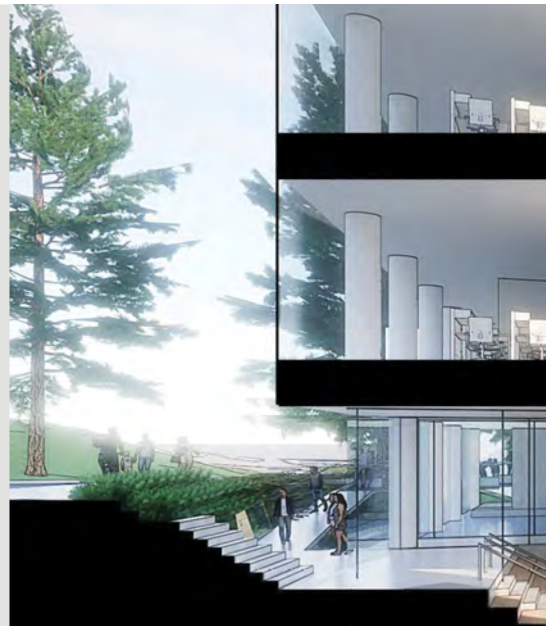
—**JOHN MARKELS,** *Ph.D. '93,* ChemE, President, Merck Vaccines

which include increasing our financial strength; fulfilling our public education, research, and service mission; and enhancing our academic excellence and worldwide reputation. The Advisory Board is focused on the following five strategic objectives: student-alumni engagement; revenue generation; development; reputation and brand; and diversity, equity, and inclusion.

Currently, the Advisory Board consists of 22 alumni and key corporate partners of the College of Chemistry, and is chaired by John Markels *(Ph.D. '93, ChemE)*, President of Global Vaccines at Merck. Our Advisory Board represents a diversity of industries and functions, and includes scientists, business leaders, venture capitalists, entrepreneurs, and intellectual property attorneys across the biotech-pharma, energy, chemicals, and materials industries with representatives from Amgen, Applied Materials, BASF, Chevron, Dow Chemicals, Fosun Pharma, Lam Research, Merck, PMP Tech, Sangamo Therapeutics, among others.

We greatly value diversity on the Advisory Board. Over the last few years, we have increased our representation of women to 30%. Read about our current members online at chemistry.berkeley.edu/advisory-board. As we look to the future, we hope to expand our Advisory Board's membership to a cadre of 30 to 40 alumni and corporate partners.

➤ If you are interested in learning more about participating on the Advisory Board, please email Laurent "Lo" de Janvry at ldejanvry@berkeley.edu

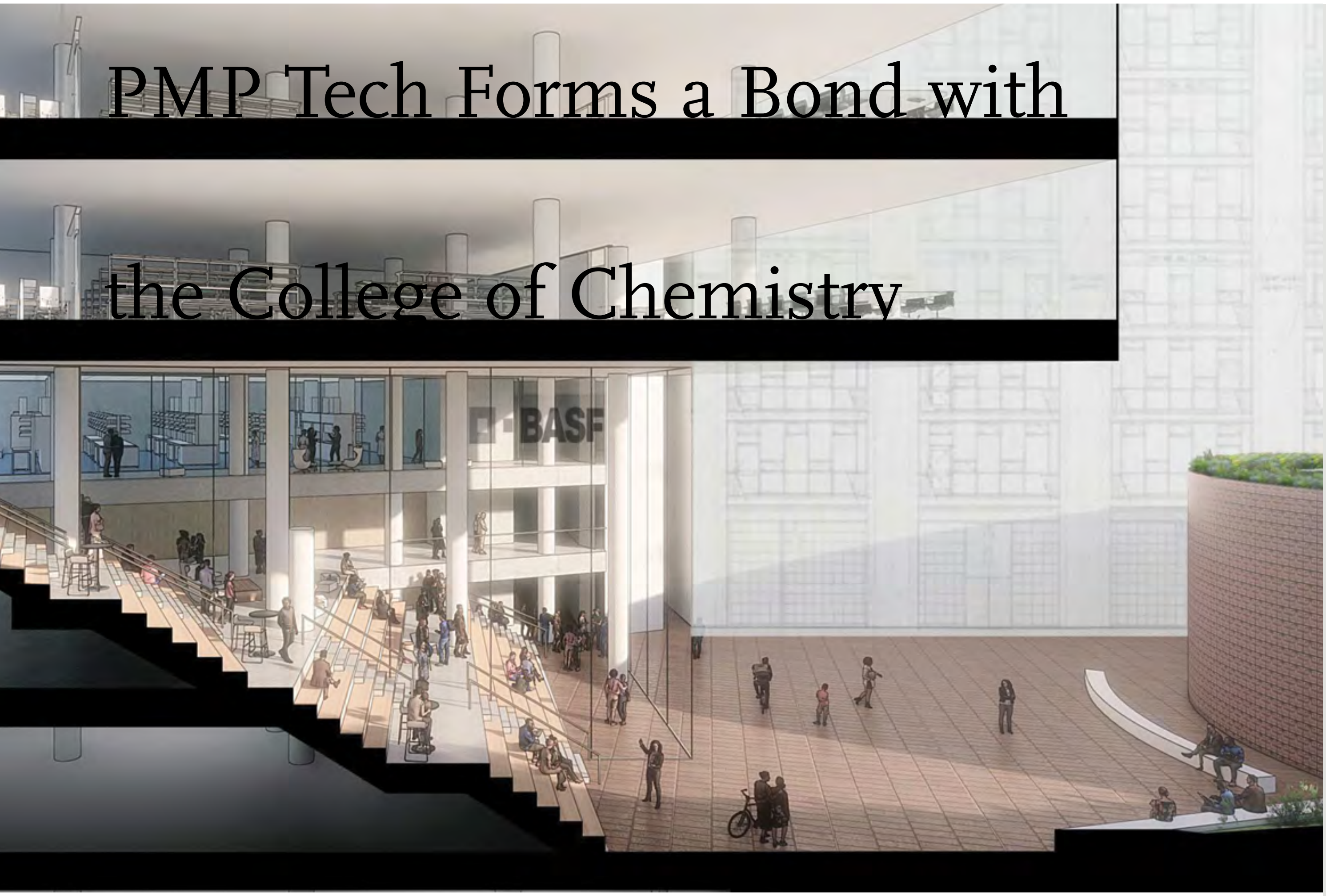


A $10 million commitment from Taiwan-based company Pioneer Material Precision Tech (PMP Tech) will catalyze educational opportunities for future generations of Berkeley chemistry, chemical engineering, and chemical biology students and help realize a vision of constructing a ground-breaking building to house the world's most advanced community of chemical scientists and engineers.

Last year, the company — a leading global manufacturer of innovative high-tech elastomers and other environmentally friendly rubber products for consumer electronics — contributed $3.6 million to establish the PMP Tech Chancellor's Chair in Chemistry, currently held by chemistry professor T. Don Tilley.

Now PMP Tech has strengthened its bond with Berkeley by investing in a top cam-

PMP Tech Forms a Bond with the College of Chemistry



paign priority for both the campus and the College. Heathcock Hall will enable expansion of research and undergraduate teaching in state-of-the-art laboratories and collaborative spaces, while providing facilities where faculty and student entrepreneurs can commercialize discoveries and innovations. When completed, the new building will define the eastern entrance into campus and be a gateway to the College complex. It is the first building on campus proposed to be named by an alumnus in honor of a living professor, Clayton Heathcock, professor emeritus of chemistry and former dean of the College. This naming opportunity was made possible by a generous commitment from Tori and Terry Rosen. Terry Rosen *(Ph.D. '85, Chem)* was a graduate student with Heathcock.

Chancellor Carol Christ said, "Heathcock Hall is vital to the College of Chemistry's educational and research mission and Berkeley's capacity to change the world. This extraordinary commitment from PMP Tech will truly make a difference in advancing the project forward."

"Heathcock Hall is going to provide new and unprecedented opportunities to translate discoveries from the laboratory into innovations that will directly benefit society," said College of Chemistry Dean Douglas Clark. "This amazing contribution will help ensure that we realize our vision of building a world-class facility."

PMP Tech's partnership with Berkeley began with an introduction from Ted Hou *(Ph.D '95, Chem)*, a general partner in the Berkeley Catalyst Fund, which provides early-stage venture capital support for science-based startups launched by Berkeley students, faculty, and alumni.

Rubber and Joy Chen (who serve as CEO and CFO, respectively) founded PMP Tech in 1978, the same year that Rubber Chen received his degree in chemical engineering from National Taipei University of Technology. He has also directed philanthropy to his alma mater, including funding for a research and manufacturing institute as well as for building a landmark bell-tower inspired by Berkeley's Campanile.

The Chens consider education to be their most rewarding and valuable investment. Having directly observed the educational excellence of Berkeley through the example of their nephew, Wei Lun Chen M.S. '17, they were initially moved to visit the campus.

"It is my honor to work with Berkeley in nurturing hard-working talent and supporting advanced research to make the world a better place," Rubber Chen said. "I truly believe that Berkeley is devoted to the highest quality of education."

➤ Learn more about the Heathcock Hall project: https://chemistry.berkeley.edu/heathcock-hall

The Appetite for Diversity, Equity, and Inclusion is Now

BY BRICE YATES, PH.D.

It is an honor and privilege to serve as the inaugural Chief Diversity, Equity, and Inclusion (DEI) Officer in the College of Chemistry, working alongside renowned faculty, exceptional staff, and students who will be future trailblazers in both academia and industry. My research has focused on the impact of DEI at predominantly white institutions (PWIs) and as a Black male, my lived experiences make me aware of the importance of DEI.

Diversity, equity, and inclusion are my passion. I do not take the role lightly. Serving as the College's Chief DEI officer means understanding the importance of creating an equitable and inclusive environment for all our faculty, staff and students. Universities have long talked about the importance of diversity and more recently equity and inclusion, but at times these words can appear to be buzzwords as opposed to action words. The appetite for DEI is now and as a College, we are actively working to ensure DEI is authentically embedded in the College's fabric.

Conversations around the topic of DEI are continuing to permeate the national landscape as well as college campuses. The past year has been tough as we have felt the impact of COVID-19, which has highlighted various inequities including racial/ethnic inequity, financial inequity, and academic inequity. With Berkeley largely utilizing online learning since March 2020, students as well as faculty and staff have had to adapt to the shifting educational landscape. With this shift, it has been imperative that students feel connected to campus learning, resources, and services which may be challenging in a virtual setting. I applaud the work of the College's faculty which has committed to providing learning space for students to be successful in a virtual setting and staff which has implemented virtual programming and support initiatives.

It is also important to note and recognize the impact social justice movements have had around the country and on college campuses. It is imperative that institutional programming and support initiatives are representative of all individuals. Representation matters. Students, whether undergraduate or graduate, want to see individuals who represent their cultural or ethnic identities within the College and the University as a whole. We must become cognizant of space that is present on campus. Do these spaces create welcoming environments or are they viewed as exclusionary? For minoritized individuals within the College, it is important that representation such as DEI programming initiatives are implemented intentionally in recruitment and retention of minoritized students, faculty, and staff on a continuous basis, and that physical representation in spaces within the College highlight and showcase minoritized individuals.

Creating a sense of belonging, and a welcoming environment, is important for students, faculty, and staff. Programming initiatives have often been reactive as opposed to proactive. For this role to be impactful and successful, I will be reaching out to all constituents within the College in order to capture their needs and perspectives regarding DEI. In order to be intentional, the narrative must change from wanting and wishing to create equitable and inclusive environments and programs to the narrative of being willing to establish an inclusive environment and inclusive programs. Wanting and wishing allows individuals to remain in a place of passive planning with no action. Being willing demonstrates the action to create the needed change.

Willingness to implement needed change can be seen through retention efforts. Throughout my decade long service of DEI work in higher education, various shifts have occurred around DEI. It is imperative that higher education institutions' retention efforts match institutional recruitment efforts. We cannot solely focus on recruiting and enrolling minoritized individuals. A simultaneous focus must also be on the retention of minoritized individuals. Realizing the importance of this fact, the College is working to establish sustainable programs that not only benefit students but also the College as a whole.

Many great things are happening around DEI within the College and numerous initiatives have been implemented by our graduate students. Within the Chemistry department, the Chemistry Graduate Life Committee (CGLC) has developed, and continues to annually administer, the Departmental Climate survey and accompanying Sense of Belonging survey. Also, the CBE Graduate Student Advisory Committee (GSAC) administers an annual climate survey. These surveys have revealed the importance of issues of diversity, equity, and inclusion to graduate students in the College.

Currently we are developing a 5-year DEI strategic plan for the College. The plan is comprised of four leading goals that we

aspire to accomplish in order to assist our DEI efforts. The strategic plan is slated to be finalized and made publicly available by the end of the spring semester. Having a pulse of the College climate is integral as we continue to enhance the College's DEI program.

The College recently launched our Graduate Diversity Program comprised of 29 students who are developing various initiatives. These include working to improve the pipeline of minoritized students into graduate school, recruiting and supporting DEI in the College graduate student population, and working with College leadership to improve the climate with the College of Chemistry.

College level faculty and staff climate surveys are also being developed to assist in recognizing our areas of strength, weakness, and opportunities. These surveys will be disseminated every two years which will allow for measurement and tracking areas of success and areas of improvement. A similar climate survey is also being developed at the undergraduate level.

As I discussed earlier, representation matters. Programming initiatives are being developed that assist with undergraduate student acclimation and sense of belonging within the College. In support of increasing and engaging DEI content and knowledge, College-wide monthly emails will be sent out highlighting the various heritage months. Emails will provide educational and celebratory information on minoritized individuals who have contributed to the fields of chemistry and chemical engineering. Lastly, College level trainings are being developed that will address topics such as unconscious bias, microaggressions, and civil discourse. A truly exciting era for the College!

Our alumni have responded enthusiastically to our new DEI initiatives. It is my hope to engage with alums in the near future to highlight our continuous DEI developments and initiatives within the College. I am excited and honored to serve as the inaugural Chief DEI officer in the College, and to work on making a positive impact for students, faculty, staff, and alumni.

Go Bears!

Learn more about the diversity programs at the College: https://chemistry.berkeley.edu/diversity

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Shop personnel (l to r) Jihad Poole, Jody Brenner, and Ryan Woloshyn.
PHOTO BY IRENE YI, UC BERKELEY

We are still here!

Many essential College workers continued to come onto campus throughout the last year, staying socially distant and working to keep the buildings open and operational. We honor all those who came to work daily and all staff who were required to work remotely. We made it through the last year because of your amazing support and dedication.

Thank you!

Stay connected with the College @ **chemistry.berkeley.edu** and online at Linkedin, Twitter, Facebook, and Instagram.

Berkeley College of Chemistry