SPRING 2020

CONVERGENCE

The magazine of engineering and the sciences at UC Santa Barbara

FOCUS ON: REVERSE ENGINEERING THE BRAIN

FOUR PROJECTS ON THE LEADING EDGE

"SYCAMORE" BREAKS THE SPEED LIMIT

ACHIEVING QUANTUM SUPREMACY

GEARING UP FOR DATA SCIENCE

NSF GRANT SUPPORTS UNDERGRADS

FIXING L.A. TRAFFIC?

APPLYING MACHINE LEARNING TO THE 405

HYDROGEN FROM FOSSIL FUELS...

...WITHOUT ATMOSPHERIC CO_2

UC SANTA BARBARA

MESSAGE FROM THE DEANS

ROD ALFERNESS
Dean and Richard A. Auhll Professor, College of Engineering

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Susan & Bruce Worster Dean of Science, College of Letters & Science

We open this issue of *Convergence* with greetings from our respective homes, where we, like you, are spending a great deal of time during this period of social distancing imposed by the coronavirus outbreak.

For now, our campus is largely vacant, labs are temporarily closed, students are attending courses remotely, and only skeleton staff remain to handle essential procedures. It is difficult for everyone, but by honoring the social-distancing mandate that has dispersed us, we are all doing our part to save lives and bring an eventual end to the pandemic.

Because this issue was well into production before the UC Santa Barbara campus was closed, we continued to work on it. Our printer has remained open, because it serves the health-care industry and was able to print the magazine without bringing additional people to their plant. Hopefully, the stories here provide you with a welcome reminder of what happens in engineering and the sciences at this university when the labs are open, the classrooms are full, and our beautiful campus is buzzing with life, purpose, and vision.

In this issue, you will find coverage of UCSB's response to the outbreak, such as what was involved in temporarily closing research labs and moving to remote teaching, as well as a group of faculty who created coronavirus test kits and another professor who is using artificial intelligence to model the spread of COVID-19.

The section titled "FOCUS ON: Reverse Engineering the Brain" presents four stories about cutting-edge research involving two computer scientists, a physicist, and faculty members from the Department of Molecular, Cellular, and Developmental Biology and the Department of Psychological and Brain Sciences, who seek to uncover important secrets of how the human brain does what it does. You will also find news about an NSF-funded initiative to support undergraduate education in data science; a Q & A with **John Martinis,** the UCSB physicist who leads the local Google team behind the quantum computer "Sycamore," which, last fall, achieved the elusive goal of quantum supremacy; modeling the dynamical system of Los Angeles traffic; identifying and eliminating a newly discovered type of computer security leak; using gene-sequencing technology in a novel way, with possible medical applications; and coaxing hydrogen fuel from fossil fuels without increasing atmospheric CO_2.

Reading these articles, we hope you will recall more-normal times and the important accomplishments that take place at UCSB during them. We will get through this together and eventually return to normalcy, stronger and more unified than ever in our commitment to creating a better world.

Be well, stay safe, and keep in touch.

Rod Alferness Pierre Wiltzius

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UC SANTA BARBARA
College of Engineering

NEWS BRIEFS

APEEL MAKES *TIME* MAGAZINE'S 100 TOP INVENTIONS LIST

TIME magazine's annual list of what it deems the 100 Best Inventions of the year is a big deal, and for 2019, Goleta-based Apeel Sciences was included. Founded by UCSB alumnus **James Rogers** (right) in 2012, the year he earned a master's degree in economics and two years before he received his PhD in materials science, Apeel now has more than 250 employees and offices on four continents.

"It's cool," said Rogers of being included among the list of inventions and innovative products that are selected based on such key factors as originality, creativity, influence, ambition, and effectiveness. "Those recognition lists are nice because they distill a lot of work into sound bites that people can search for or find. It's an honor for the team and nice for our brand, too."

Operating under the idea "We Use Food to Preserve Food," Apeel Sciences produces a barrier made from edible plant materials that is applied to produce after harvesting to slow the rate of spoilage. Since its founding with funding from the Bill and Melinda Gates Foundation, the company has thrived and grown while attracting hundreds of millions of dollars in capital.

Roughly thirty to forty percent of all harvested food in the world is thrown out because of spoilage. In founding Apeel, Rogers sought to do something about it. "Food spoilage is a $2.6 trillion problem, and this company has developed a plant-based coating to reduce waste," he says. "Making any small dent in that is significant. It's enjoyable work, because you feel that what you're doing isn't just a business; it's working on a problem that needs to be solved."

In addition to its Goleta headquarters, Apeel now has offices in Mexico, Peru, Spain, and the Netherlands and is in the process of opening one in South Africa. It has established a partnership with Kroger's, the largest grocery chain in the United States, which plans to sell Apeel avocados — the company's main treated produce to date — in its 2,800 stores, and also has contracts with leading grocers in Germany and Denmark.

The company includes point-of-sale informational labeling. "The reason for this," Rogers explains, "is that we want you to be able to find Apeel produce so you can lessen your food waste at home. Our produce carries no additional cost to the consumer, so it's an easy way to make a big difference. Reducing food waste was recently found to be the number-one way to reverse climate change, so we want to help get the word out in grocery stores and beyond so this transformation can happen."

Photograph courtesy of Apeel Sciences

James Rogers surrounded by fruit treated with the Apeel Sciences coating at company headquarters in Goleta.

ANTHONY CHEETHAM KNIGHTED

Anthony Cheetham, founding director of UC Santa Barbara's world-renowned Materials Research Laboratory (MRL), has joined elite company as a Knight Bachelor of the United Kingdom. The honor, conferred by Queen Elizabeth II, allows Cheetham to receive the title of "Sir" and for his wife, Janet, to bear the title "Lady Janet Cheetham."

The Knights Bachelor honor is a component of the 2020 New Year Honours, an annual list recognizing the outstanding societal contributions of people from across the U.K. Cheetham was cited for "services to Material Chemistry, U.K. Science and Global Outreach."

"The knighthood is very special in a number of ways," said Cheetham, also a member of the Royal Society of London and the American Academy of Arts and Sciences. "First, it was awarded not only for my scientific achievements, but also in recognition of my international outreach efforts, especially to developing countries. The latter has been a passion of mine for more than twenty-five years."

After earning his PhD and accepting a faculty position at the University of Oxford, Cheetham joined UCSB's Materials Department in 1991. The following year, he became the founding director of the MRL, widely recognized as one of the top five such facilities in the world. Cheetham became director of UCSB's International Center for Materials Research in 2004, before returning to the United Kingdom in 2007 as Goldsmiths' Professor of Materials Science at the University of Cambridge. After retiring from Cambridge, he rejoined the MRL at UCSB as a research professor in January 2018.

"My sixteen years on the faculty at UCSB were pivotal in terms of my personal career development. Not only did they mark a step change in the quality of my own research, but being director of the MRL gave me the opportunity to help build one of the top materials science programs in the world," said Cheetham. "It gives me great pleasure to know that the MRL has continued to thrive, first under the excellent leadership of my successor, **Craig Hawker,** and currently under the outstanding guidance of **Ram Seshadri.**"

Anthony Cheetham, professor emeritus.

Cheetham's research focuses on the synthesis and characterization of functional inorganic and hybrid materials. He has worked on developing advanced methods for the chemical and structural characterization of polycrystalline materials. His current interests are in the field of functional metal-organic frameworks and hybrid perovskites.

"The Materials Department is exceptionally proud of this honor for Tony," said **Michael Chabinyc,** professor and chair of the Materials Department at UC Santa Barbara. "He has made a significant impact on the department and UCSB, particularly as the founding director of MRL."

The Imperial Society of Knights Bachelor was officially founded in 1908, though the honor of knighthood dates back to medieval chivalry, as does the method used to confer the knighthood — the accolade, or the touch of a sword by the sovereign. Only British people can be made Knights Bachelor, but foreigners can be given an honorary KBE.

Honorees will receive their medals from the Queen or other members of the Royal Family during investiture ceremonies at Buckingham Palace or Windsor Castle. Cheetham said his ceremony will take place this summer.

ENGINEERING ALUMNUS WINS UC STARTUP PITCH SHOWCASE

Damien Kudela (PhD Materials '15) has won the 2020 UC Startup Pitch Showcase. In February, the co-founder and CEO of Cayuga Biotech bested four other UC finalists to win the system-wide pitch competition, which was attended by more than nine hundred corporate capital investors. The win earned him a spot at the Extreme Tech Challenge, a global pitch competition scheduled to take place in Paris, France, this June (but perhaps delayed due to the COVID-19 outbreak). At that event, 35 startups will pitch to some of the world's largest venture capitalists and corporate leaders.

"I felt a tremendous sense of pride about winning," said Kudela, who was a finalist in UCSB's New Venture Competition in 2014. "We often joke that biotech companies are always the bridesmaid but never the bride at these events, because of their high-risk reward. It's really encouraging and validating to have people see value and worth in our company and believe in us and our technology."

Kudela's company manufactures an injectable drug to accelerate clotting and reduce blood loss following injury. Hemorrhaging, or the loss of blood from the cardiovascular system due to traumatic injury, is the leading cause of death among Americans between the ages of one and forty-four and is responsible for nearly half of all battlefield deaths during military combat.

"Our drug contains a polymer called polyphosphate, which acts as a catalyst to speed up the blood-clotting process," said Kudela, who met his chief technical officer, **Kyle Ploense** (PhD '16), when they were both PhD students at UCSB. "We believe our clotting catalyst can provide a safer and more effective method to keep people alive and let surgeons do their job."

Damien Kudela displays the trophy he received for winning the 2020 UC Startup Pitch Showcase.

Cayuga has received about $2 million from the Department of Defense to fund its research. Kudela wants to raise a Series A round to pay for the Investigational New Drug (IND) application, the first step in the drug review process by the U.S. Food and Drug Administration; to manufacture the drug; and to complete testing.

"If we can raise those funds by the end of the year, we hope to be approved for clinical testing by the end of 2021," said Kudela. "We're really trying to move things forward to get it onto the battlefield and into hospitals as quickly as possible to start saving lives."

Cayuga is also one of twelve finalists in the U.S. Army's Expeditionary Technology Search. Scheduled for March, the event, which awards the winner $250,000, was postponed as a precaution during the outbreak of COVID-19.

Kudela admits that the start-up process has been stressful, but he focuses on the positives, such as successful rounds of testing, positive data results, and winning the UC competition. He attributes his perseverance and progress to the support he received at UCSB, starting with materials professor **Galen Stucky,** his PhD advisor, and the Office of Technology and Industry Alliances (TIA).

"There would be no Cayuga Biotech if I didn't have an opportunity to work with and learn from Professor Stucky and be part of one of the top materials departments in the world," said Kudela. "**Sherylle [Mills Englander]** and the TIA office familiarized us with the entrepreneurship process, and events like Grad Slam and the New Venture Competition trained us to get our point across quickly during a pitch."

COE MATERIALS STUDENT AWARDED TOP POLYMER PHYSICS PRIZE

Nicole Michenfelder-Schauser, a PhD student in the UC Santa Barbara Materials Department, has received the Frank J. Padden, Jr. Award, the nation's most prestigious student polymer physics prize, from The American Physical Society. The annual award recognizes a single PhD student for excellence in polymer physics research, with judges basing their selection on the quality of nominees' research, oral presentations during the Padden Award Symposium, and responses to questions.

Materials PhD Student Nicole Michenfelder-Schauser.

"I am honored to receive the Padden Award. It was a very competitive field of finalists performing innovative research," said Michenfelder-Schauser, who is co-advised by **Rachel Segalman,** professor and chair of the Chemical Engineering Department, and materials professor **Ram Seshadri,** director of the Materials Research Laboratory (MRL). "I think this award serves as continued validation of UCSB's innovative and collaborative approach to materials research."

Michenfelder-Schauser's research centers on a relatively new class of materials called *polymeric ionic liquid*s (PILS). The materials are highly conductive, they demonstrate thermal and chemical stability, and they function in the absence of water, which allows them to operate in high temperatures and provide greater flexibility of design to incorporate a range of useful functions.

Motivated by a desire to maximize energy efficiency and sustainability, Michenfelder-Schauser says that her primary goal is to design materials, like next-generation polymer electrolytes, that can advance novel battery architectures. Her interest in using polymer physics as a solution for energy-storage applications began when she was an undergraduate at UC Berkeley and has expanded during her time at UCSB, as she now explores the connections among polymer structure, ion transport, and macroscopic properties.

"Using the model polymer platform I created, I can systematically tune the various factors that may be important for governing ion transport in polymers," Michenfelder-Schauser said. "Currently, Professor Segalman and I are collaborating with Mitsubishi Chemical and two additional research groups at UCSB to explore how we can further improve the performance of these polymer electrolytes to be used in lithium batteries."

In addition to the APS award, Michenfelder-Schauser and fellow Materials PhD student **Andrew Rowberg** were among 660 young scientists from 101 countries invited to attend this summer's Lindau Nobel Laureate Meeting in Germany. The annual gathering provides students and postdoctoral scholars with the unique experience of meeting and learning from dozens of Nobel Laureates.

A $2 MILLION STARTUP BOOST

Four years ago, a team of enterprising UC Santa Barbara students came up with the idea for a wearable device that could monitor blood-alcohol content (BAC) in real time. The inventors, known as Milo, won UCSB's 2015 Technology Management New Venture Competition, an annual showcase of talented young tech entrepreneurs.

Last year, the company pivoted away from a BAC sensor that consumers *might* want to have, and toward a product essential for self- or supervised monitoring of alcohol consumption. The company — now Milo Sensors, Inc. — also received a $2 million Small Business Innovation Research (SBIR) Phase II grant from the National Institute on Alcohol Abuse and Alcoholism, part of the National Institutes of Health.

"There is a real need for improved tools to monitor alcohol consumption that overcome the inconvenience and stigma of breathalyzers and ankle bracelets; the ION™ wearable fills that need," says **Bob Lansdorp** (PhD '15), Milo CEO and principal investigator, who joined fellow teammate and UCSB alumnus **Evan Strenk** (BA '14) to start the company in 2016. Together, and with the help of countless advisors, they developed a biosensor that taps into the flow of molecules leaving the skin and sends continuous, real-time information about the wearer's BAC via a cloud-enabled smartphone app.

Milo's funding to date includes a $100,000 NIH Challenge Prize in 2016, an NIAA $223,000 SBIR Phase I grant in 2017, the $75,000 Grand Prize at the UC Startup Showcase in 2018, and now the Phase II SBIR grant.

"The grant is a big deal," according to **Tal Margalith,** executive director of technology at UCSB's California NanoSystems Institute (CNSI), which hosts the wet-lab incubator where Milo conducts its R&D activities. The new funding allowed them to rent office space in downtown Santa Barbara and round out their staff.

Lansdorp says that the new grant has allowed Milo Sensors also to hire its "dream team." In addition to himself and Strenk (currently Head of Operations), it includes Test Engineer **Rashad Hamid,** Research Scientist **Dr. Peter Lamberg,** Mechanical Engineer **Archika Poria,** and Technical Project Manager **Stephanie Schudel.**

The team is currently shipping pre-beta units of the ION™ to early adopters and research customers, receiving feedback from testers, and incorporating it into their next-generation product.

"In the long-run," says Landsdorp, "we aim to help millions of people lead happpier, healthier lives by improving the quality of Alcohol Use Disorder treatment in a way that provides a direct link of support and accountability between patients and their support network."

The Milo Sensors "dream team" (from left): Bob Lansdorp, Evan Strenk, Stephanie Schudel, Archika Poria, Rashad Hamid, Peter Lamberg.

Responding to COVID-19

The university adjusts to life during the pandemic

An uncharacteristically empty Elings Hall lab during the COVID-19 campus closure.

University labs are hives of activity where experiments are conducted, materials grown, and discoveries made night and day. We don't think of them as being closed — ever. But on March 18, **Vice Chancellor for Research Joseph Incandela** ordered all labs at UC Santa Barbara to be closed temporarily and all research halted, except for a few exceptions, in response to the COVID-19 pandemic. As the virus spread, most faculty PIs across campus saw the closure coming and immediately joined their graduate students and lab staff to take the necessary steps to prepare. Here's how the process looked to some and how it might impact research going forward.

Materials professor **Stephen Wilson** and his graduate students grow many of their samples in a furnace lab in Elings Hall, and that equipment, he says, "can simply be turned off." He currently does a weekly safety walk-through of the lab and says that the biggest challenges of the closure were "the administrative delays and figuring out how to run our group remotely."

The collaborative nature of Wilson's work, however, means that partners feel the ripples of the closure. "We provide samples for people to study nationally and internationally," he says. "Collaborators are waiting for us to provide them with samples, and we have no idea when we will be able to do that again."

"Some processes can be stopped and some cannot," says **Ram Seshadri,** professor of materials and chemistry and director of the UCSB Materials Research Laboratory. "This is definitely a setback. You can't immediately stop and start."

"It's incredibly painful for the researchers, because lab work is at the core of what they do," says **Kurt Olsson,** who manages the MBE (molecular beam epitaxy) lab. Because Olsson's position requires him to "plan for the unexpected," he was able to put equipment in a safe state and stop processes without losing work over the course of a week. "Nothing is lost except time and opportunity," he says.

Still, he adds, "The PIs and researchers work so hard towards their goals, and having to pause is really devastating. We're trying to operate at as low a level as possible to save power and consumables, like liquid nitrogen, without turning everything off and costing researchers time and money."

The MBE process involves bringing materials to high temperatures to deposit thin films of low-defect crystals, and the ultra-high-vacuum MBE chambers where that occurs need to be as clean as possible to produce high-quality films. "It is important to minimize maintenance," Olsson says. "If we were to completely shut down everything, we would have to open the systems to reload materials, which is an extremely expensive process. We have molten metals in the systems, and if they freeze, they'll damage the equipment. We've essentially idled the systems, leaving critical components on and turning off as much as we can. Once research resumes, we can bring everything back up in a matter of days."

Graduate students in materials and other labs are feeling the effects of the COVID shutdown.

"In our group, we grow and measure a lot of samples, and we had to stop all of that activity," says Wilson. "Depending on where students are in their dissertation work, some have enough results so that they can pivot during this pause from doing lab work to writing up their results. But a lot of first- and second-year students don't have enough results, so the shutdown is holding them back."

Seshadri echoed that. "If my students are very early in their PhDs, they're learning; those who

> "A lot of first- and second-year students don't have enough results, so the shut-down is holding them back."
>
> STEPHEN WILSON

have results are analyzing them and writing them up," he says. "For those who are not writing, our group has received a lot of submissions of resources where others can find material that will help them in their careers. And I have suggested to all of them that they use the time to teach themselves new skills, such as Python programming. Having said all this, it's not easy to focus on research when the news is so dire, so I'm sympathetic if they are not able to get a lot done. I hope they take the time to focus on their physical and mental health as well."

Before the campus closure, Cassidy Arnold feeds stem cells, which are now in cryogenic storage.

"A lot of people in the stem cell lab have experiments running that took months to get where they are."

CASSIDY ARNOLD

For **Cassidy Arnold,** laboratory director of the Center for Stem Cell Biology & Engineering, the directive to shut down labs meant determining which experiments could continue and which had to be stopped, transferring to cryogenic storage the lab's newly cultured stem cells as well as those that were not yet involved in experiments, and establishing a protocol for operating the lab with about ninety percent of its operations suspended and a drastically reduced staff.

"Stem cells can self-renew, so we can freeze them and thaw them later," Arnold says. "We have a very well-established process for doing that, and it typically doesn't introduce too many abnormalities, although it does take a while to get them up and running again."

Still, the timeline to close the lab was short. Arnold heard the first rumors of a lab shutdown order just three days before it came. "We went from planning to freeze some cells to freezing pretty much all of them," she says.

The only exceptions, determined by petition, would be experiments that were either of vital importance or would be set back by several months to a year or more if stopped. That was difficult, Arnold says, because, "A lot of people in the stem cell lab have experiments running that took months to get to where they are, and a shutdown could set them back years. We were hopeful that all these experiments would get the approval to proceed."

Arnold and a few other researchers are currently in the lab about twice a week, maintaining the cells involved in experiments, processing biohazardous waste, and doing regular lab maintenance, such as routinely monitoring the levels of liquid nitrogen in the tanks for the cryogenic freezers."

The difficulty of closing down a lab varies depending on the type of experiments that are being run and the complexity of the equipment and instrumentation housed in it. For **Chris Bates,** assistant professor in the Materials Department, the process was a reasonably straightforward one-day undertaking that took "a little bit of planning."

"We do synthetic organic chemistry, so our lab is not particularly complicated," he says. "We don't have complex equipment that requires supervision, so we can basically turn it off and stop whatever reactions are underway. And we had the Environmental Health and Safety Office pick up chemical waste and chemicals that we don't want to leave lying around for a long time."

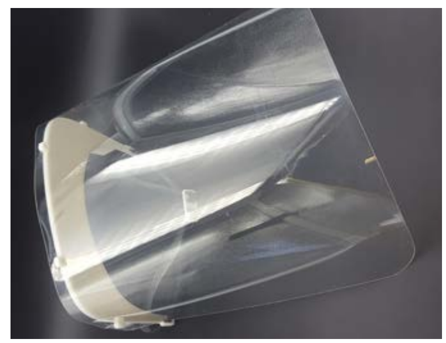
Closing his lab meant "getting any experiments to a safe state and then refrigerating or freezing the chemicals, which is a standard way to store them," Bates says.

Some UCSB PIs who can work remotely were immediately engaged in addressing the pandemic. Mechanical engineering professor **Igor Mezić,** fifth-year PhD student **Allan Avila,** and a group of international collaborators have been working for the Defense Advanced Research Projects Agency (DARPA), using artificial-intelligence algorithms to predict the spread of COVID-19.

Several UCSB labs began making their own hand sanitizer before the campus was shut down, and **David Bothman,** who manages the California NanoSystems Institute's Microfluidics Lab, and CoE Machine Shop Superintendent **Andy Weinberg** have fabricated protective face shields for Cottage Hospital health-care workers. Bothman also set up an online portal where people from UCSB can sign up to offer their services.

One team of UCSB researchers acted well ahead of the official lab shutdown in order to provide a reagent for COVID-19 testing, which would soon be in short supply.

Professors **Max Wilson, Carolina Arias, Kenneth Kosik,** and **Diego Acosta-Alvear,** all from the Department of Molecular, Cellular, and Developmental Biology, collaborated to produce six hundred "reactions," which were then donated to Cottage Hospital to help the medical facility there cope with the rapidly spreading virus.



This 3D-printed mask for health-care workers was made by David Bothman in the California NanoSystems Institute.

Testing protocols for the novel coronavirus, as developed by the World Health Organization and the U.S. Centers for Disease Control, rely on a polymerase chain reaction (PCR) test, which hones in on the presence of the SARS-CoV-2 virus's genetic material in a tissue sample and amplifies the signal by duplicating the target RNA to a level that can be detected.

As the pandemic spread through Europe and Asia, the researchers knew it would soon reach the United States, so they took action and stocked up on the reagents.

Even in times of crisis, collaboration and innovation remain the collective signature of UCSB researchers.

Going Remote

When the COVID-19 outbreak hit, UCSB faculty and administrators rushed to switch over to remote, online instruction for the spring quarter. Here are excerpts from a conversation about the process with chemical engineering professor **M. Scott Shell.**

Zooming in on a health crisis: M. Scott Shell (top row, second from left) teaches graduate students via the popular online app.

PLANNING At the department level, we anticipated a potential move to online classes early on and explored options for delivering remote lectures and for collecting and grading coursework through Zoom, Gauchospace, and GradeScope. A few of our faculty had experience using these tools, so when the university announced the transition, we quickly met to demonstrate procedures and best practices. Also valuable was the university's quick expansion of an Instructional Continuity website as a single go-to resource providing faculty with detailed resources for the many issues that need to be resolved with such a transition.

THE EXPERIENCE I am teaching a graduate core course, Advanced Equilibrium Statistical Mechanics, and it's full! Many graduate students are taking advantage of the shutdown to invest in coursework and literature reviews. During the last week of winter quarter, I figured out how to use a virtual whiteboard on my iPad while monitoring student questions through chat on my desktop screen. I've also been recording all lectures and uploading through our GauchoCast site, and posting all of my iPad whiteboarding to the course Gauchospace site. It's incredibly useful for students to be able to rewind and work through lecture material. I also deliberately slowed down the pace of the material, given that Q&A in an online class isn't quite as effective as in person. So far, things have been going well; the students seem to be completely on-board with the technology, and we've had no major technical problems!

KEEPING THE CHEMISTRY With my research group, I am holding group "game time" Friday afternoons, where everyone plays an interactive game via Zoom, just to touch base and remember that we're all in support of each other. The group also holds a Wednesday virtual lunch, where outside speakers discuss a topic of interest beyond our expertise. Our Chemical Engineering Graduate Student Association is organizing social activities, such as Zoom coffee hours and Netflix parties, so that graduate students can keep in touch.

THE TAKEAWAY As an academic institution during this crisis, we are incredibly lucky to be able to continue in our mission to educate the next generation of scholars and leaders. It gives us an end goal that keeps us all thinking, learning, and interacting. We are all working hard to make sure this time becomes one of productivity and progress for our students, who are ultimately our legacy. Personally, the most remarkable aspect of recent events has been witnessing the immense and rapid demonstration of incredible commitment, adaptability, and compassion from my colleagues, the administration, and, of course, our students.

> "Continuing our mission to educate... gives us an end goal that keeps us all thinking, learning, and interacting."
>
> M. SCOTT SHELL

FACULTY AWARDS

A sampling of honors received by faculty from June 2019 to February 2020

1. **Kaustav Banerjee**
Electrical and Computer Engineering
2019 Highly Cited Researchers List, Clarivate Analytics. Ranked in the top one percent of his field in terms of references and citations in journals published from 2008-'18.

2. **Christopher Bates**
Materials
Young Investigator Award, American Chemical Society. Recognized as an early-career emerging leader who has made significant contributions in his field within polymer materials science and engineering.

3. **Guillermo Bazan**
Materials
2019 Highly Cited Researchers List, Clarivate Analytics. Ranked in the top one percent of his field in terms of references and citations in journals published from 2008-'18.

4. **Elizabeth Belding**
Computer Science
Fellow, American Association for the Advancement of Science. For "distinguished contributions to the field of networking, particularly network architectures, protocols, and measurement of mobile networks."

5. **Daniel Blumenthal**
Electrical and Computer Engineering
2020 C.E.K. Mees Medal, Optical Society. For "innovation in ultra-low-loss photonic integrated circuits and their application to ultra-low-linewidth lasers, optical communications, signal processing, optical gyroscopes, and atom cooling."

6. **Michael Chabinyc**
Materials
Fellow, National Academy of Inventors. For demonstrating "a highly prolific spirit of innovation in creating or facilitating outstanding inventions that have made a tangible impact on the quality of life, economic development, and welfare of society." Fellow, American Physical Society. "For contributions to the understanding of relationships between structure and electronic properties of conjugated polymers, and the translation of these relationships to functional devices, such as transistors and solar cells."

7. **Phillip Christopher**
Chemical Engineering
Presidential Early Career Award for Scientists and Engineering (PECASE). Received the highest honor bestowed by the U.S. government on outstanding scientists and engineers who are beginning their research careers and show exceptional promise for leadership in science and technology. Early Career in Catalysis Award, American Chemical Society. For accomplishments and innovation of unusual merit completed in the early stages of his career.

8. **Elliot Hawkes**
Mechanical Engineering
NSF Early CAREER Award.
To study the factors that govern the movements of soft robots, which could lead to the design of new vine robots for potentially life-saving applications.

9. **Alan Heeger**
Materials
2019 Highly Cited Researchers List, Clarivate Analytics. Ranks in the top one percent of his field in terms of references and citations in journals published from 2008-'18.

10. **Matt Helgeson**
Chemical Engineering
Science Award, Neutron Scattering Society of America. For scientific contributions made within the past five years using neutron scattering techniques.

11. **B. S. Manjunath**
Electrical and Computer Engineering
Edward J. McCluskey Technical Achievement Award, IEEE Computer Society. "For contributions to image search, retrieval, and bio-image informatics."

12. **Sanjit Mitra**
Electrical and Computer Engineering
Fellow, National Academy of Inventors. For demonstrating "a highly prolific spirit of innovation in creating or facilitating outstanding inventions that have made a tangible impact on the quality of life, economic development, and welfare of society."

13. **Galan Moody**
Electrical and Computer Engineering
Young Investigator Award, U.S. Air Force. Selected in support of his project aimed at creating an optical quantum computing platform in which all of the essential components are integrated onto a single semiconductor chip.

14. **Yasamin Mostofi**
Electrical and Computer Engineering
Fellow, Institute of Electrical and Electronics Engineers. "For contributions to control and communications co-optimization in mobile sensor networks."

15. **Arnab Mukherjee**
Chemical Engineering
Young Investigator Award, National Institutes of Health. Selected in support of research efforts to develop new reporter proteins that tackle existing challenges of "invisible dark matter."

16. **Kunal Mukherjee**
Materials
NSF Early CAREER Award. Selected to support a project that focuses on exploring a different class of electronic materials known as IV-VI semiconductors, which have very unusual atomic bonding. (See page 30.)

17. **Shuji Nakamura**
Materials / Electrical and Computer Engineering
Fellow, Royal Academy of Engineering (U.K.). Recognized for invention of blue light-emitting diodes, which enabled development of white LEDs. Hall of Fame Inductee, Consumer Technology Association.
Recognized as a technology leader who advanced innovation and improved consumers' lives. 2019 Leigh Ann Conn Prize for Renewable Energy, University of Louisville.
For "outstanding innovation and its translation into clearly impactful technology related to renewable energy."
2020 Industrial Application of Science Award, National Academy of Sciences. For "pioneering discoveries, synthesis and commercial development of Gallium nitride LEDs and their use in sustainable solid-state light sources, which are reducing global greenhouse gas emissions while also reducing costs to those adopting this technology,"

18. **Michelle O'Malley**
Chemical Engineering
Early Career Applied and Biotechnological Research, American Society for Microbiology. Presented to an early-career investigator with distinguished research achievements in the development of products, processes, and technologies that have advanced the microbial sciences. Scientist to Watch, *Science News.* Selected as one of ten scientists to watch, based on her innovative research and contributions to the field of microbiology. Fellow, American Institute for Medical and Biological Engineering (AIMBE). Honored for "innovative research and significant contributions to the biological engineering field."

19. **Tresa Pollock**
Materials
Robert Franklin Mehl Award, Minerals, Metals and Materials Society. Awarded one of TMS's most prestigious honors in recognition of her "extraordinary contributions to the improved understanding of high-temperature alloys and coatings, and for being an inspirational role model for young engineers of both genders."

20. **Omar Saleh**
Materials
Fellow, American Physical Society. Honored for "outstanding contributions to single-molecule biophysics, including development of magnetic-tweezer instrumentation and its use in elucidating electrostatic and self-avoidance contributions to biopolymer structure, as well as mechanics of motion of ring-shaped ATPases along DNA."

21. **Spencer Smith**
Electrical and Computer Engineering
Presidential Early Career Award for Scientists and Engineering (PECASE). Received the highest honor bestowed by the U.S. government on outstanding scientists and engineers who are beginning their research careers and show exceptional promise for leadership in science and technology.

22. **Megan Valentine**
Mechanical Engineering
Fellow, American Physical Society. "For pioneering research in the development of microbiology and the applications of biomechanics at multiple length scales to diverse biological systems."

23. **Chris Van de Walle**
Materials
2019 Highly Cited Researchers List, Clarivate Analytics. Ranked in the top one percent of his field in terms of references and citations in journals published from 2008-'18.

24. **William Wang**
Computer Science
Future of Computing Academy, Association for Computing Machinery. Selected to participate in its Future of Computing Academy, which is intended to engage and empower the next generation of computing professionals. IBM Faculty Award and Facebook Research Award.

25. **Yuan Xie**
Electrical and Computer Engineering
Fellow, American Association for the Advancement of Science. "For distinguished contributions to the field of computer architecture and electronic design automation, particularly three-dimensional integrated circuits and memory." Fellow, Association for Computing Machinery. "For contributions to the design technology and tools for their implementation and evaluation of computer architecture." Edward J. McCluskey Technical Achievement Award, IEEE Computer Society. "For contributions to technology-driven computer architecture and to tools for their implementation and education."

CoE Welcomes Fourteen New Faculty in 2019-'20

In a continuing hiring surge (nineteen new faculty were hired during the 2018-'19 academic year), fourteen faculty members have joined UC Santa Barbara's College of Engineering during the 2019-'20 academic year. Their realms of expertise range from quantum materials to machine learning, and from recovery technology to stem cells and virtual reality.

"I am proud to welcome them to UC Santa Barbara. Each one brings impressive academic credentials, research achievements, and life experiences," said **Rod Alferness**, the Richard A. Auhll Professor and dean of the College of Engineering. "The college prides itself in hiring the best faculty, who will be recognized for their innovative research that addresses society's biggest challenges. This new group continues that tradition and adds to our strengths. I look forward to seeing them thrive in our collaborative culture."

The fourteen faculty were added to six departments and programs within the college. Twelve of the new hires are assistant professors, and five are women. Five assistant professors joined the Computer Science Department. Three assistant professors and one lecturer were added to the Mechanical Engineering Department, and two faculty joined the Electrical and Computer Engineering Department. The Chemical Engineering Department, and the programs of Technology Management and Media Arts and Technology each added one assistant professor.

Here are the College of Engineering's newest faculty members:

PRABHANJAN ANANTH ***Assistant Professor, Computer Science***
Research Interests: Focuses on theoretical aspects of cryptology, program obfuscation, and secure multiparty computations.
PhD, UC Los Angeles; postdoctoral research, Massachusetts Institute of Technology

MICHAEL BEYELER ***Assistant Professor, Computer Science***
Research Interests: Develops novel methods and algorithms to interface sight-recovery technologies, such as retinal implants and the human visual system, with the ultimate goal of restoring useful vision to the blind.
PhD, UC Irvine; postdoctoral fellowship, University of Washington

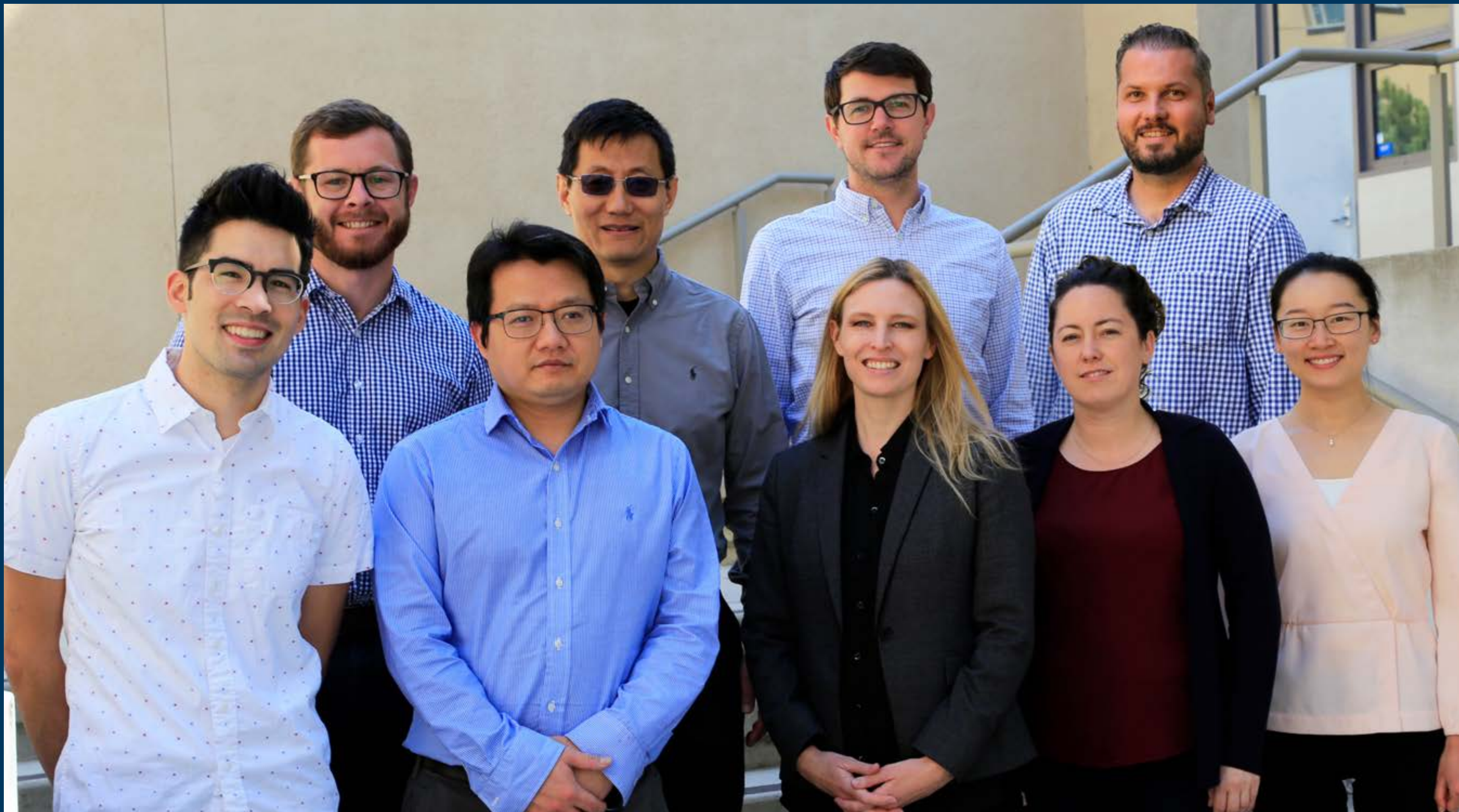
ADELE DOYLE ***Assistant Professor, Mechanical Engineering***
Research Interests: Studies stem cell responses to mechanical forces and cues during system development and maintenance; examines molecular circuits that enable specialized mechanosignaling.
PhD, Georgia Institute of Technology and Emory University; UCSB lecturer and researcher since 2013

YU FENG ***Assistant Professor, Computer Science***
Research Interests: Builds automated tools that guarantee the desired behavior of a system in a sound, precise, and scalable way; applies static analysis and tackles smartphone security problems.
PhD, University of Texas at Austin; postdoctoral research, University of Washington

ARPIT GUPTA ***Assistant Professor, Computer Science***
Research Interests: Designs systems to solve real-world network problems at the intersection of networking, cybersecurity, and machine learning.
PhD, Princeton University; postdoctoral research, Columbia University

JENNIFER JACOBS ***Assistant Professor, Media Arts and Technology***
Research Interests: Develops expressive computational tools, software, and computer languages to support expressive computer-aided design.
PhD, Massachusetts Institute of Technology; postdoctoral research, Stanford University

PENG LI ***Professor, Electrical and Computer Engineering***
Research Interests: Works at the intersection of integrated circuits, neuroscience, machine learning, applied statistics, and electronic design automation; aims to engineer smart circuits and systems that are efficient and can process large amounts of data.
PhD, Carnegie Mellon University; joined UCSB after serving on faculty at Texas A&M University from 2004-19



New faculty for 2019-20 (clockwise from bottom right): Yangying Zhu, Adele Doyle, Jessica Santana, Yu Feng, Geoffrey Tsai, Ryan Stowers, Peng Li, Galan Moody, Michael Beyeler. Not pictured: Prabhanjan Ananth, Arpit Gupta, Jennifer Jacobs, Misha Sra, Sho Takatori

GALAN MOODY *Assistant Professor, Electrical and Computer Engineering*
Research Interests: Fabricates and characterizes integrated quantum photonic devices and quantum materials relevant to quantum information processing, communications, and metrology.
PhD, University of Colorado at Boulder; joined UCSB after serving as research scientist and postdoctoral fellow at National Institute of Standards and Technology

JESSICA SANTANA *Assistant Professor, Technology Management*
Research Interests: Studies the role of networks in innovation and entrepreneurship; utilizes insights from organizational theory, economic sociology, social psychology, and network science.
PhD, Stanford University; Master of Information Management and Systems, UC Berkeley

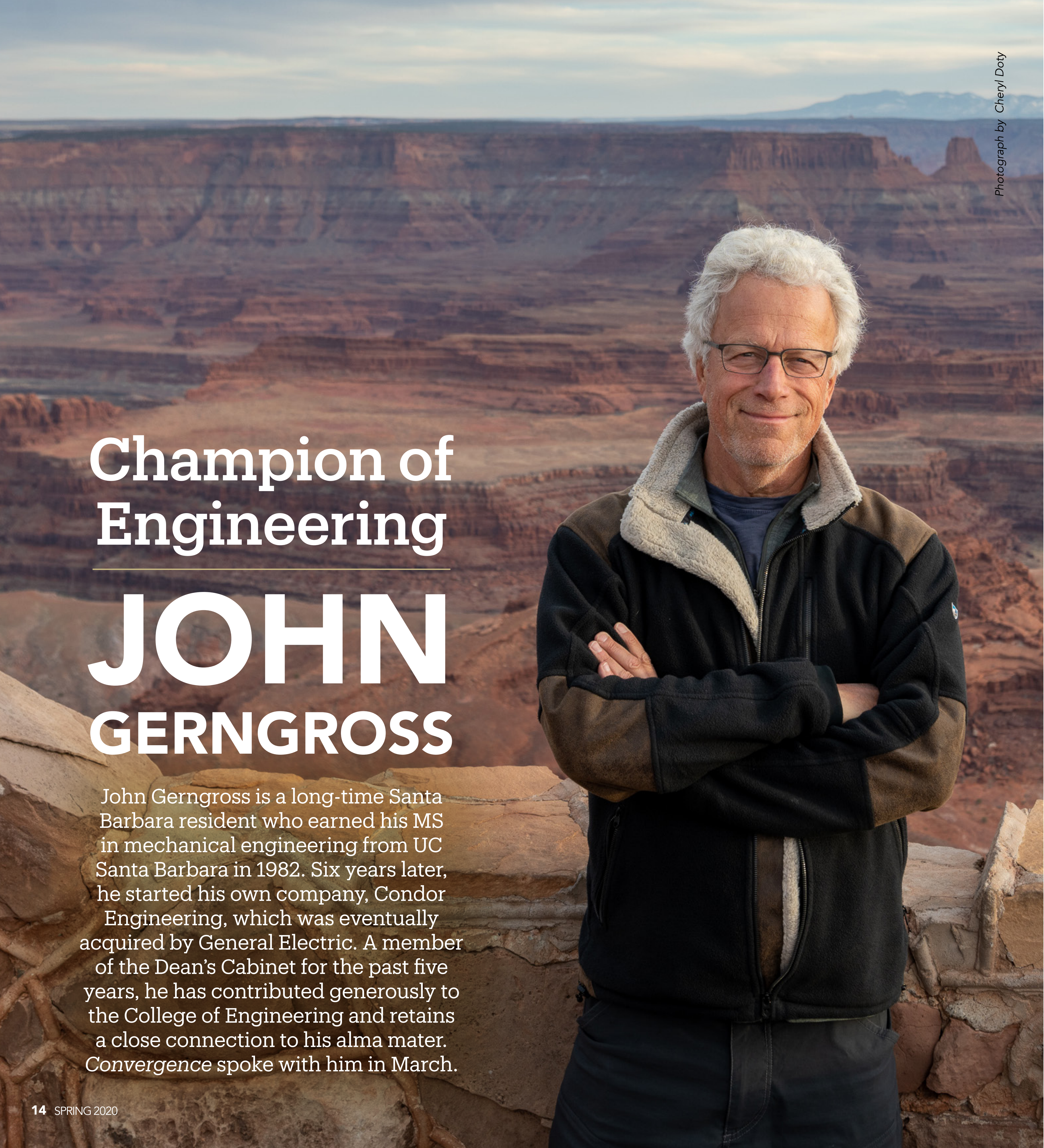
MISHA SRA *Assistant Professor, Computer Science*
Research Interests: Specializes in perceptual engineering, which is building systems and devices to modify and manipulate a user's sense of space, place, and body.
PhD, Massachusetts Institute of Technology

RYAN STOWERS *Assistant Professor, Mechanical Engineering*
Research Interests: Develops 3D hydrogel cell-culture platforms to mimic native extracellular matrix properties with the goal of determining molecular mechanisms that regulate cell phenotype.
PhD, University of Texas at Austin; postdoctoral research, Stanford University

SHO TAKATORI *Assistant Professor, Chemical Engineering*
Research Interests: Aims to understand and engineer unconventional, nature-inspired soft materials by combining theoretical fluid dynamics and statistical physics with biomolecular experiments.
PhD, California Institute of Technology; research fellowship, UC Berkeley

GEOFFREY TSAI *Lecturer, Mechanical Engineering*
Research Interests: Explores the process of designing, building, and presenting new products and systems.
PhD, Massachusetts Institute of Technology

YANGYING ZHU *Assistant Professor, Mechanical Engineering*
Research Interests: Addresses thermal management challenges of electronic devices, batteries, and electrocatalytic systems; focuses on using thermo-fluid engineering approaches to create future electronics and sustainable energy solutions.
PhD, Massachusetts Institute of Technology; postdoctoral research, Stanford University



Photograph by Cheryl Doty

Champion of Engineering

JOHN GERNGROSS

John Gerngross is a long-time Santa Barbara resident who earned his MS in mechanical engineering from UC Santa Barbara in 1982. Six years later, he started his own company, Condor Engineering, which was eventually acquired by General Electric. A member of the Dean's Cabinet for the past five years, he has contributed generously to the College of Engineering and retains a close connection to his alma mater. *Convergence* spoke with him in March.

Convergence: What motivated the $250K gift you and Cheryl [Doty, his wife] made to establish a chair in computer science, a gift that was matched by an anonymous donor?

John Gerngoss: No matter what your business, to be the best, it is critical to have the best people working for you. The academic world is a case in point. To maintain and improve the high quality of the College of Engineering, we need great professors at all levels, and the best and brightest are in high demand. Funding is one of the important incentives to help people make the decision to come here. Supporting the creation of a chair is our way of providing for this important need.

It was very gratifying to be able to name the chair in honor of my parents, who came from poor backgrounds and leveraged engineering and chemistry degrees to provide for their family which, in turn, allowed me to find my own success. It is our privilege to be able, in this small way, to pay it forward.

C: Can you discuss any other facets of the university generally, and of the College of Engineering, specifically, that inspire you to support it?

JG: I find the university in general and the college specifically to be inspirational places. I constantly learn of new, exciting, and important work. Twice a year at the Dean's Cabinet meeting, **Rod [Alferness,** dean] has professors discuss their work, and we occasionally tour labs. I think it is important to support the profoundly important research being done here, and when you give to the university, you are supporting programs that have the potential to be life changing, if not planet changing.

C: As an entrepreneur, you founded and had great success at Condor Engineering, which was sold to General Electric in 2006. How do you see the entrepreneurial tech world evolving at UCSB, and affecting the Santa Barbara/Goleta area?

JG: When I came to Santa Barbara in 1979, its tech world was dominated by three large corporations. The opportunities for entrepreneurship were limited by the high cost of entry to engineering development and the scarcity of good tools. Today, there are startups and entrepreneurs everywhere. The reason for this is the tremendous availability of affordable tools, building blocks, and support systems for startups. The capstone program is a perfect example. Every year, I see sophisticated student projects that would have taken a professional engineering department many person-years to do back in the eighties. And every year I am more impressed than I was the year before.

Our entrepreneurship recipe in Santa Barbara is brilliant. We have a top-tier engineering college, where highly motivated students have access to affordable and powerful development tools. We have an experienced and engaged professorship, mentorship, and investing community backing them up, and our Technology Management Program is a great resource, with the New Venture Competition one example of its value. The university also is very supportive of its entrepreneurs and wants to help them be successful, even providing resources like lab access, IP protection, and incubator space. We have every ingredient needed for success. Just add a great idea and stir.

C: What was your mindset when you started Condor? Were you gung-ho? Nervous? What made you take that leap six years after earning your master's degree? Take us through that process a bit, if you will.

JG: When I started Condor I was totally gung-ho. I wasn't nervous because I knew that if things didn't work, out I could always go back to my regular job. I didn't need much start-up capital, just a lot of engineering hours, which I provided by working night and day. I was self-funded, so I didn't have to report to investors. The worst case was that I would lose career-development time and some of my savings.

I used my MS degree during the six years after graduation to leverage myself into increasingly sophisticated engineering jobs and to refine my skills. In 1988, I was working in aerospace and realized that, with the advent of the IBM PC, test equipment was evolving from expensive, dedicated, single-function devices to PC clones with generic communication equipment and specialized software — a fundamentally more powerful, flexible, and cheaper solution. I used that opportunity to start Condor Engineering, which made communication products for military and commercial aerospace applications. After some early missteps in the sales and marketing arena, the company started growing rapidly. It was built on the ethic of delivering top-quality products and great customer support.

C: You have previously donated to support undergraduate capstone projects in the CoE, which are important in imparting collaborative skills. Can you talk a bit about the importance of collaboration?

JG: Today, collaboration is more important than ever. Systems are generally complex and often interdisciplinary. Multiple people with different skill sets are required to work together. I really appreciate the way the capstone programs in the CoE provide an opportunity for students to learn and start to appreciate the complexities of communication and organization for group projects. These are some of the most difficult but important skills graduates can bring to their jobs. It is not enough just to be good technically; to be successful, you also need to be able to collaborate.

Faculty Q&A

JOHN MARTINIS

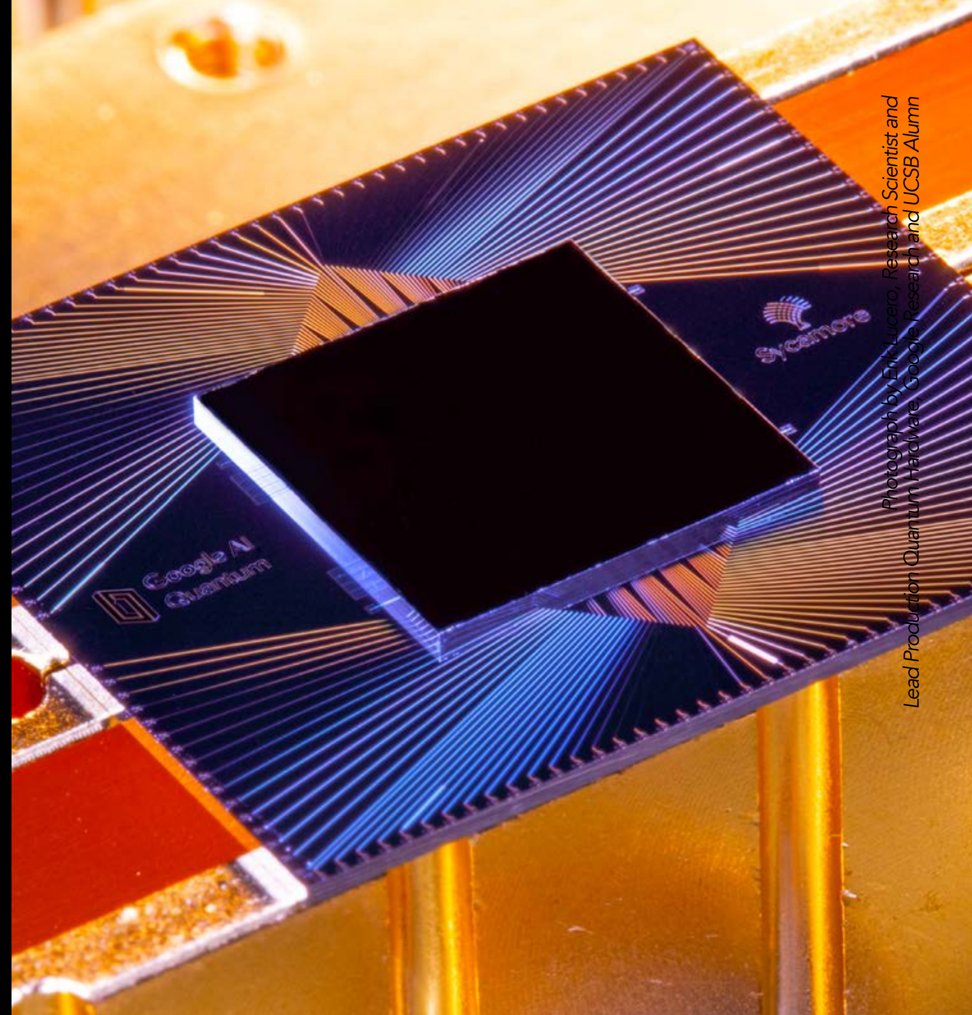
"Sycamore" Breaks the Speed Limit

UCSB physicist **John Martinis** leads the Goleta-based Google team that achieved quantum supremacy

Last fall, a paper in the journal *Nature* described how Google's 53-qubit quantum computer, named "Sycamore," had achieved "quantum supremacy" by solving a massive sorting problem in a couple of minutes that Google said would have taken ten thousand years to solve on the world's most powerful supercomputer.

IBM, which built that supercomputer, named "Summit," balked at the claim, arguing that certain data-packaging strategies would have enabled its sprawling machine to solve the problem in a period closer to two and a half days than to ten thousand years.

To longtime UCSB physics professor **John Martinis,** now chief scientist and head of the hardware group that is building Sycamore, which hangs suspended like an elegant,



Photograph by Erik Lucero, Research Scientist and Lead Production Quantum Hardware, Google Research and UCSB Alumn

Artist's rendition of the Sycamore processor mounted in the cryostat, Forest Stearns, Google AI Quantum Artist in Residence

With its number-crunching capacity enabled by 53 qubits, like the one shown (top), "Sycamore" (above) provided a powerful proof of the quantum-computing concept.

copper-wire-clad chandelier in an industrial park near UCSB, the debate is moot. The point, to him, is that Sycamore is faster, a lot faster; exactly how much faster is not so important, because the speed advantage will grow exponentially as new qubits are added. If another 53-qubit chip (actually, it has 54-qubits, but one failed during the test) were added to Sycamore, Martinis suggests, a digital supercomputer would need to be the size of a city to compete.

Regardless of one's take on the test, it was perhaps the most exciting moment in quantum computing to date, making this a good time to catch up with Martinis. *Convergence* spoke with him at Google's Goleta lab in February.

> "It was amazing that basically everything else worked and we could do the experiment."

Convergence: *So, where are you in the development of this machine?*

John Martinis: The fifty-three-qubit Sycamore device is a functioning quantum computer, and we actually have a practical application for it. But if you want a quantum computer that can solve practical problems that you can't solve with a supercomputer and do it without errors, you'll need something like a hundred thousand to a million qubits. That's kind of how we're thinking about it in the long term. So, we're just going to make this thing bigger and bigger. There is a lot of overhead associated with error correction, which makes it hard.

C: *You ran the quantum-supremacy test with 53 qubits on a 54-qubit chip. What happened to the 54th?*

JM: The qubit was good, but there was a partial short on one of the wirings on the mount circuit board. We knew that the fault existed when we cooled it down a year ago. [The qubits have to be cooled to barely above absolute zero for quantum computing to occur.] But it was our first chip, and we thought, *It's only one qubit, and it's off to the side, so if it doesn't work, it doesn't matter anyway because there's going to be something else we have to fix.* When you do something for the first time, nothing ever works perfectly. It was amazing that basically everything else worked, and we could do the experiment. That was not expected, and it was great.

C: *On your way to one hundred thousand, or a million, qubits, when do you make the next incremental increase?*

JM: We're working to make the chips better, so they have fewer errors. We want to reduce the errors by a factor of about five. That's good enough to do error correction, and then we have to scale up.

C: *If and when quantum computers become part of the "regular" computing landscape, how do you think they will be accessed and used?*

JM: We think the natural way to use the quantum computer we have now and will have in the future is to have cloud access, which is essentially how supercomputers are used now. No one sits next to one and types in their program; they access it on the internet. Your laptop and your cellphone — they're both just interface devices, because most of the computation is done in the cloud these days. So, going to that kind of a model is perfectly sensible. This is really hard to build, and it may never be small and portable like a classical computer, but on the other hand, when classical computing started, no one believed that we could build it at the sizes we do now.

C: *Do you foresee any materials solutions to quantum-computing challenges, and are you working with anyone at the new NSF–funded UC Santa Barbara Quantum Foundry?*

JM: It's fundamentally impossible to make a perfect qubit. Nature is working against you, and you're always going to have errors. Classical information can be fundamentally stable, but quantum computing is fundamentally unstable, because quantum systems are by their nature, environmentally sensitive and therefore inherently unstable. There are a lot of open questions in materials that we need to understand, and we communicate that to people we're working with, both at the university — and some of them are affiliated with the new foundry — and at other outside entities. At this point, though, a lot of the work we're doing is a bit proprietary.

C: *How did you come to your position with Google?*
JM: I've been working on quantum computing since the mid-1980s. Six years ago, we had got far enough along with our research at UCSB that Google took note and started thinking about having a hardware effort.

I wanted to build a quantum computer, our UCSB team wanted to build one, and Google wanted to build one. Our desires kind of lined up, and it was the right time. We had just got some results and wanted to do something more complicated and keep the team together, and that's hard to do at a university. Building a machine seemed a little more industrial, so moving from academia to an industrial setting seemed the right thing to do.

Working with industry, you don't have issues with government funding. The engineering and physics challenges are so hard that, at the university, you bring people in as PhD students and you train them up, and then they leave. This way, we're focused on the work, we have all the funding, our researchers can start families and buy homes, and I can focus all my effort on building this thing instead of continuously raising money.

What was very nice was how well UCSB and the Office of Research worked with Google to come up with an arrangement that makes sense. There's a lot of benefit for everyone, and I really thank UCSB for being understanding of the situation and working hard to make it work.

C: *What are your thoughts on the security concerns related to quantum computers, i.e. that they will be able to hack into systems in seconds, and is that something you concern yourself with at this point?*
JM: People use RSA [Rivest-Shamir-Adleman] algorithms for security encryption, which is based on the fact that it's easy to take prime numbers and multiply them and the resulting number is very hard, exponentially hard, to factor. The current thinking is that if you can make fast, high-quality qubits — and we don't know if that can be done — you would need twenty million to fifty million physical qubits to do the RSA hacking.

People who worry about and work on security know that RSA is not quantum-safe, but they know that there are other algorithms that are quantum-safe. They're working on it. There's a program at NIST [the National Institute of Standards and Technology] to come up with something to replace RSA. The world has a decent amount of time — probably twenty years — before it has to worry about a quantum computer. Every security and cryptosystem ever built has a finite lifetime, because new technology comes around and people figure it out, so to expect RSA to last forever is silly. It's not something we think too much about, because we believe that our value is added in other things and not that.

> “I wanted to build a quantum computer, our UCSB team wanted to build one, and Google wanted to build one. Our desires lined up, and it was the right time.”

Photograph by Eric Lucero

UCSB physicist John Martinis in Google's "Sycamore" lab.

Purposeful Mutations

Michelle O'Malley's lab develops a new technique that may have medical benefits

UC Santa Barbara chemical engineer **Michelle O'Malley** focuses much of her research on identifying and engineering unusual enzymes from nature to build fuels and chemicals. But a new paper published in the February 4 issue of the journal *Nature Communications* describes work led by author **Justin Yoo,** a recently graduated PhD student from O'Malley's lab, in a different but related area — engineering a membrane protein receptor to bind pharmaceuticals better.

The human adenosine A2a receptor is a medically relevant G protein coupled receptor (GPCR). GPCRs are a major family of membrane proteins in humans, which are implicated in diseases ranging from cancer to heart disease. "For some GPCRs, we understand how drugs (ligands) interact with them to change what cells do, and for others we don't. Understanding the structure-function relationship of a human GPCR that's involved in disease is really important," O'Malley notes. "This paper is about using new advances in DNA sequencing to track and evaluate how millions of receptor variants bind to drugs, which is related to the broader goal of understanding how to design drugs that interact with their targets more effectively."

For some time, researchers have been engineering proteins — a process called *directed evolution* — by causing changes to their amino acid building blocks. "Mutations are happening all the time in cells," O'Malley says, "but in the field of protein engineering, you make mutations to proteins either randomly or strategically to mimic nature's natural evolution process, apply selective pressure to filter the mutants, and then tune a protein toward a function it didn't have before.

"That's the broad problem we're addressing in this paper," she continues. "We're introducing a new protein-engineering technique that relies on high-throughput DNA sequencing to tell us exactly which protein variants survive our selection, and which don't. Part of what we're trying to do is understand which parts of the human A2a receptor play a role in binding drugs, and to identify variants, or mutants, of the receptor protein that are better than others at binding certain therapeutics."

Typically, O'Malley explains, directed evolution of this type would involve making some spot mutations to the A2a receptors, building a library of those variants, and then sorting through them to identify a "winner."

What you don't get with that approach, however, is a picture of what happened along the way or why the losers lost. "That's what this technology is getting at," she says. "It addresses protein epistasis — how multiple mutations combine for an added positive or negative benefit on the overall function of the protein, which cannot be predicted from the protein sequence itself or from the behavior of multiple individual mutants."

The project required developing a new data-processing pipeline called BRIDGE, which stands for *bridge reads and distal sites within genes*. "Essentially, we use state-of-the-art Illumina technology to sequence each receptor variant that we made and screened," O'Malley says. "But, by stitching together short sequencing fragments, we can identify and survey exactly where each mutation occurred over millions of different A2a receptor variants."

"It's complicated," O'Malley says, "but if you unwind an A2a receptor, you have the amino acid sequence and can then make a mutation where you choose in its corresponding DNA. DNA is bound to a flow cell, where it forms "clusters" that are sequenced by tracking small bursts of fluorescence that correspond to the DNA base pairs. But, if you made two mutations that are relatively far apart — e.g. three hundred base pairs or so — in the A2a gene, the sequencing technology would allow you to sequence each block separately, but not together. So, you could get information on mutation 1 and mutation 2, but you wouldn't know that mutation 1 and 2 co-occurred in the same gene variant."

Yoo discovered a use for an additional layer of information from Illumina sequencing that typically is ignored when processing data. "When you bind DNA to the Illumina flow cell, you can match DNA fragments with non-overlapping segments by locating their specific (x,y) coordinate on the flow cell – essentially stitching together mutations from A2a variants on the same gene," O'Malley explains. "It's an extra layer of data that pretty much everybody has just thrown out. Justin recognized that it could be used to build a library of A2a variants that, when coupled with a ligand binding screen, could tell us exactly which variants were great at binding drugs and which were poor."

Thanks to advances in sequencing technology, she adds, "The team could not only sequence all the variants and mutations they made, but also say quantitatively which protein mutations were good, which were bad and, surprisingly, which ones led to a combined function that we could never have predicted through conventional methods.

"There's this idea in the field that if you make a mutation, it's usually bad and wrecks protein function, and sometimes you make a mutation that's good and helps protein function," she adds. "In reality, you're mutating multiple sites, and it can be hard to tell how to combine mutations to get a certain effect."

As part of this work, Yoo wrote a software program for researchers who have next-generation data and want to know how to sort through a pile of variants they created and understand how interesting mutations made the protein better or worse. "It's a pipeline that somebody could follow to say, 'I want to make this protein that has improved functions, and I want to understand why I got the result that I did,'" O'Malley says.

"Understanding how natural variations in human receptors lead to different interactions and outcomes with pharmaceuticals is really powerful," she concludes. "It could lead to personalized medicine and many technologies that are not currently possible."

GEARING UP FOR DATA SCIENCE

A National Science Foundation grant enables UC Santa Barbara to lead a multi-campus initiative aimed at supporting undergraduates' data-science pursuits

Eight years ago, venture capitalist Geoffrey Moore tweeted a prescient assertion that read, "Without big-data analytics, companies are blind and deaf."

Increasingly, data runs our lives. It allows companies to compete, drives web advertising, and supports policy-making. It can lead to improved performance by farmers, airlines, athletes, highway systems, and banks. It fuels artificial intelligence and the Internet of Things, and catalyzes scientific discovery on many levels and in nearly any subject area one can imagine.

But, on its own, data is just raw information. It takes people — data scientists, in particular — to give meaning to the numbers. With their unique skill sets, data scientists are able to extract knowledge and glean insights from the extensive datasets that society now generates every second of every day. As a result, data science is, increasingly, where the jobs are.

To answer the growing demand for data scientists while addressing the increasing integration of data into every aspect of modern life, the National Science Foundation (NSF) has awarded UC Santa Barbara a three-year, nearly $920,000 grant to fund what is known as the Central Coast Data Science Initiative. The muti-campus initiative — partner schools are Cal State San Bernardino, Cal Poly San Luis Obispo, and Santa Barbara City College — will support coursework and project-based classes aimed at both generating awareness of and interest in data science and at providing programmatic support and hands-on experience to undergraduate students. The NSF grant totals more than $1.2 million across the four institutions.

The initiative will include classes and student projects as well as a collaboration of data scientists. Most of the funds will go toward undergraduate fellowships for these new data scientists, explained **Tim Robinson,** an academic coordinator in the Department of Computer Science. UC Santa Barbara plans to provide 65 fellowships over a two-year period.

"The overall idea is to build a culture around data science on campus," said computer science professor **Ambuj Singh,** who leads the university's working group on data science and is the principal investigator on the NSF project. His co-PIs at UCSB are **Mike Ludkovski,** professor and chair of statistics and applied probability; **Alexander Franks** and **Sang-Yun Oh,** assistant professors of statistics and applied probability; and computer science lecturer **Yekaterina Kharitonova.**

Unlike most other disciplines, which are defined by a set of common topics of interest, data science — encompassing aspects of mathematics, statistics, and computer science — is a collection of tools and techniques that make it possible to glean patterns, insights, and knowledge from data related to any topic or discipline. It is a practice applicable to any pursuit.

As a result, demand for data science courses and projects has soared among students. For instance, the number of majors

Data-driven: Co-PIs on the data science initiative (from left): Mike Ludkovski, Ambuj Singh, Alexander Franks, and Sang-Yun Oh.

in the Department of Statistics and Applied Probability (PSTAT) has more than tripled in the past six years, due in part to the surge of interest in data science.

"Our students desperately want research projects," said Ludkovski. The NSF grant will enable the university to expand its offerings to meet this burgeoning interest.

The computer science and PSTAT departments are collaborating to establish a series of three courses, open to all majors, though prerequisites will be required for courses beyond the first one in the series. The final course includes a year-long capstone project in data science involving small groups of two to three students working on actual data sets for some of the many industry partners PSTAT has developed over the years.

The three-course sequence is modeled on PSTAT's highly successful actuarial-science capstone project and on a very popular capstone-course sequence in computer science. A mix of faculty from the two departments will teach the series, with the first course scheduled to be offered in fall 2020.

The NSF grant and the data-science courses and capstone projects reflect keen and growing student interest in the subject. Close to two hundred students participate in UCSB's very active student-run Data Science Club, which hosts workshops and speakers and organizes quarterly data science projects, providing students from various departments with a place to develop their data science skills, regardless of how much or how little they know coming in.

> "Data science is a super-hot topic. It gets applied in every field, so it's very marketable as a career."
>
> NATALIE ROZAK

Natalie Rozak, a senior who is graduating a year early as a third-year statistics major and is one of the club's project-group directors, demonstrates that interest. "Working with such great professors and having great classmates and mentors in the club made me realize that I love using data," she says. "Through the media, one can see that data science is a super-hot topic. It gets applied in every field, so it's very marketable as a career."

Rozak, who has a job as a data scientist with the chemical company BASF waiting for her after she graduates, is excited about the new initiative and the capstone projects it supports.

"In class, we learn the theory behind key data science concepts, and we apply those methods to homework assignments and projects," she says. "It's wonderful that the grant will allow professors to teach more data science techniques and include hands-on projects in the curriculum, because both are very important and rewarding for students."

The university's interdepartmental effort in data science reflects the interdisciplinary nature of data science itself. "You can situate data science in a single department and let that department expand, or you can create something new," says Singh. "We're leaning toward the latter approach. It requires more work up front, but we hope that a broader perspective will bring together faculty and students from different streams and departments, resulting in a more unified approach."

"The program will provide a pathway for a number of community-college students to explore data science and move into a four-year university," said Robinson. "It also connects the more practically minded Cal State University system with the research-oriented UC system."

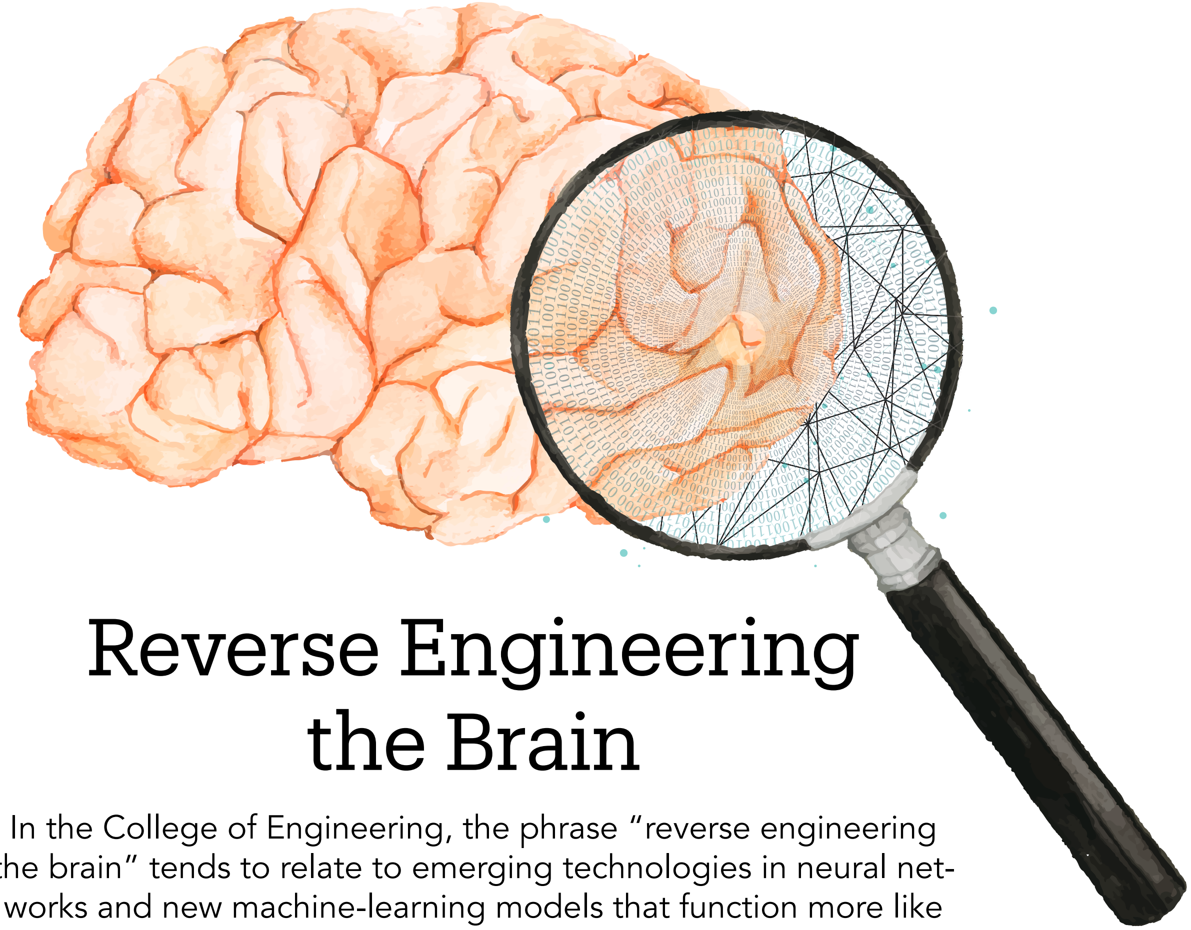
The data science consortium is part of a growing emphasis UC Santa Barbara is placing on data science. Most recently, the Bren School of Environmental Science & Management announced that it will offer a Master of Environmental Data Science, in addition to its existing Master of Environmental Science and Management degree and its doctoral program. The inaugural data science class will be offered in fall 2021.

Photograph by Robert Rozak

*Third-year data-science major **Natalie Rozak** reflects growing student interest in data science. She became active in the Data Science Club and is now graduating a year early with a job awaiting her at the chemical company BASF.*

"We hope that a broader perspective will result in a more unified approach."

AMBUJ SINGH



Reverse Engineering the Brain

In the College of Engineering, the phrase "reverse engineering the brain" tends to relate to emerging technologies in neural networks and new machine-learning models that function more like the human brain. That work relies on other research that unravels how the brain operates — how it does what it does. In this FOCUS ON: section, we present four examples of such research that is ongoing at UC Santa Barbara.

Michael Beyeler: "Fooling" The Mind To See

"There is research to try to understand the brain — how it works on a mechanistic and algorithmic level — and then there's applying that to an engineered system that can interface with the brain," says **Michael Beyeler**, an assistant professor in Computer Science and Psychological & Brain Sciences, in providing context for his research, which lies in the emerging interdisciplinary field of neuroengineering.

"Brain-computer interfaces can be used both for treating neurological and mental disorders as well as for understanding brain function," he says. "Eventually, they should also allow us to restore vision to the blind." The work involves neuroscience, computer science, and, because subjective perception is involved, psychology.

Beyeler's research focuses on visual prostheses (aka "bionic eyes"), which are being developed for those rendered blind by diseases of the eye, such as retinitis pigmentosa or macular degeneration. "The idea is that when individuals, due to various diseases, no longer have their photoreceptors — the light-gathering cells in the back of the eye — we can replace those cells with a microelectrode array that mimics their functionality. The question is just how to stimulate the surviving cells in order to avoid confusing the brain."

Beyeler has spent the past several years

"The question is just how to stimulate the surviving cells in order to avoid confusing the brain."

— Michael Beyeler

extensively studying the neural circuitry of the visual system to understand how to stimulate the system so that a person can see an intended image.

"Once a person loses the photoreceptors in their eyes, other cells start to die as well. Eventually the neural circuitry in the eye rewires completely," Beyeler explains. "That's why, when we put in a chip, the result depends on the patient's history and the state of the retina.

"Unfortunately, with current technology, it turns out to be really hard to mimic the neural code in the eye and the visual cortex to fool the brain into thinking that it saw something meaningful. This is where I come in."

Beyeler conducts psychophysical experiments and builds computational models to determine how to go from camera input to electrical stimulation and come up with a code that the visual system can interpret. "We ask implantees to draw what they see when we stimulate different electrodes. We then use insights from these experiments to develop software packages that predict what people should see for any given electrical stimulation pattern, which can be used by the device manufacturer to make the artificial vision provided by these devices more interpretable for the user.

"By averaging the drawings from multiple trials with a single patient and then overlaying them over the electrode, and doing the same for all the electrodes, we get an idea of what the array produces," he says. "For one person, it might be all lines. For another person, it might be triangles, wedges or other shapes. What we find is that the vision produced by current devices is distorted — it is far from a low-resolution pixel display, and it is far from natural vision. The question now becomes how to make things better — with preprocessing, with novel stimulation strategies, with better computational models of the eye. That's where my research is going."

"It's early days," he says, although some five hundred people in the world have the chips. "They see motion pretty clearly," and the shape of what is moving. "A lot of people are very happy with them. People learn to use them. It's a new code, a new way of seeing."

Kenneth Kosik: Electric Neurons

For nearly his entire career, **Kenneth Kosik**, Harriman Professor of Neuroscience in the Department of Molecular, Cellular, and Developmental Biology at UCSB, and co-director of the university's Neuroscience Research Institute, has studied neurons from the perspectives of molecular and cellular biology as they relate to gene expression, specifically in Alzheimer's disease. Recently, he branched out to study neurons from what he describes as "a neurophysiological or electrophysiological perspective."

Kosik and colleagues — UCSB physics professor **Paul Hansma**, computer science professor **Linda Petzold**, and research scientist **Ken Tovar** — developed a novel analytical approach for understanding the complex electrical connection among neurons.

The experimental setup begins with neurons that have been dissociated from a mouse brain, or even human neurons derived from stem cells. Kosik places about 100,000 neurons onto a square surface 1.2-millimeters on a side, beneath which is a multi-electrode array (MEA) containing 120 electrodes. The neurons spontaneously form connections that can be tracked by action potentials traveling along axons and across synapses, and the electrodes pick up the signals. "I believe that we can extract certain principles of neural connectivity from this model system," Kosik says.

Previously, researchers using MEAs encountered too much variability from one experiment to another to be able to extract general principles about basic neurophysiology. "I think we overcame that problem," Kosik says, "and it started with one simple but important insight."

Kosik's group realized that, as a neuron sends a signal down its wire-like axon, the axon crosses over a number of electrodes, and that its pattern as it fires above electrode 1, then 2, then 3 is an extraordinarily accurate maker for a single neuron extending its axon over the distance across the grid. The pattern of spikes separated by a millisecond or less occurs over and over in the same order and with high fidelity. That, Kosik says, "is an indisputable signal of axon potential traveling down the axon." He was surprised that others had not previously appreciated this method to extract axonal signal propagation velocities of multiple neurons from a single culture.

With many neurons firing simultaneously, it is challenging to correlate specific pulses in the MEA with individual neurons. For that, researchers generally use a computational assessment called *spike sorting,* which involves looking at the waveform. But, says Kosik, "The waveform will always vary depending on how far the electrode is from the neuron. That created the variability, which, in my opinion, is what has prevented progress with MEA technology.

"For one electrode pulse, multiple neurons could be firing, but if you actually do what's called signal averaging, so that you line up the signal in electrode 1 that corresponds, timing-wise, to the signal in electrode 2, and you ignore all the other signals from other neurons that are present but don't fit in that sequence, you now have a novel way to sort the spikes. We started doing it manually, but then, **Destinee Cheng**, a talented PhD student in Linda Petzold's lab, wrote an algorithm to automate the process."

"The computer program transforms the electrical pulses into very long sequences of zeroes and ones — mostly zeroes — with zeroes representing neurons that are not firing and ones representing neurons that are firing," Petzold says. "From that, we try to determine how the neurons represented by those electrodes are wired together. We're just trying to infer what the network looks like."

In one array, Kosik, says, "We can measure the velocity of the action potential in about fifty different neurons. Previously, no one had been able to do that over a large number of neurons in a high-throughput way."

Kosik has used the same system to calculate the rate of firing across synapses. Based on work by **Elmer Guzman**, a graduate student in the Kosik lab, he says, "We can put all these data together, all the latencies over the whole array, and actually build a network and see how these neurons are connected to each other."

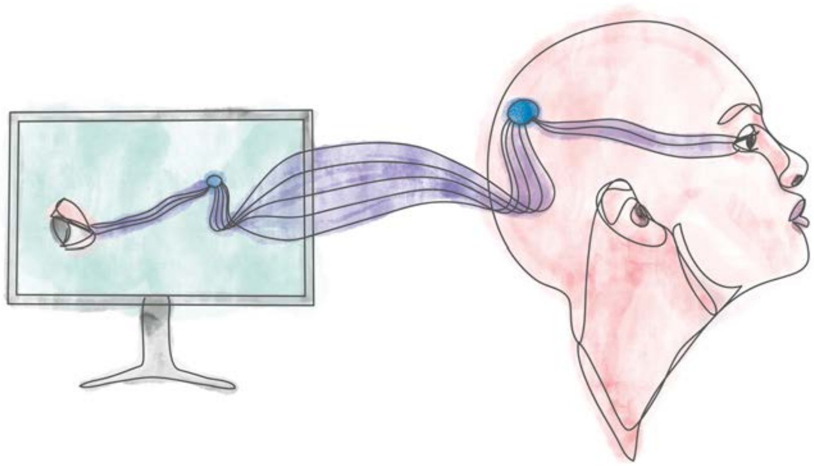
The process could give rise to multiple applications. "These neurons are revealing to us a very fundamental aspect of neurobiology, which is the action potential and synaptic transmission," Kosik says. "And then we can see how it's altered by drugs or mutations or diseases that affect axons, for instance. It could be diagnostic for a mutation or a toxin, or it could be used as a drug screen. Suppose you want drugs that can change the speed of conduction in diseases where the transmission of an action potential is impaired. If you have a drug you think might be efficacious, you can see its effect in this system."

"That pattern of spikes is an extraordinarily accurate maker for a single neuron extending its axon across the grid."

— Kenneth Kosik

"We're trying to determine how the neurons are wired together. We're trying to infer what the network looks like."

— Linda Petzold



"A lot of current vision systems are just not very robust in dealing with some of these things that the brain has learned to cope with."

— Miguel Eckstein

Miguel Eckstein: Modeling Vision

"Vision can seem like a trivial thing," says **Miguel Eckstein**, professor in the Department of Psychological and Brain Sciences, "but a fourth to a third of the human brain is dedicated to it. There is a vast world of problems and challenges you encounter in trying to model this for AI."

As examples of such difficulties, he recounts two nearly identical incidents in which Tesla vehicles set on Autopilot collided with semi-trucks that blocked nearly the entire field of view. "The autonomous vehicle was not trained to deal with it and thought there was nothing there," says Eckstein, who leads the Vision and Image Understanding Laboratory at UCSB. "A lot of the vision systems are just not very robust in dealing with some of these things that the brain has learned to cope with."

Eckstein develops algorithms that reflect how humans process images and incorporates them into AI computer models with the goal of improving such functions as face recognition and search, tasks, he says, "that seem trivial but are very complicated for computers. Some of my work is reverse engineering to understand how state-of-the-art machine vision differs from how humans do the task and how to incorporate into machine vision some of the processes the brain uses to solve a problem."

Among Eckstein's wide-ranging research in this area was a project he did with UCSB mechanical engineer **Franceso Bullo** involving the increasingly common prospect of AI and humans working together. Bullo wanted to coordinate twenty drones to gather information over a vast geographical area. Once collected, the information would be passed to a human decision-maker.

"There's a lot of complicated math involved in developing the strategies to ensure that the drones complement each other and efficiently cover everything, and getting the human into the loop is non-trivial," Eckstein says. "To combine the efforts of a human and a machine effectively, you need to know the capabilities and limitations of both and build on them. If you don't do that, you can end up with a bit of a disaster, in which the human receives too much information or ignores the machine because he doesn't trust it."

In a new project that also combines AI and humans and is scheduled to begin in May (but will perhaps be delayed because of the COVID-19 outbreak), Eckstein will work with Dutch scientists on a €3 million project called The Accurate and Intelligent Reading for EArlier breast cancer Detection (aiREAD). Their goal will be to understand and improve the integration of AI and radiologists to optimize diagnostic performance and medical outcomes.

In another type of seeing that Eckstein studies, he examines the differences between how a human finds an object in a scene versus how the same task is done by machines, which are getting much better at it. The key difference is that when AI looks for an object, it looks exhaustively at tiny details of that one object without taking into account the context — the object's relationship with the rest of the scene — as the human brain does.

Eckstein makes the point with a composite photo illustration he created that ran in the *New York Times.* It's a picture of a bathroom and an assembly of objects in it. A human who is asked to find the toothbrush will do so easily, spotting one on the counter near a sink. But that same human will nearly always miss the five-foot-long toothbrush standing against the wall beside the toilet, while a machine would never miss it.

"You miss it because your brain processes everything in the scene," Eckstein explains. "There's an expectation. That compensates for the fact that our vision outside our point of focus is pretty bad. If you try to read from the corner of the eye, you just get a little blur. That's why your brain relies a lot on size relationships across objects. Without the heuristics [rule-of-thumb strategies] the brain uses, we'd be pretty bad at recognizing the world around us."

> “How many different kinds of learning algorithms does a human brain actually use? How many mechanisms does it have for learning?”

Scott Grafton: Brain Voxels

People who have suffered a stroke or a traumatic brain injury recover to various degrees through learning. **Scott Grafton**, a professor in the Department of Psychological and Brain Sciences at UC Santa Barbara who has worked extensively with such patients, knows that learning occurs on many different time scales.

“The classic example is, I give you a phone number, and you can remember it instantly,” he says. “Then, if I give you a new phone, you have to learn to use it. That learning happens on a different time scale. And after you’ve called your beloved a thousand times, you can do it automatically without thinking about it, so you have that long-term automaticity. And if the phone’s center of mass is a little off, just lifting it forces your fingers to learn to adjust to the object, and they remember features about the object. In our group, we study human physical learning that takes place on different time scales.”

One of the big sets of breakthroughs in computer science and artificial intelligence has been algorithms for learning that make it possible to train robots, create deep neural networks, and more. One question that comes up in those endeavors, Grafton says, “relates to how many different kinds of learning algorithms a human brain actually uses, how many mechanisms it has for learning. That’s where we are in this space.”

Grafton uses fMRI (functional magnetic resonance imaging) to capture the activity of different brain systems as they relate to different time scales of learning. “We’re seeing not just whether an area of the brain is more or less active,” he notes. “We can actually look at the patterns of activity in that given area and ascertain, for example, before a person even lifts an object, the degree to which they’re anticipating the dynamics of the object.”

He explains that an fMRI measures blood flow in the brain, which serves as an indirect measure of brain activity: “It’s a signal that is kind of delayed and dispersed in time, but one we can measure at a fine spatial scale.”

Grafton uses that information to create a model, which allows him to simulate how changes in the activity in various areas of the brain affect learning. “We model a chunk of brain maybe the size of a sugar cube, and within that is packed a bunch of 2x2x2-millimeters voxels,” he explains. “That whole array of voxels has a pattern of activity, and in that volume of activity, I can determine whether someone is picking up an object that has a right- or left-oriented center of mass.”

One current hot area in engineering is brain implants, he explains: “So, say, you’re paralyzed, and we put these electrodes in you and try to read your mind. But that works only if your brain is good and there’s a disconnect between your brain and your muscles. What has always drawn me to this is, what if your brain is damaged?

“There, you’re not just trying to bypass something that’s broken; you have to figure out how to rewire what’s left,” he continues. “So, you really need to understand what’s left and how it learns, how it reorganizes itself. Those are all time-scale questions about how different parts of the brain learn in different ways. And if you know that, you have a basis for new ideas about what to do for stroke patients.”

> “We can actually look at the patterns of activity and ascertain the degree to which someone is anticipating the dynamics of the object.”
>
> — *Scott Grafton*

Fixing LA Traffic?

Igor Mezić applies Koopman Operator theory to understanding dynamical systems — like the 405 freeway

Traffic has been vexing drivers since not long after the first Model T's rolled off Henry Ford's assembly line. And while the cause of traffic may seem obvious — too many cars using a stretch of roadway at a certain time — the dynamics that lead to congestion are not.

That's because traffic is, as described by **Igor Mezić,** professor of mechanical engineering at UC Santa Barbara, a dynamical system, that is, one that is in constant flux, with an almost infinite number of ever-changing inputs dictating how efficiently the system functions at any given time.

In a paper to be published in an upcoming issue of the journal *Nature Communications,* Mezić and **Allan Avila,** a fifth-year PhD student in his lab, describe their research, which makes use of Los Angeles freeways, some of the busiest in the nation, as a test case for a new approach to understanding and forecasting traffic patterns. Their method employs a sophisticated mathematical approach known as Koopman Operator theory, a subject on which Mezić is a widely recognized expert.

The research was funded as part of a $6.5 million U.S. Army Multidisciplinary University Research Initiative (MURI) project focused on developing methods to describe and predict the behavior of dynamical systems generally. Traffic is such a system, as noted above, and the data was available, so, Mezić and Avila took on the challenge.

For decades, says Avila, the approach to trying to understand traffic as a dynamical system has been "to write some sort of evolution equations to describe how traffic dynamics evolve in time."

Avila explains the problem with that approach: "Whenever you're trying to develop such a mathematical model of a system, you make assumptions that allow you to simplify your equations. For example, you may assume that the highway system consists of only a single lane and has no exits or entrances."

In other words, you get an incomplete picture of the reality of the dynamical system.

There are good reasons for that, Avila says. "It's very difficult to get those equations right even for a single-lane road, and it's much more difficult to get a multi-lane description correct, because then you have to account for the complexities of lane-changing behavior and vehicles exiting and entering."

The Koopman Operator method requires no assumptions and enables accurate short-term predictions based on limited real-time data. That is in contrast to machine-learning (ML) techniques, considered today's state-of-the-art for traffic modeling, which require large amounts of training data to learn traffic dynamics. Unfortunately, even with voluminous data, they are contextually limited.

Mezić notes, "If you show one of these machine-learning methods a stretch of freeway in L.A. and then try to use the same model to apply what you learned somewhere in San Francisco or Denver, often times it starts to perform poorly, and you need to retrain it based on data for the new location."

Mezić and Avila's method overcomes several problems inherent in mathematical and machine-learning models, the most obvious one being that forecasts often fail to match what actually happens. "With our method, we don't need to write down equations explicitly," Avila explains. "Instead, we take observations of the dynamical system

in the form of data from sensors on the road and analyze the data via Koopman Operator methods." (For this project, they used data sets from the Federal Highway Administration and the California Department of Transportation.)

In application, the Koopman Operator theory works by breaking down — "decomposing" in the language of the theory — the observed data into subpatterns, along with their respective frequency of repetition and time of persistence (duration). Avila explains, "If we then combine the individual sub-patterns, we can recover the observed data, indicating that the extracted subpatterns are physically meaningful. Most importantly, the decomposition can be used to draw forecasts beyond the observed data."

Mezić adds, "Our method doesn't depend on where a road is or whether it's one lane, multi-lane, or a network of multi-lane highways. And it requires only the previous fifteen minutes of data to predict the next fifteen minutes or the next hour. It's really a type of AI that learns in a very short time, that scales, and that powerfully predicts the evolution of the system with a very limited amount of data."

Mezić and Avila would like to compare their method against some standard machine-learning methods, but that's difficult, because in developing ML models for traffic, researchers often smooth out "noisy" data and limit the data they use to, say, non-holiday weeks when it didn't rain. Effectively, Avila says, "they're describing only a subset of the dynamical system, whereas our method maintains its performance regardless of weather conditions, holiday season, or time of day. We don't smooth noisy data or prefer one type of condition or roadway over another.

"We can pick a highway and a certain time of the year, when the traffic is heavy," he continues. "We do the Koopman Operator method in little steps, so if we have data for an hour, we apply it to maybe every ten minutes and keep sliding it forward and drawing forecasts. The Koopman Operator propagates that function forward in time. And since real data exists, we can subtract our forecasted results from the actual measured reality and quantify our error."

While the project was intended to shed light on dynamical systems generally, Mezić believes that the impact of the research can spill over into the public domain in the form of improved roadway design and emergency preparation. "Understanding these traffic patterns on freeways for egress — remember what happened in New Orleans after Hurricane Katrina — is of national importance," Mezić says. "It's important to test the capacity of roadways before something happens. What if everyone suddenly starts leaving during a fire or after an earthquake? So, it's not just for traffic prediction; it's also useful for informing road design to handle emergencies."

New Math: III-V Plus IV-VI Equals an NSF Career Award

Kunal Mukherjee's lab group seeks to combine semiconductors for strength and defect immunity

Kunal Mukherjee (left) and student Eamonn Hughes in the molecular beam epitaxy lab.

For the past four-plus decades, the vast majority of semiconductors used in LEDs, optical communication, and light detection have been "III-V" materials, so called because they are compounds made by combining elements from groups III and V in the periodic table.

Kunal Mukherjee, an assistant professor in the Materials Department in the UC Santa Barbara College of Engineering, works extensively with III-V materials, but as a materials scientist, he is also interested in exploring new systems and developing new approaches to using familiar ones. He recently received a five-year, approximately $593,000 National Science Foundation Early CAREER Award to study IV-VI semiconductor materials, which are made of elements from those groups in the periodic table.

IV-VI materials predate III-V materials. Their properties were discovered around the 1870s, but they have been largely abandoned in electronics, because they are inherently soft and slow and can be easily damaged under the stresses of manufacturing.

IV-VI materials may have value, though, in addressing an inherent limitation of III-V materials. All crystalline materials have defects in their atomic structure, and provided the crystals are grown carefully, the defects in III-V materials are not problematic in most electronic applications; however, when III-V materials are used to make cost-effective devices that emit or receive light in the infrared spectrum, defects degrade performance. IV-VI materials, on the other hand, might be immune to some of the impacts of defects and loss when operating in the infrared.

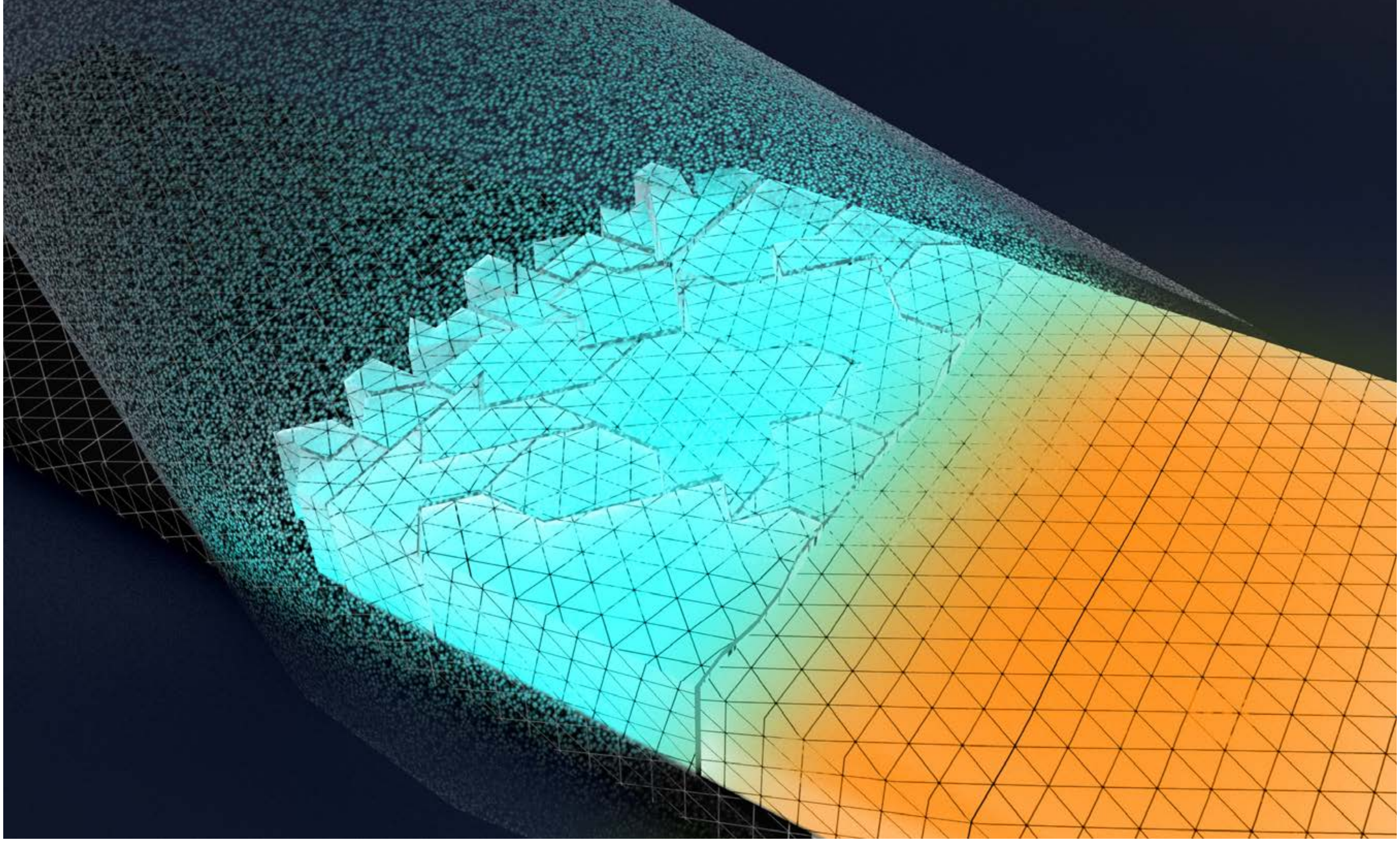
"When you make devices to emit and detect at these [infrared] wavelengths, you have to grow them very, very carefully; otherwise, you can have whole rows of atoms that are not in the right place," Mukherjee says. "A defect of this kind grows over time in the device as you're running it, causing it to malfunction. We've seen how bad defects can be in III-V infrared lasers, so our long-term thinking was, can we find a material that has the intrinsic properties of a III-V material but is not as sensitive to defects in the infrared?"

The team hypothesizes that a unique mixture of metallic, covalent, and ionic bonding of atoms in a IV-VI materials is what lends immunity to defects. "To address one part of the proposal, we want to try to verify this. We want to prove scientifically that there is immunity in the IV-VI, and then uncover the mechanism that confers the immunity," Mukherjee says.

The researchers also want to know if III-V materials can be combined with IV-VI materials to create a kind of "best of both worlds" material that is structurally stiff, like III-V materials, but also immune to crystal defects in the infrared. Their initial attempts have involved using molecular beam epitaxy (MBE) to create a substrate of III-V materials, and then to grow IV-VI materials on top of them.

"The nature of the bonds between atoms in a material determines the properties of that material," the team writes in the proposal. They want to see how the IV-VI material bonds atomically to the III-V and whether that changes the property of the semiconductor. Their challenge lies in the fact that the crystal structures for the III-V and the IV-VI are similar but different.

The team spent the past year learning how to overcome the difficult challenge of getting the IV-VI material to sit on top of the III-V substrate. "The interface is a new environment for the atoms, so they don't know what's going on," Mukherjee says. That causes some of them not to seat properly. "You have to coax the



Artist's depiction of IV-VI atoms (blue and orange) assembling into a crystal on a III-V substrate (black). A hotter growth temperature (yellow) leads to a well-aligned first layer of IV-VI atoms. Multiple crystallites of inferior quality (cyan) are depicted, resulting from growth at colder temperatures (cyan).

> "A defect of this kind grows over time in the device as you're running it, causing it to malfunction."
>
> KUNAL MUKHERJEE

first layer of IV-VI atoms down onto the III-V substrate."

Because the substrate is unfamiliar to the IV-VI atoms that are condensing onto it in the MBE chamber, sometimes the atoms land incorrectly. To overcome that, Mukherjee explains, "We gave the atoms time and a lot of second chances to correct the errors."

They did that by making the substrate very hot. Mukherjee explains: "If an atom went down incorrectly, the heat gave it enough energy to pop back out and rearrange itself in a correct position. The substrate was not so hot, though, that it caused atoms that settled correctly to re-evaporate. Once the atoms were in place, the substrate was allowed to cool, and from that point, it was easy to grow more layers of IV-VI to achieve the desired thickness. Growing the top layer of III-V materials will likely involve overcoming similar challenges."

Now that the team has reached this point, they can pursue the other challenges in the proposal. One of those is to use electron microscopy to understand why IV-VI materials have immunity to defects.

"We have a wonderful electron microscopy facility in our department, and we can actually locate an individual defect and then observe how that defect is sucking up all the charge in the material," Mukherjee explains. "We'll then change some of the properties of the material and the interface to see how that influences the defect."

The team has deep expertise in III-V materials and is simultaneously growing them to provide a benchmark to use in comparing how IV-VI materials behave differently.

Another goal of the research is to attempt to create the materials in some exotic phases, such as topologically ordered states, which are of interest to those working in the new NSF-funded UC Santa Barbara Quantum Foundry.

Researchers have three chances to apply for an NSF Early CAREER Award; this was Mukherjee's first try. "It's such a relief to get the award," he says. "The thing I like about it is that everything we submitted was homegrown by my students **Brian Haidet** and **Eamonn Hughes** in the past year to year and a half. It's validation that it sometimes pays to take risks. I was trained in III-V materials and did all the III-V things, but we decided to go out on a limb to look at some more exotic systems that we can grow. The reviewers liked that we are a III-V group and can therefore more objectively evaluate the IV-VI system. To have a panel of exterior reviewers say it's a risk worth taking is rewarding."

Hydrogen from Fossil Fuels — without CO_2

Changing the carbon cycle: Currently (top right), trains carry coal to coal-fired power plants, which produce electricty and abundant CO_2. In McFarland's approach (bottom right), natural gas would produce hydrogen to fuel a zero-emission power plant, and the same train tracks would be used to deliver leftover solid carbon to retired coal mines for burial and sequestration.

UCSB professor seeks to scale up hydrogen production and bury solid carbon in coal mines

In the search for zero-emissions alternatives to fossil fuels, UCSB chemical engineer **Eric McFarland** is betting on…fossil fuels. "Our strategy is to build a bridge technology that will allow us to get to a non-fossil-fuel future, which is ultimately going to happen, because fossil fuels are finite," he says. "The lowest-cost way of doing that may be to use fossil fuels differently, so that they don't produce CO_2. Our goal is to minimize atmospheric CO_2."

His approach, which he has been developing since 2016 in collaboration with fellow UCSB chemical engineers **Michael Doherty** and **Mike Gordon** and UCSB chemistry professor **Horia Metiu,** and with support from the U.S. Department of Energy and, now, Royal Dutch Shell, is to develop a method for creating clean-burning hydrogen fuel by stripping the hydrogen away from natural gas and leaving behind solid carbon. McFarland says that the solid carbon byproduct is much easier to store than carbon dioxide and could be buried, for example, in currently shuttered coal mines.

"It's a win-win," he says. "Rather than being the enemy, the fossil-fuel industry will be producing low-cost zero-emission fuel for society. Currently, we harvest carbon-containing natural resources and burn them in a way that produces CO_2; our vision is basically to reverse that flow to obtain fuel without atmospheric CO_2."

Further, McFarland explains, existing infrastructure could be used to make it work: "A coal plant today has a grid connection and a train track for bringing in the coal. We can replace the coal plant with a gas plant that runs on hydrogen derived from natural gas. Everything else stays the same. We have two million miles of high-pressure natural-gas pipeline in the U.S., which can be used to move the fuel, and the same train systems that formerly brought coal from the mine will now take the solid carbon back to the mine. The grandchildren of coal miners will have jobs filling the holes their grandfathers dug. The cost should be about the same $15 per ton it costs now to take coal from the ground and deliver it to a coal-burning power plant."

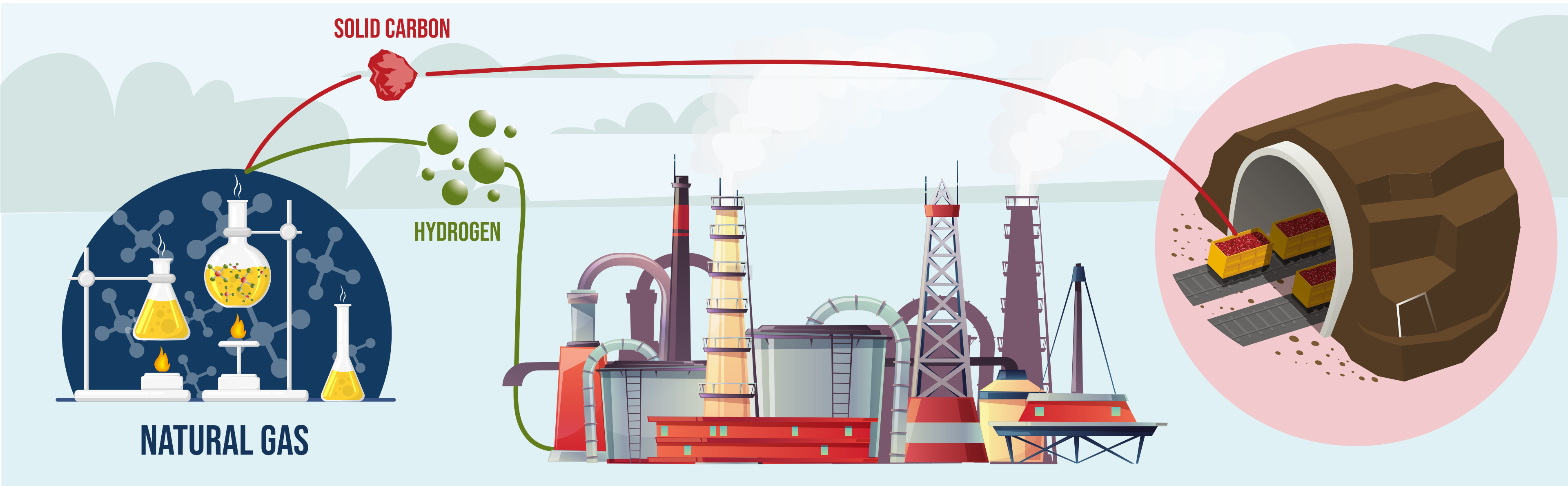
The final piece of the puzzle, he says, is that "Hydrogen is viable as a transport fuel. Long-haul trucks can be converted to hydrogen very easily, ships have been run with it, and GE already makes a hydrogen-fueled jet engine. It's not an unusual fuel that hasn't been looked at carefully before."

McFarland and Metiu have been working on understanding and controlling reactions of methane, the major component of natural gas, for over a decade. Producing hydrogen (H_2) from methane (CH_4) via the pyrolysis reaction $CH_4 \rightarrow 2H_2 + C$ requires very high temperatures or the use of a catalyst, traditionally a solid. But solid catalysts get clogged with solid carbon (C) in a process called *coking,* causing them to lose their activity.

The group began investigating reactions of natural gas on high-temperature *liquid* catalysts to produce hydrogen in 2016, as a means for solving the coking problem. As methane is bubbled into the high-temperature liquid environment, the liquid catalyst at the gas-liquid interface is continuously renewed. The solid carbon floats away in the process and can be removed. The first paper about the work ran in the journal *Science* in 2017 and described the team's discovery of catalytic molten metal alloys and their mechanism of catalysis. "We leverage a lot of what is already known," McFarland says. "Our contribution was to identify liquids that are good at converting methane into carbon and hydrogen."

The molten-metal catalysts can also be used on mixtures of methane and carbon dioxide. In their recent paper published in the January 20, 2020, issue of *Nature Catalysis,* the team showed how molten-metal alloy catalysts transformed mixtures of carbon dioxide and methane into *synthesis gas,* a mixture of hydrogen and carbon monoxide (CO) that can be used to make methanol or fuel-like molecules. "There are many gas fields on earth that have a large amount of CO_2 with the methane, and they're largely thought to be pretty useless, because it's hard to separate them," McFarland explains, "but, if you do what is called a *dry reforming* and react methane and CO_2 together, you can produce carbon monoxide and hydrogen, which, in the right ratio, can allow you to make methanol and other fuels." McFarland and Metiu's catalysts make it possible to control the H:CO ratio and also prevent coking.

The team is now focused on investigating the use of molten salts as catalysts specifically for making hydrogen from natural gas. It is important that the solid carbon that is removed from the reactor be free of contamination from the liquid catalyst so that it can be disposed of cheaply. That's difficult with molten metals, because the metal sticks strongly to the carbon, and lost metal is expensive. The researchers have published several recent papers identifying new molten-salt catalysts, which produced the cleanest carbons from natural gas pyrolysis.



“It is better to build out and pay for the infrastructure while making use of the lowest-cost zero-emission hydrogen.”

ERIC MCFARLAND

Having come this far, McFarland says, “You have to make it work cheaply. From a process point of view, you have to take the natural gas into a facility, put it into a high-temperature reactor, make the solid carbon, and get the carbon out. And you have to do all of that at a competitive cost.”

The group’s work on obtaining hydrogen from the methane in natural gas has had considerable interest from industry, and McFarland’s Shell-backed startup, called CZero, is licensing the intellectual property owned by the University of California to commercialize the process.

The company hopes to help California achieve its low-carbon goals by providing affordable hydrogen with zero CO_2, leveraging low-cost natural gas until alternative means are found for using renewables to produce cost-effective hydrogen. McFarland points out, “It is better to build out and pay for the needed hydrogen infrastructure while making use of the lowest-cost zero-emission hydrogen than to use the very expensive hydrogen produced from renewables and not be able to pay for infrastructure while simultaneously offering an affordable hydrogen product.”

Currently, he says, “We’re nearly ready to go to a demonstration-scale. We have a concept that can produce several kilograms of carbon per day. From there, if we get it right, we may be able to go to a commercial pilot scale.”

Side Ways

Computer scientists discover a software vulnerability that is akin to an information "leak" — and propose a way to isolate it

Every day, we trust computer systems with our sensitive data. The more we do so, the more devastating are the results of increasingly common cyber attacks that result in the theft of confidential information. While many software-development practices are aimed at protecting the confidentiality of private data, according to a team of UCSB computer scientists, numerous software systems still contain serious security vulnerabilities, allowing information to be "leaked" through what are referred to as side channels.

Side channels are a class of information leaks that can allow a hacker to capture secret information by observing the non-functional side effects of software systems, such as their execution time, their memory usage, their power consumption, and the size and timing of their network packets.

Side-channel leaks are the subject of two recent papers by UCSB researchers, one to be presented at the 41st IEEE Symposium on Security and Privacy (S&P), held in San Francisco from May 18-20, and the other to be delivered at the 42nd International Conference on Software Engineering (ICSE), scheduled in Seoul, South Korea, from October 5-11. S&P and ICSE are the top publication venues in computer security and software engineering research, respectively.

In the papers, co-authors **Tegan Brennan** and **Seemanta Saha,** PhD students in VLab, directed by UC Santa Barbara professor and computer science chair, **Tevfik Bultan,** who is also their PhD advisor, and former VLab postdoctoral researcher **Nicolas Rosner** (now at Amazon) report a new type of side channel that leaks information in modern software systems.

The new class of side-channel vulnerabilities are called *JIT-induced side channels.* The key insight behind their discovery is that just-in-time (JIT) compilation — crucial to the performance of modern programming languages, such as Java and Javascript — can introduce timing side channels into a program as it performs its function, which is to convert source code, or bytecode, into machine code while the program is running and optimizing the machine code for the most-common-use cases.

What Brennan, Bultan, and Rosner show in their paper, titled "JIT Leaks: Inducing Timing Side Channels through Just-In-Time Compilation," to be presented at S&P 2020, is that a hacker can leverage this optimization process to learn sensitive information.

In one scenario described in the paper, a low-privileged user can use an authentication system that is supposed to be secure to detect if and when a high-privileged user logs into a computer system. At a classified facility, the presence of a high-privileged user could be sensitive information itself. A JIT information leak could allow that information to be captured by other users. Another example demonstrates that a user of an online map service can detect if and when another user makes a routing request that is larger than a distance threshold. "We can think of many ways this new side channel can be exploited," Bultan said, "but we should be more worried about the exploits we cannot think of yet."

VLab researchers do not know if malicious hackers have been exploiting this type of information leak; however, other types of leaks have had very serious consequences. For example, the Meltdown and Specter exploits, reported in 2018, demonstrated that nearly all processors produced since 1995 were susceptible to attacks that can steal users' data. Both Meltdown and Specter exploited a well-known *cache* side channel that exists in computer hardware. JIT-induced side channels discovered by VLab researchers is a new type of side channel that can lead to new exploits.

Brennan discovered the vulnerability while taking a course on runtime systems and, at the same time, working on a challenge problem to identify information leaks in software systems as part of a Defense Advanced Research Projects Agency (DARPA) project, says Bultan. "When she started learning about the just-in-time compilation strategies used by runtime systems in class, she suspected that they might leak information and decided to investigate." Encouraged by Bultan, she recruited other researchers from VLab to work on the problem, leading to the discovery of JIT-induced side channels.

In the second paper on this topic, titled "JVM Fuzzing for JIT-Induced Side-Channel Detection," to be presented at ICSE 2020, Brennan, Saha, and Bultan describe an automated approach for detecting and evaluating JIT-induced side channels in programs. It allows software developers to automatically evaluate whether a Java program might be vulnerable to this class of side channels and under what runtime conditions. It also allows a developer to detect JIT-induced side channels automatically before a software system is deployed and can be exploited.

The team is currently working on mitigation techniques that would eliminate JIT-induced side channels in programs once they are detected.

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Lasting connections are particularly meaningful in this moment of COVID-19–induced social distancing. As this issue of *Convergence* goes to press, we are in the midst of the pandemic, but when things eventually return to normal, the strength and support of our community will be more important than ever.

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The beginning of spring quarter found the UC Santa Barbara campus empty and the usually busy bikepath that passes the Materials Research Lab (upper right) uncharacteristically free of traffic.