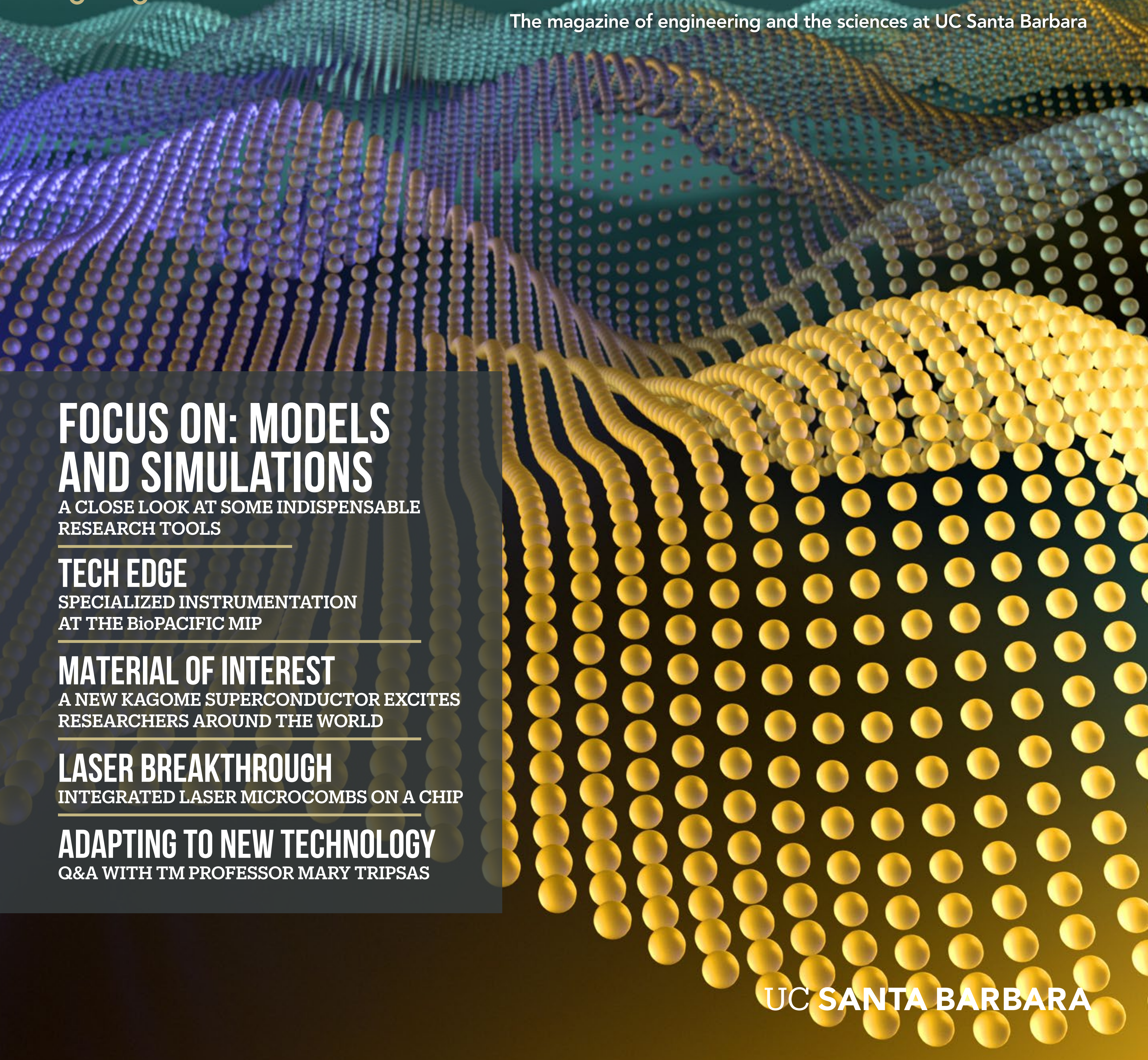
FALL/WINTER 2021

CONVERGENCE

The magazine of engineering and the sciences at UC Santa Barbara



FOCUS ON: MODELS AND SIMULATIONS

A CLOSE LOOK AT SOME INDISPENSABLE RESEARCH TOOLS

TECH EDGE

SPECIALIZED INSTRUMENTATION AT THE BioPACIFIC MIP

MATERIAL OF INTEREST

A NEW KAGOME SUPERCONDUCTOR EXCITES RESEARCHERS AROUND THE WORLD

LASER BREAKTHROUGH

INTEGRATED LASER MICROCOMBS ON A CHIP

ADAPTING TO NEW TECHNOLOGY

Q&A WITH TM PROFESSOR MARY TRIPSAS

UC SANTA BARBARA

MESSAGE FROM THE DEANS

TRESA POLLOCK
Interim Dean, College of Engineering; Alcoa Distinguished Professor of Materials

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

The most important two words we can say right now just might be "Welcome back." Welcome back to students, who have been dispersed for so long but are again filling walkways, bike paths, classrooms, and labs. Welcome back to faculty and staff, who have returned to teaching and supporting, amid renewed appreciation for the familiar rhythms and daily routines of campus life. And welcome back to members of the greater community, who can again visit the university.

The effort needed to re-establish these familiar campus routines is, perhaps, the biggest collaboration ever undertaken at UC Santa Barbara. That's saying something. After all, we pride ourselves on accomplishing great things and providing a world-class education to so many by coordinating efforts, sharing resources, and taking bold strides to connect disciplines in ways that fuel innovation and help to improve the world. As always, this issue of *Convergence* is filled with the results of such efforts.

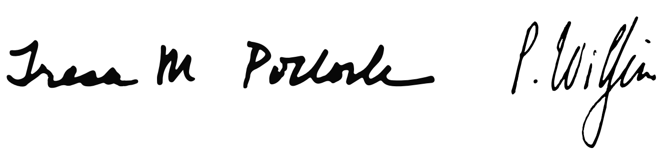
For instance, we share with you a breakthrough in miniature on-disc laser technology (P. 12), the fruition of years of work in the labs of **John Bowers** and his collaborators. We also not only tell you about a promising new superconducting material developed in materials professor **Stephen Wilson**'s lab (P. 16), but also share the fascinating story of how it came to be (P. 18).

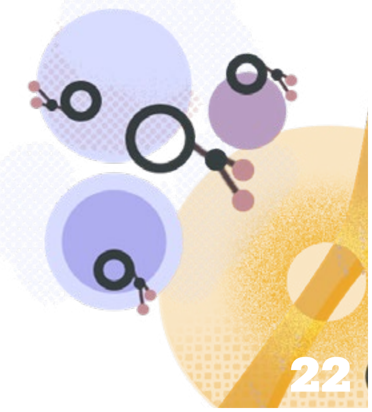
This issue's "FOCUS ON:" section (P. 22) is devoted to models and simulations, which many people know of but not necessarily about. We spoke with six researchers in a range of disciplines who helped us gain a deeper understanding of these important tools, which are indispensable to research efforts everywhere.

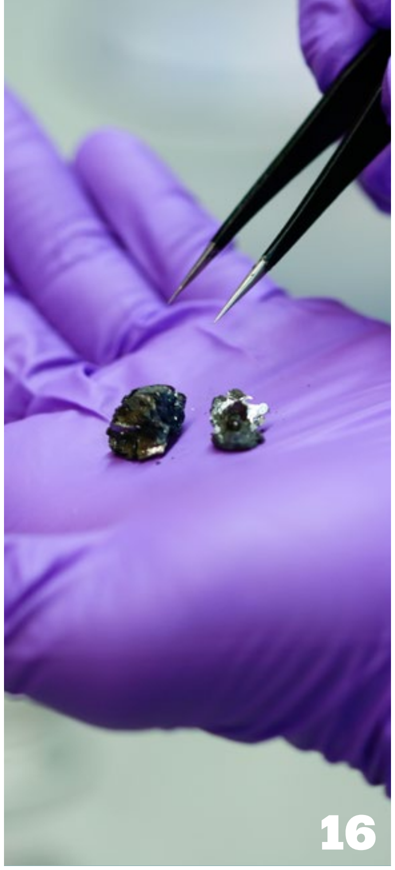
We offer a Q&A with dynamic new Technology Management professor **Mary Tripsas** (P. 14), and another with **Jim Frank** (P. 20), a major UCSB and College of Engineering donor who leads the Goleta-based Raintree Foundation, established by his late father, **Harold Frank,** for whom Harold Frank Hall is named.

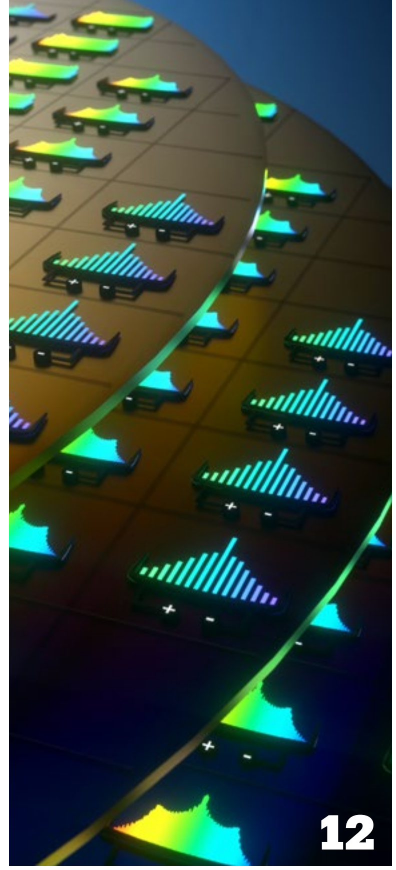
Finally, a new section called "Tech Edge" (P. 8) debuts in this issue, providing a behind-the-scenes look at state-of-the-art equipment and instrumentation that enables engineering and science research at UCSB. We begin with the rapid-chemistry platform, the additive manufacturing (3D printing) facility, and the X-ray diffraction facility, each a fundamentally enabling element of the NSF–funded BioPolymers, Automated Cellular Infrastructure, Flow, and Integrated Chemistry Materials Innovation Platform (BioPACIFIC MIP).

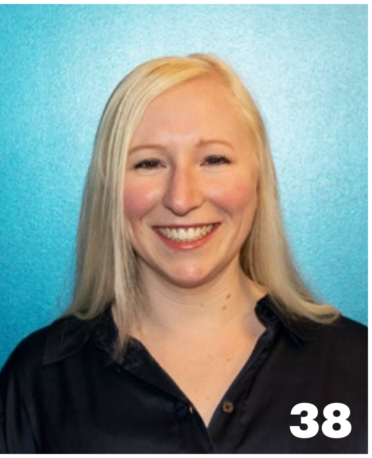
We hope you enjoy the issue, and again, welcome back!

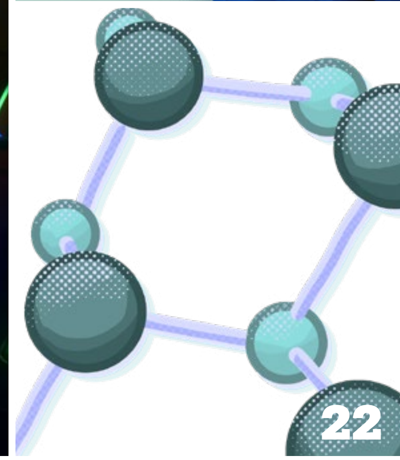












CONTENTS

CONVERGENCE

The Magazine of Engineering and the Sciences at UC Santa Barbara
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UC **SANTA BARBARA**
College of Engineering

NEWS BRIEFS

ROD ALFERNESS RETIRES; TRESA POLLOCK NAMED INTERIM DEAN

Tresa Pollock became the COE's interim dean after Rod Alferness retired.

Materials professor **Tresa Pollock** has been named interim dean of the UC Santa Barbara College of Engineering, following the retirement of **Rod Alferness,** which became effective Sep. 21.

"We are grateful for Professor Pollock's dedication and willingness to assume the responsibilities of this important leadership position," said **Chancellor Henry Yang** in a letter announcing her appointment.

Pollock, the Alcoa Distinguished Professor of Materials and a world-renowned metallurgist known for her creativity as a researcher, has served as the COE's associate dean since 2018 and will lead the college until a new permanent dean is identified following a thorough national search.

"It is an honor to serve the college in the role of interim dean at this critical time," Pollock said, "and I am grateful for the leadership that Rod provided throughout his tenure as dean."

"My association with Tresa goes back quite a number of years, to when she served as chair of the Materials Department, and more recently, as a fellow associate dean," said **Glenn Beltz,** the COE's Associate Dean for Undergraduate Studies and a professor of mechanical engineering. "The diversity of experience she has gained during her distinguished career in both industry and academia gives me tremendous confidence that she will continue to advance the stature of the College of Engineering on both the research and the education fronts. I look forward to working with her."

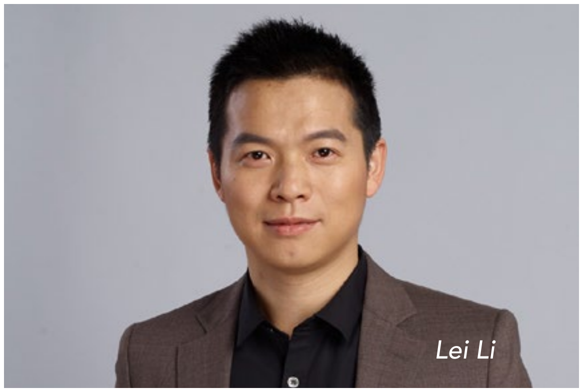
During his ten years as COE dean, Alferness provided steady leadership that led to increased standing and recognition for the college. Under his watch, important new buildings were completed, key faculty members were hired and retained, and the college made the transition to and from remote learning during the COVID pandemic, to mention only a few of many important milestones. While Alferness will be missed by all who know him, he left the college well positioned to move boldly into the future.

Please join us in welcoming Dr. Pollock to her new role, and in wishing her abundant success in the months ahead.

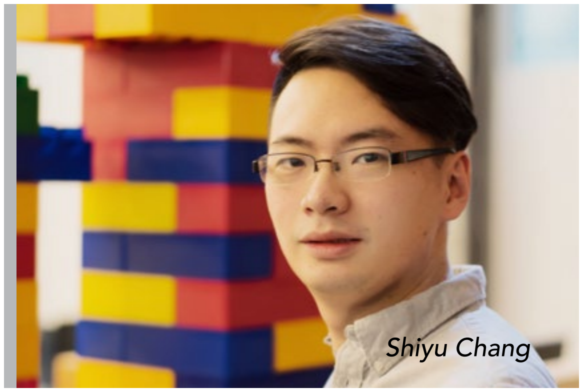
"RISING STARS" JOIN COMPUTER SCIENCE FACULTY

The Computer Science Department in the UC Santa Barbara College of Engineering has earned a solid reputation in many areas, one of them being natural language processing (NLP), a sub-specialty within machine learning (ML) and the greater realm of artificial intelligence (AI).

The department's standing in NLP, especially, will undoubtedly rise further with the addition of two new faculty members: **Lei Li,** formerly of ByteDance AI Lab, the company behind TikTok and other prominent mobile apps, where he was founding director, and **Shiyu Chang,** previously a research scientist at the Massachusetts Institute of Technology's IBM Watson AI Lab. They joined the CS faculty this summer.



Lei Li



Shiyu Chang

Computer science professor and department chair, **Tevfik Bultan,** said of the two hirings, "UCSB CS has become a center of excellence, with stellar students and faculty, and this enables us to attract the best talent in the world, as demonstrated by Lei's and Shiyu's decisions to leave lucrative research positions in industry and join our department. They will further strengthen our leadership in NLP and help us to address the exploding demand for research and education in ML and AI."

"This is excellent news for our program

and very important for our campus," said **William Wang,** computer science associate professor and co-director of UCSB's Natural Language Processing Group and its Center for Responsible Machine Learning. "Both Lei and Shiyu are rising stars in AI and NLP, and their presence here means that our students will be able to take more, and more diverse, AI courses, and allow us to build one of the strongest natural language processing groups in the world."

Li earned his bachelor's degree at China's prestigious Shanghai Jiao Tong University and his PhD in computer science from Carnegie Mellon University in 2011. He then spent three years as a postdoctoral researcher at UC Berkeley before eventually finding his way to ByteDance. Chang received both his BS and his PhD from the University of Illinois at Urbana-Champaign.

The common theme in much of Li's work is a focus on developing new technologies to improve the efficiency and efficacy of how people create, communicate, and consume informational content, mainly in the areas of ML, NLP, and machine translation, as well as in such innovative project areas as intelligent robotics.

A machine-writing system (Xiaomingbot) that Li developed to automatically create news articles from table data was used to generate media reports on some four hundred competitions in the 2016 Rio Olympics, and in August, he and his team won the best paper award, out of more than three thousand submitted, at the Annual International Conference of the Association of Computational Linguistics.

He says that coming to UCSB made sense: "I had a chance to visit Santa Barbara previously and was really impressed by the extraordinary group of scholars and the hospitality of the region. Plus, there are many people here I admire or know very well, such as [CS professors] **Ambuj Singh** and **Xifeng Yan.** I have been reading their papers since my graduate school years. Also, William Wang and I have collaborated on multiple papers." Finally, the vice president of ByteDance, **Dr. Weiying Ma,** is a UCSB alumnus who, Li said, "kept telling me good things about UCSB."

Chang says that his interest in teaching was kindled by his late advisor at the University of Illinois. "A teacher changed my life," he said. "I want to have the same impact on my students, and I would like to use my passion and enthusiasm to encourage young people to devote themselves to this field, just as my school and my advisor did for me. This is why I am committing myself to pursuing an academic career."

Chang's research is focused on advancing the application of deep-learning algorithms, which, he said, "have achieved unprecedented success across many benchmark tasks but see only limited application in mission-critical deployments, such as medical applications, owing to the lack of an efficient communication channel between humans and machine-learning algorithms."

In a conventional ML paradigm, he explains, humans communicate with neural networks primarily by providing them with training and testing data, and the neural networks communicate back with a single, inscrutable neural prediction. There are few opportunities for humans to inject additional intuitions, experience, or other guidance into these "black-box" systems.

Chang's most recent work has focused on "deep rationalization," that is, using a language he calls "rationales" — human-interpretable explanations of neural network predictions — to enable efficient two-way communication between humans and complex neural networks.

Both Li and Chang say that they are looking forward to working with the UCSB NLP group and other scholars in CS.

"I firmly believe in the power of teamwork, and I have benefitted a lot from it," Chang noted. "The UCSB NLP group is one of the most reputable research groups worldwide. I look forward to working closely with all of the talented faculty members and students in the group to develop more impactful research."

"Together with my colleagues, I hope to strengthen and further promote UCSB as a nationally and internationally recognized center on AI, machine learning, and NLP," Li said, "and to cultivate next-generation scientists as leaders in academia and industry."

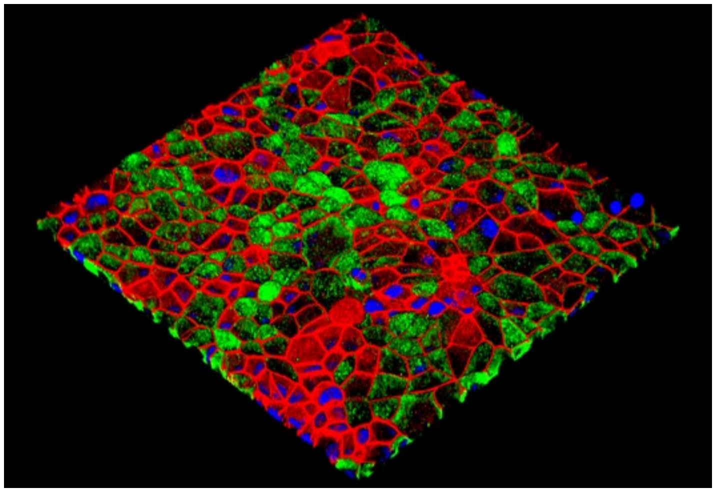


Image of retinal pigment epithelial cells on a scaffold after recovery from cryopreservation, stained for the ZO-1 protein (red), the BEST-1 protein (green) and nuclei (blue). Illustration by Jeff Bailey

FREEZING HEATS UP POSSIBILITIES FOR MACULAR-DEGENERATION THERAPY

In 2016, UC Santa Barbara biochemist **Dennis Clegg** published a paper describing a treatment he had developed for age-related macular degeneration (ARMD), the leading cause of blindness in aging populations. The process involves attaching ocular cells, created from pluripotent stem cells, to a flexible scaffold that is implanted into the eye. Clinical trials of the treatment are currently under way.

Now, Clegg and collaborators at UCSB, the University of Southern California, and the biotechnology company Regenerative Patch Technologies (RPT) have reported a new methodology for preserving RPT's stem cell-based therapy. The results, published in *Scientific Reports,* demonstrate that the implant can be frozen, stored for long periods, and distributed in frozen form to clinical sites, to be thawed and immediately implanted into the eyes of patients experiencing macular degeneration. The technique will extend the shelf life and enable on-demand distribution of the treatment to distant clinical sites, increasing the number of patients able to benefit from it and other cell-based therapeutics.

"This is the first published report that demonstrates high viability and function of adherent ocular cells following cryopreservation, even after long-term frozen storage," said lead author, **Britney Pennington,** who is head of process development at RPT and assistant project scientist at UCSB.

The study demonstrates that cryopreserved implants are comparable to their non-cryopreserved counterparts in appearance, gene expression, and cellular function. "It's a major advance in the development of cell therapies using a sheet, or a monolayer, of cells, because you can freeze them as the final product and ship them all over the world," said Clegg, who is senior author on the paper.

Data Driven Biology Fellows (from left): Gabriella Villalpando Torres, Rebecca Martin, Daniella Walter, and Samuel Rosen.

NEW PROGRAMS IN BIOENGINEERING FOR PHD STUDENTS IN MULTIPLE DISCIPLINES

PhD students in multiple disciplines are taking advantage of two new training programs launched during this fall quarter at UC Santa Barbara: the Interdisciplinary Training Program in Quantitative Mechanobiology, funded by a National Institutes of Health (NIH) T32 institutional training grant, and the Data Driven Biology (DDB) training program, funded by the National Science Foundation's (NSF) National Research Traineeship (NRT) program.

Beth Pruitt, mechanical engineering professor, director of UCSB's Center for BioEngineering, and PI of both training grants, says that the grants provide new opportunities for UCSB graduate students to work collaboratively and become better prepared for careers in academia, industry, national labs, and government.

Both programs accept PhD students from multiple departments and programs at UCSB, including the newly approved Biological Engineering PhD program, which will begin matriculating graduate students in fall 2022. The programs offer participants novel coursework and hands-on research experiences, plus opportunities for internships, externships, professional development, networking, and mentoring.

The NIH-funded Interdisciplinary Training Program in Quantitative Mechanobiology brings together biologists, physicists, and engineers to train predoctoral researchers in mechanobiology, which is focused on the relationships between molecular events and mechanical forces in living systems. The program enhances students' training in quantitative bioscience methods and engineering models and devices, while also offering multidisciplinary training to develop and apply quantitative approaches to problems in mechanobiology.

The program recently welcomed its inaugural cohort of Mechanobiology Fellows, comprising six PhD students representing the Departments of Chemical Engineering, Mechanical Engineering, Physics, Biomolecular Science and Engineering (BMSE), and Molecular, Cellular and Developmental Biology.

The NSF-funded DDB program is intended to train a new generation of biological scientists and engineers who are fluent in data analytics and experimental methods and can work across disciplines to advance fundamental research in quantitative biology and bioengineering. The program enhances students' PhD research by enabling them to integrate machine learning, data science, and quantitative image and bioinformatic analysis into their work.

The program welcomed its first cohort of five Fellows, from the Departments of Mechanical Engineering, BMSE, and Electrical and Computer Engineering.

KNOWLEDGE SHARING BEGINS AT THE BIOPACIFIC MIP

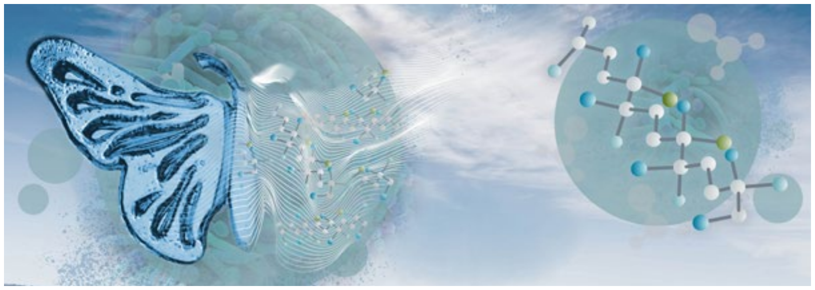
Virtual "summer school" was in session August 2-5 as the BioPolymers, Automated Cellular Infrastructure, Flow, and Integrated Chemistry Materials Innovation Platform (BioPACIFIC MIP), a $23.7 million NSF-funded collaboration between UC Santa Barbara and UC Los Angeles, offered a series of online training and information sessions to potential users.

The week-long summer school gave students, postdocs, faculty, technical staff, and industry researchers the opportunity to learn more about scalable production of bio-derived building blocks and polymers from yeast, fungi, and bacteria. The MIP incorporates automated high-throughput synthesis and characterization of bio-derived polymers with the goal of accelerating discovery and development of new high-performance materials.

The MIP is intended to be used by researchers from across the broad biomaterials community, with a vast network of users sharing knowledge. "Knowledge sharing is one of the key pillars that the NSF expects of MIPs," said UCSB MIP executive director, **Tal Margalith.** "We wanted to leverage the summer school to introduce the biomaterials research community to the MIP and its available equipment [see P. 8 for more on MIP instrumentation] and expertise while also creating a community around BioPACIFIC MIP and providing networking opportunities for students, especially with industry. The industry career panels were particularly well received, and the technical sessions were all well attended."

Outreach of the kind offered at the summer school is key, because half of the available platform time is reserved for external users, who need to be aware of what it offers in order to take advantage of the MIP's vast potential. To that end, said Margalith, UCSB and UCLA MIP faculty and staff reached out to experts in academia whose research is aligned with the MIP's capabilities, including experts in such key areas as high-throughput automated flow chemistry and creating nomenclatures for organizing polymer databases. Industry speakers attended from companies that either make tools used at the MIP or are using automation to develop biomaterials. More than thirty experts presented at the event, including MIP co-directors **Javier Read de Alaniz** (UCSB) and **Heather Maynard** (UCLA).

The summer school focused on introducing attendees to automated high-throughput synthesis and characterization of bio-derived polymers; hierarchical computational tools and theory to enable flexible, inverse design; the Design-Build-Test-Learn (DBTL) experimental design, intended to accelerate discovery of new high-performance materials; and the capabilities of the state-of-the-art equipment available at BioPACIFIC MIP while also providing mentorship and networking for graduate students.



KEEPING UP WITH COVID

*With the UC Santa Barbara campus reopened even as variants continue to be a challenge, particularly in areas that have low vaccination rates, we caught up with **Carolina Arias,** an assistant professor in the UCSB Department of Molecular, Cellular and Developmental Biology and an expert in virus-host interactions, to discuss her current focus with respect to the diminished, though continuing, pandemic. Arias recently received the prestigious 2021-'22 Harold J. Plous Award from the College of Letters & Science. The award is given annually to an assistant professor from the humanities, social sciences, or natural sciences who has shown exceptional achievement in research, teaching, and service to the university.*

Convergence: What is keeping you busy these days?

Carolina Arias: Variants. As viruses replicate, they accumulate mutations, and that leads to new variants; it's a normal part of viral replication. Right now, my lab is continuing to support Cottage Hospital and the California Department of Public Health to sequence viral variants, to help them figure out which ones are circulating, and to keep tabs on any that either the CDC or the WHO, or both, refer to as "variants of concern."

At the start of the pandemic, we saw a mix of variants, the majority of which were neither "of concern" nor "of interest." Then, the West Coast variant became dominant throughout California. The Alpha strain, from Great Britain, was then prominent for a while. The next significant variants were Beta from South Africa, Gamma from Brazil, and now, Delta from India. The virus is constantly changing. On the West Coast and across the U.S., it's all Delta now. In Santa Barbara, Delta came in and replaced all the other variants in a couple of weeks.

2021-'22 Harold J. Plous Award winner, Carolina Arias.

> WHEN YOU ARE VACCINATED, YOUR IMMUNE SYSTEM IS READY TO GO, SO YOU CONTROL THE INFECTION AND YOU CONTROL IT EARLIER.

C: *How do you keep track of the evolving variants?*

CA: We talk to each other a lot. For instance, we have a regular meeting with the people at Cottage Health. There are repositories of information, including good, up-to-date websites where you can go to track the variants and see where we've had outbreaks and whether a certain variant is represented more in the U.S. or California. We get information from WHO, the CDC, and even just the news, like Reuters. And we constantly monitor the archives of research journals.

C: *Are you still involved in testing?*

CA: Yes; even though we have very high vaccination rates among the UCSB population, testing will continue to be important until we can control transmission and see cases dropping around the world. We have to be vigilant, and we have to test to be aware of any new variants that might show up. As long as it's spreading, it will continue to mutate.

C: *What are your thoughts on vaccines, eleven months after the first one came out?*

CA: The vaccines are safe, they work as they should, and side effects are rare. And you are much more likely to become severely sick or to die of COVID if you get infected and are not vaccinated. The evidence is there. Many people think that the vaccines should completely prevent transmission and we should not have breakthrough cases, but that's not the case.

We know that people who are vaccinated are not ending up in the hospital, but it doesn't mean that we are completely immune. The vaccine was not designed to prevent transmission completely. It was proven to prevent severe disease, and it is doing that in normal vaccinated people who do not have other underlying factors, such as a compromised immune system.

When you are vaccinated, your immune system is ready to go, so you control the infection, and you control it earlier. The vast majority — in the upper ninety percent — of people who are severely sick right now and have filled our ICUs recently are unvaccinated. Recent outbreaks have been outbreaks of the unvaccinated.

***C:** Why do some vaccinations, such as those for measles and polio, prevent all cases of disease, while others seem to provide less complete protection?*

All vaccines are different, and the type of protection they provide against different pathogens is going to be different, too; it's not one recipe fits all. That's why we don't have a vaccine for every single pathogen out there, because they all behave differently, so how your system responds and how the vaccine targets the virus or the pathogen will be different, too.

We've been working on an HIV vaccine for decades and still don't have it. It gives you a little pride in the community that we were able to develop several vaccines that actually work against this virus. Otherwise, we'd be in more trouble than we are in now.

TECH EDGE

Leading-edge Instrumentation that Makes the BioPACIFIC MIP Go

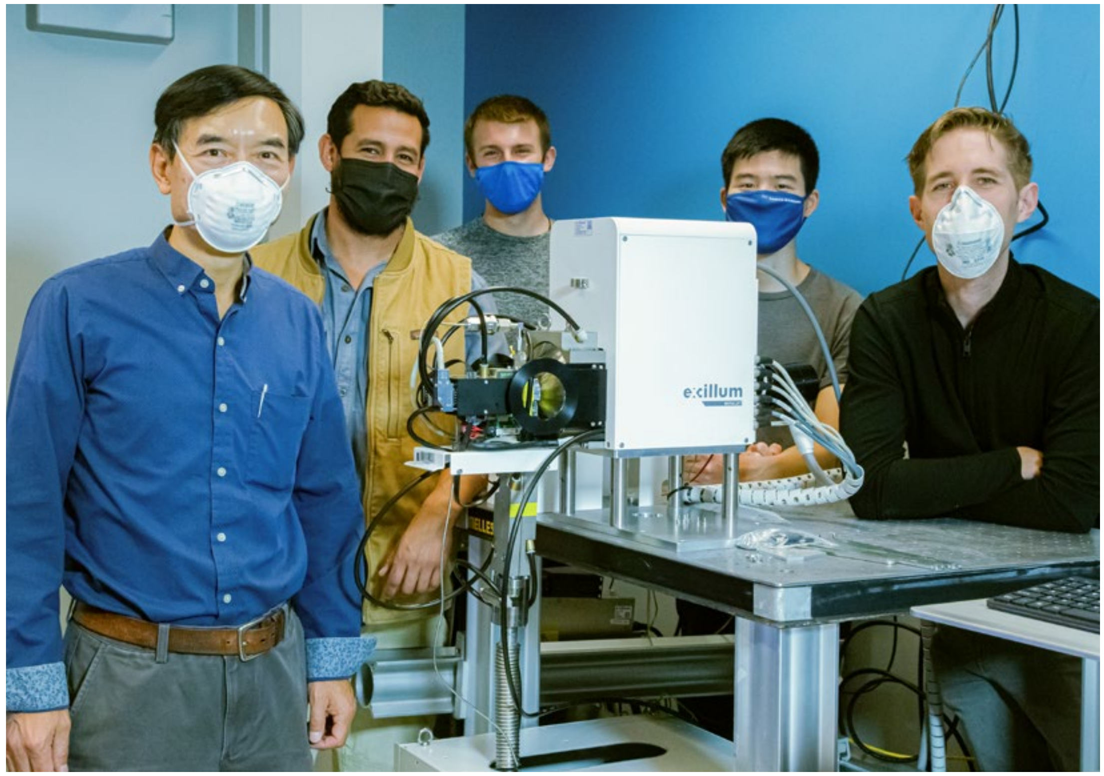
When it comes to collaborating, few R1 universities can match UC Santa Barbara, especially in engineering and other instrumentation-intensive STEM disciplines. The ability and willingness of diverse departments to cooperate — and the support for such reciprocal sharing provided by **Chancellor Henry T. Yang** and other key administrators — have been critical to enabling UCSB to achieve world standing in multiple STEM disciplines.

That uniquely collaborative environment — reflected to tremendous effect in the College of Engineering — has been instrumental in securing major funding for such entities as the Materials Research Science & Engineering Center (MRSEC, aka the Materials Research Lab), the Quantum Foundry, and, most recently, the BioPolymers, Automated Cellular Infrastructure, Flow, and Integrated Chemistry Materials Innovation Platform (BioPACIFIC MIP).

Such grants have also enabled UCSB to build a world-class array of leading-edge laboratory equipment and instrumentation. In this new series, "Tech Edge," we will highlight some of those instruments and how they serve the research enterprise, while meeting some of the people who operate and maintain them. We begin with three facilities — for small-angle X-ray diffraction (XRD), for additive manufacturing (aka 3D printing), and for automated chemistry, all part of the BioPACIFIC MIP. The five-year, $23.5 million collaboration with UC Los Angeles is aimed at building and operating a first-of-its-kind platform dedicated to the accelerated discovery and development of new high-performance, bio-derived materials. As an NSF platform program, the MIP is intended to provide tools and techniques to enable new approaches to scientific discovery.

"High-throughput" is foundational to the MIP, and everything related to it is being built or modified with the goal of rapidly discovering and synthesizing promising new materials, characterizing those materials at atomic and molecular scales, computationally simulating their behavior across a range of spatial and time scales, building libraries of new molecules and polymers for researchers around the world to use, and providing feedback to inform further refinement and discovery. Each of the three facilities described in this edition of "Tech Edge" is essential to that collaborative effort.

X-ray Diffraction: Youli Li



Concentrated on diffraction (from left): facility director, Youli Li, R&D engineer Miguel Zepeda-Rosales, undergraduate assistants Ryan Williat and Alvin Pan, and staff specialist Phillip Krohl with new X-ray source.

Microscopy and X-ray diffraction (XRD) are two of the most commonly used techniques for characterizing the structure of new materials. A highly advanced small-angle X-ray scattering (SAXS) instrument, which is a special application of the XRD technique for large-scale structures, is being built at UCSB to study the nano-structures of new materials produced in the BioPACIFIC MIP.

In traditional optical microscopy, light and lenses combine to provide direct observation of a sample magnified many times. Electron microscopy (EM) employs electrons, which have much shorter wavelengths than photons, to achieve the much-higher resolution required to "see" the atomic structure of a material. Electron microscopy, however, is primarily a *surface* imaging tool. The electrons from the beam interact strongly with the material, so they are absorbed quickly within the surface slice, preventing them from penetrating deeper and conveying information from any sub-surface region of the material.

X-ray diffraction, says **Youli Li,** who leads UCSB's XRD facility, "is quite the opposite." He explains that X-rays can penetrate deep into a material, with some X-rays bouncing off the electrons along the beam path, in a process called *scattering,* to produce a diffraction pattern that resembles an image of peaks and valleys. A computer is then used to mathematically transform that pattern into an image revealing how the atoms and molecules are arranged throughout the entire volume of the material. Thus, the information provided by X-ray diffraction is complementary to that of electron microscopy.

"The X-rays we use are well suited for looking at atomic and molecular structure, because their wavelength is so small, about the size of an atom, and that is the yardstick you're using to make measurements," Li explains. "In the optical range, the wavelength is on the order of a few thousand angstroms — a few hundred nanometers — so you can see detail down to the micron size. X-rays are about a thousand times smaller, providing a clear advantage."

For the MIP, Li and his team are expanding and enhancing the COE's XRD capability to facilitate high-throughput characterization of new materials. "We have been doing XRD for a long time and are well known, especially in small-angle X-ray scattering of biological and polymer structures, like those to be made in the MIP," Li notes. "When we applied for the MIP, we asked ourselves what tools we would need and how we could advance the SAXS technique to speed up discovery and give us one of the best instruments in the world."

An XRD consists of a source to pump out X-rays and a detector to read them. Li and his team decided to pursue an SAXS system that would have the brightest X-ray source available for a non-national lab setting in the world, coupled to the most advanced high-sensitivity detector to count individual x-ray photons.

"Our competitor will be the network of billion-dollar national facilities, called synchrotrons," Li says, "but we will have an instrument that allows you to just walk in and do a measurement."

And do that measurement quickly, leading Li to say that the new SAXS instrument "absolutely fits in" with the high-throughput nature of the BioPACIFIC MIP, thanks to engineering his team has done in building it. "High throughput means being able to examine multiple samples, quickly and efficiently, while minimizing dead time between them," he says. "You want to be able to load as many samples as possible, and we're building in a lot of automation and robotics so that you can automatically align the sample quickly and point an X-ray at it, normally a time-consuming process.

"Part of the reason we decided to build the instrument ourselves was because this combination of the brightest source and the best detector is not commercially available," he adds. "Additionally, building in the high-throughput capability to process samples rapidly allows us to serve a larger number of user groups. More important, in my mind, is that we can develop the instrument to meet the needs of possible future applications. The focus of research can shift over time, and we want this tool to be adaptable. We don't want to build a big, fancy, expensive tool to do just one thing."

He concludes: "We are hugely grateful to have received this NSF funding, and we're excited for the opportunity to design, engineer, and develop this high-performing instrument for the MIP. We hope that it will allow us to push the envelope in terms of developing new X-ray diffraction techniques, approaches, and methods that other researchers can use as well."

Printing Functional Biomaterials: Juan Manuel Urueña

New materials discovered in the BioPACIFIC MIP will, in turn, enable new technologies to arise in the form of novel biomaterial-based devices, treatments, or products. Additive manufacturing, or 3D printing, will play a key role in creating one-off objects made from novel materials for use in a wide variety of applications. Many additive manufacturing techniques are well suited for creating complex structures from very soft solids composed of bio-derived materials.

The BioPACIFIC MIP Additive Manufacturing Facility is directed by MIP project scientist **Juan Manuel Urueña.** His doctoral research was focused on the energy-dissipation mechanisms of soft aqueous gels, and during his postdoctoral research, he developed microgels for 3D bioprinting and designed infrastructure to support long-term, continuous in-vitro cell and tissue culture in 3D. He says he joined the BioPACIFIC MIP "to engage in collaborative research focused on soft bio-derived materials discovery and to expand 3D manufacturing techniques for new biological and bio-inspired materials."

Juan Manuel Urueña in the Additive Manufacturing Facility, where novel materials can be printed for the MIP.

The facility supports state-of-the-art 3D printing platforms designed specifically for bio-inspired, bio-derived materials providing an alternative to petroleum-based polymers. Conventional manufacturing processes, such as machining, are used to produce solid workpieces that are generally isotropic; that is, they have the same material properties throughout. Additive manufacturing, however, enables the fabrication of soft, anisotropic objects, in which different regions might be chemically and mechanically distinct so that they are optimized for specific functions.

The wide variety of 3D printing approaches employed in the facility includes a custom process developed by UCSB professor of materials and chemistry and MIP co-PI **Craig Hawker.** Called Solution Mask Liquid Lithography (SMaLL), it enables users to create such intricate anisotropic biomaterial-based structures having a range of material properties within the same 3D printed object.

In addition, the MIP has invested in a suite of 3D printers designed to work with biological samples, such as the Cellink BioX bioprinter, which is capable of precisely arranging living cells and cellular components in a three-dimensional environment. The combination of expertise and state-of-the-art equipment positions the facility to have a big impact on such diverse fields as flexible electronics (used in wearable devices and biosensors), smart materials, encapsulation technologies (i.e. enclosing materials into capsules before delivering them into a system), and personalized medicine (such as drug-delivery devices).

In his role leading the Additive Manufacturing Facility, Urueña provides detailed training to those using each of the machines in it, as well as technical advice when users are testing new materials or developing new protocols. "Users benefit from consulting with me and other project scientists to ensure that their experiments go as smoothly as possible," he says. "I provide technical help and encourage users to submit proposals so that we can provide feedback."

In terms of what lies ahead for him in the hugely collaborative BioPACIFIC MIP, Urueña says, "I enjoy the scientific challenges that come with working with users from a wide variety of academic backgrounds, and I'm fortunate to be part of a very supportive, collaborative, and multidisciplinary team. A team made up of members who have diverse backgrounds leads to very creative solutions to problems and makes for an enthralling journey to the solution."

> *Additive manufacturing enables the fabrication of soft, anisotropic objects, in which different regions might be chemically and mechanically distinct...optimized for specific functions.*

Automated Chemistry Platform: Morgan Bates


Morgan Bates

Morgan Bates, a project scientist at UCSB who earned her PhD in chemical engineering with a background in chemistry and synthesis, is in charge of the MIP's "quick chemistry" component, which relies on a unique high-throughput instrument called an *automated chemistry platform.* "As one of several instruments geared for making the synthesis of biopolymers and related materials easier, more reproducible, and high-throughput," Bates says, "the platform's function is basically to mimic all of the synthetic manipulations a chemist would do."

The system, valued at roughly $1 million, is doubly unique. First, the manufacturer, Chemspeed, is the world's only supplier of an automated chemistry platform having such automated and robotic capabilities, and second, it had not previously put together a system having as many different functions as the BioPACIFIC MIP team requested.

The box-shaped platform, which was to arrive in November and is about the size of a small car, has a work surface contained within an acrylic enclosure to seal it away from oxygen or other atmospheric contaminants. On the work surface, called a *deck*, is a series of robotic tools that can dose, or add, reagents in powder or liquid form to a large series of reactors, performing as many as 96 reactions in a single run, something a human would be unlikely to attempt. The choice of a specific reactor type depends on whether the reaction requires unique kinds of stimuli, such as light and high pressure or, perhaps, very high or very low temperatures, in order to occur.

Bates explains that, collectively, the robotic tools on the instrument work together to set up and run reactions and do some of the purification steps, such as filtration, drying, centrifugation, and solid-phase extraction, that are commonly employed to isolate a small molecule or a polymer.

The instrument's robotics could also be leveraged by researchers who are examining physical phenomena, enabling them to study a much larger swath of that parameter space than would be possible if the formulations were prepared by hand. A grad student may make only a few samples, because doing so can require significant physical effort, whereas a robot is fine with turning out many, many samples, making it possible to vary more parameters or produce more variations within a series of samples.

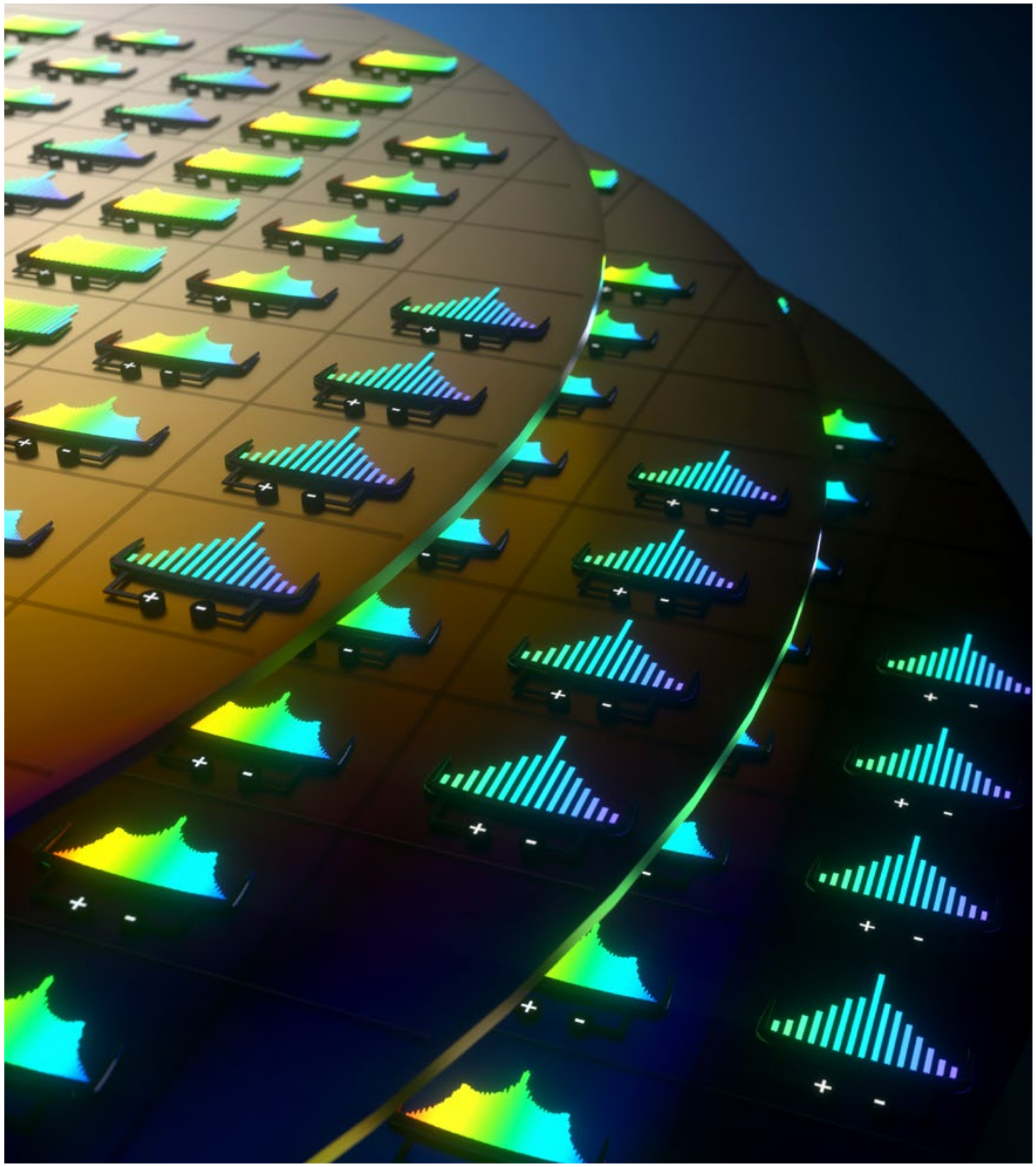
The million dollar, custom-built, automated rapid-chemistry plaform, with the most functions that German manufacturer Chemspeed has ever put into one of its systems, will enable rapid-throughput chemistry 24/7.

"The instruments in this facility will allow people to carry out science twenty-four-seven. The robots don't sleep," she says. "Their impact results from their ability to conduct non-stop exploration of an immense experimental parameter space."

The physical advantage the system provides in terms of labor-saving automation also yields a huge *intellectual* advantage for those doing the science. "When a researcher is able to rest while the physical labor still gets done, that person's untaxed mind is free to focus deeply on the questions at hand, the end goal, and the relationships that they observe in their generated data," Bates says.

Users wishing to access the UCSB BioPACIFIC site will submit a proposal and then receive instrument access based on its quality and the appropriateness of the work for the instrumentation available. If approved, Bates says, "It is then my responsibility to help researchers translate their science to our instrumentation. That might mean adapting their process to the automation or, conversely, working with researchers to modify the equipment to make it work for their process."

Concept illustration depicts how thousands of integrated frequency microcrombs might be manufactured at scale on silicon wafers. Illustration by Brian Long.



The First COMMERCIALLY SCALABLE INTEGRATED LASER **AND MICROCOMB** *on a Single Chip*

The Bowers lab and collaborators develop long-awaited breakthrough technology

Fifteen years ago, **John Bowers**, professor in UC Santa Barbara's Departments of Materials, and Electrical and Computer Engineering, pioneered a method for integrating a laser onto a silicon wafer. The technology has been widely deployed in combination with other silicon photonics devices to replace the copper-wire interconnects that formerly linked servers at data centers, dramatically increasing energy efficiency, an important endeavor at a time when data traffic is growing by roughly 25 percent per year.

For several years, the Bowers group has collaborated with the group of Tobias J. Kippenberg at the Swiss Federal Institute of Technology (EPFL), within the Defense Advanced Research Projects Agency's (DARPA) Direct On-Chip Digital Optical Synthesizer program. The Kippenberg group discovered "microcombs," a series of parallel, low-noise, highly stable laser lines. Each of the many lines of the laser comb can carry information, extensively multiplying the amount of data that can be sent by a single laser.

Recently, several teams demonstrated very compact combs made by placing a semiconductor laser chip and a separate silicon nitride ring-resonator chip very close together. However, the laser and the resonator were still separate devices, made independently and then placed close to each other perfectly aligned, a costly and time-consuming process that is not scalable.

The Bowers lab has worked with the Kippenberg lab to develop an *integrated* on-chip semiconductor laser and resonator capable of producing a laser microcomb. A paper titled "Laser soliton microcombs heterogeneously integrated on silicon," published last summer in the journal *Science*, describes their success as the first to achieve that goal.

Soliton microcombs are optical frequency combs that emit mutually coherent laser lines — lines in constant, unchanging phase relative to each other. The technology is applied in optical timing, metrology, and sensing. Recent field demonstrations have included applications in multi-terabit-per-second optical communications, ultrafast light detection and ranging (LiDAR), neuromorphic computing, and astrophysical spectrometer calibration for planet searching, to name several. It is a powerful tool, but one that normally requires exceptionally high power and expensive lasers and sophisticated optical coupling to function.

The working principle of a laser microcomb, explains lead author **Chao Xiang,** who earned his PhD in Bowers's lab in May and is now a postdoctoral researcher there, is that a distributed feedback (DFB) laser produces one laser line. That line then passes through an optical phase controller and enters the micro-ring resonator, which causes the power intensity to increase as the light travels around the ring. If the intensity reaches a certain threshold, non-linear optical effects occur, causing the one laser line to create two additional identical lines, one on either side of it. Each of those two "side lines" creates others, leading to a cascade of laser-line generation. "You end up with a series of mutually coherent frequency combs [so-called because the parallel laser lines resemble the teeth of a comb]," Xiang says — and a vastly expanded ability to transmit data.

This research enables semiconductor lasers to be integrated seamlessly with low-loss nonlinear optical micro-resonators, "low-loss" referring to the fact that the light can travel in the waveguide without losing a significant amount of its intensity over distance. No optical coupling is required, and the device is entirely electrically controlled.

Importantly, the new technology lends itself to commercial-scale production, because thousands of devices can be made from a single wafer using industry-standard complementary metal-oxide-semiconductor (CMOS)-compatible techniques. "Our approach paves the way for large-volume, low-cost manufacturing of chip-based frequency combs for next-generation high-capacity transceivers, datacenters, space, and mobile platforms," the researchers say in the paper.

The key challenge in making the device was the fact that the semiconductor laser and the resonator, which generates the comb, had to be built on different material platforms. The lasers can be made only with materials from the III and V groups on the Periodic Table, such as indium phosphide, and the best combs can be made only from silicon nitride. "So, we had to find a way to put them together on a single wafer," Xiang explains.

Working sequentially on the same wafer, the researchers leveraged UCSB's heterogeneous integration process for making high-performance lasers on silicon substrate and the ability of their EPFL collaborators to make record ultra-low-loss high-Q silicon nitride micro-resonators using a "photonic damascene process" they developed. The wafer-scale process — in contrast to making individual devices and then combining them one by one — enables thousands of devices to be made from a single 100-mm-diameter wafer, a production level that can be scaled up further on the industry standard 200-mm- or 300-mm-diameter substrate.

"The field of optical comb generation is very exciting and moving very fast," says Bowers, the Fred Kavli Chair in Nanotechnology and the director of the College of Engineering's Institute for Energy Efficiency. "The missing element has been a self-contained chip that includes both the pump laser and the optical resonator. We demonstrated that key element, which should open up rapid adoption of this technology."

"I think this work is going to become very big," says Xiang, adding that the potential of the new soliton laser technology reminds him of how the development of putting lasers on silicon fifteen years ago led to enormous progress both in research and in industrial commercialization of silicon photonics. "That transformative technology has been commercialized, and Intel ships millions of transceiver products per year. Future silicon photonics incorporating co-packaged optics will likely be a strong driver for higher-capacity transceivers using a large number of optical channels.

"We believe that our achievement could become the backbone of efforts to apply optical frequency comb technologies in many areas, including efforts to keep up with fast-growing data traffic and, hopefully, slow the growth of energy consumption in mega-scale datacenters."

"We believe that our achievement could become the backbone of efforts to apply optical frequency comb technologies in many areas, including efforts to keep up with fast-growing data traffic and, hopefully, slow the growth of energy consumption in mega-scale datacenters."

Faculty Q&A

MARY TRIPSAS

New TM Professor Brings Expertise on *How Firms Adapt To Technology*

Adapting to technology can be challenging. It requires learning and changing, and poor execution or outdated thinking can cause it to fail. **Mary Tripsas,** a newly hired professor in Technology Management, studies how organizations adapt to disruptive new technologies, with an emphasis on how the interplay of organizational capabilities, organizational identity, and managerial mental models shape strategic responses.

Prior to coming to UC Santa Barbara, Tripsas spent four years on the faculty at the University of Pennsylvania's Wharton School, thirteen at the Harvard Business School (where she had previously earned her MBA; she earned her PhD at the Massachusetts Institute of Technology), and eight at Boston College, where she served as founding director of the Edmund H. Shea Jr. Center for Entrepreneurship and led the creation of a new undergraduate concentration in entrepreneurship. Not to be overlooked: the fact that she is a lifelong musician who played oboe as part of the backup orchestra at an Indigo Girls concert in 2018.

Mary Tripsas

Convergence: ***What inspired your career path?***

MT: At a very young age, I became interested in technology and technical change. My father was born in Greece and didn't even have the opportunity to finish high school, but he became an electrical engineer, at first designing electromechanical telephone central-office switches based on relay logic. Telephone switching technology then moved to electronic and, eventually, digital systems, and he had to retrain himself along the way. That sparked my interest in a question that a lot of my research has been about: How do organizations deal with these major shifts in technology?

My mom was a math major at UCLA, and once we kids were in high school, she rejoined the workforce doing software development for the same company as my dad. In her case, software had changed a lot from when she finished college. Again, the issue of how you adapt to accommodate new technology was uppermost in my mind.

C: ***Your first job out of college was with IBM, correct?***

MT: Yes. I worked in software development for an internal shop-floor control system at a manufacturing facility. Even though we were software engineers writing code, we could also go to the plant floor and interact with the users to better understand what they wanted. Often as a software engineer, you just write the code and don't actually get to see who's using it or what they're doing with it. That was a very interesting time for me in terms of understanding the challenges of what's easy, technically, versus what people want to use.

C: ***Can you tell us about your early research while earning your PhD at MIT's Sloan School?***

MT: I was super-interested in what we now call ecosystems, or the interdependencies of different firms that come together to create new systems of products. I was especially interested in what Adobe Systems was doing. They democratized publishing by creating the first desktop publishing system that had any commercial success. The founders, who had left Xerox PARC, did something that was incredibly innovative at the time: they enlisted other firms to develop certain pieces of their solution. As part of the system, they wanted to supply users with real typographic-level fonts. So, they licensed a bunch of fonts from a company called Mergenthaler Linotype, which, my advisor and I discovered, had been licensing fonts that had been around since the 1800s.

Learning that led me to switch gears and write my thesis about the typesetter industry, which landed me on a theme that has continued through much of my work. When you're looking at making a technical transition, developing the new technical capability can often be the least challenging part of the transition. In the typesetter industry, for example, it turned out that what protected these typesetter firms over generations of technology advances were their large font libraries, which were difficult for other firms to replicate. They provided a buffer that gave the typesetter firms time to adapt to the new technology.

Since then, my most highly cited work has involved looking at the transition of photography firms from analog photography to digital imaging. And in that transition, the same thing was true. It wasn't the technology itself that was the problem. Polaroid and Kodak have some of the most highly cited patents in digital imaging. They developed digital imaging technologies early, and they did it really well. Then why did they fail so miserably? One of the answers has to do with the mental models of the management and their inability, despite having the technical capability, to shift their thinking about what the most appropriate business models would be to commercialize that technology.

At Polaroid, for instance, management was very much stuck on this belief that the "razor blade" model (in which one of two complementary products is sold cheaply to increase sales of the other product) was the only way to make money. And so, they had digital cameras that they could have released very early in the development of the market. But management wouldn't commercialize the digital camera until it could produce an instant Polaroid print, because they thought they needed the print to be able to make money. And that certainly had been true for years for Polaroid, but with digital photography, people don't want to print; they can look at their pictures on a screen. And so, overcoming the sort of mental or cognitive biases is, in the end, I think, one of the more difficult things to accomplish.

C: ***How does your research relate to your teaching?***

MT: I got my first job at Wharton, where I was asked to teach entrepreneurship. I didn't know much about it, but I had an MBA and an understanding of business, so I managed to do OK. The course evolved to focus on technology entrepreneurship, which was more related to my expertise. I started working with the folks from other parts of Penn, in particular the technology transfer office. I started having my student teams do projects in which they would evaluate the commercial potential of university technologies. And so again, this intersection of deep understanding of technology with the business side is sort of a common theme.

At the Harvard Business School, I initially taught entrepreneurship but then took over a joint course with the MIT Media Lab, where Media Lab technologists, together with Harvard MBAs, worked on projects. By the time I moved to Boston College, I had started publishing research in the area of entrepreneurship, for instance, the role of experimentation and the importance of user innovators as firm founders. I brought that research perspective and rigor to BC, where I helped to get the Entrepreneurship Center established.

C: ***Have any of your students started successful companies?***

MT: When I was at Harvard, we used to quote a statistic to the effect that, while not that many students start firms directly out of the MBA program, something like half of the students do something entrepreneurial by ten years out. So I imagine — or hope — that many of my students have started firms that I don't necessarily know about. But, of students who worked on start-up projects in my classes, probably the two most successful are Rent the Runway and Birchbox. Both of those firms have female founders, which raises another important issue: women are way underrepresented in both venture capital and as start-up founders, something that I hope I can help to address as a mentor and advocate here at UCSB.

> ***"The farmers and truckers...don't view themselves as experts in block-chain. Yet, it could end up affecting them in ways that make their products no longer stand-alone."***

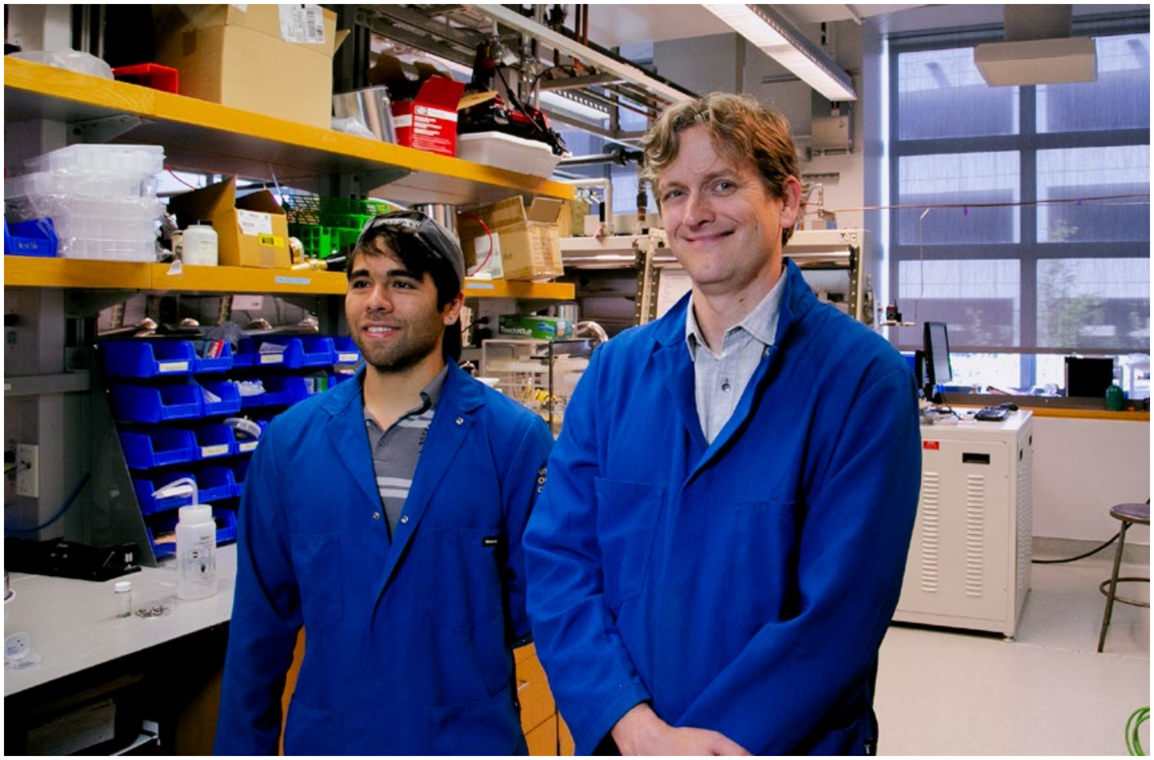
C: ***How does your past work influence your current research?***

MT: Over time, I became more interested in entrepreneurship as a research setting. I have also been looking at how developing or participating in platforms or ecosystems is challenging not only for organizations that have typically thought of themselves as technology-oriented, but also for those that have not traditionally been digital technology experts.

Right now, I'm doing some work on the use of blockchain in the food-safety supply ecosystem. If you look at the companies that have been involved in food processing historically, you have farmers, truckers, the equipment that processes the food that comes from the farm, and all the other things that go into producing food that ultimately lands on your shelf. The folks involved in that process certainly don't view themselves as experts in blockchain. And yet, it could end up affecting them in a way that makes their products no longer stand-alone. Because they're all putting information onto this blockchain, what used to be very non-technical, separate things suddenly become highly interconnected.

C: ***Why did you choose to come to UCSB?***

MT: I'm excited to be at UC Santa Barbara to further my research interests and collaborate with the outstanding team of scholars dedicated to the field. I'm also looking forward to contributing to the curriculum to support students in their quest to understand technology within the context of the current business world. The Department of Technology Management is positioned well to support this mission. I'm also excited about contributing to the Technology Management doctoral program, with students focused on the management of technology, whether it's how technology affects the operations of organizations and the way that people work together in companies or how you commercialize those technologies.

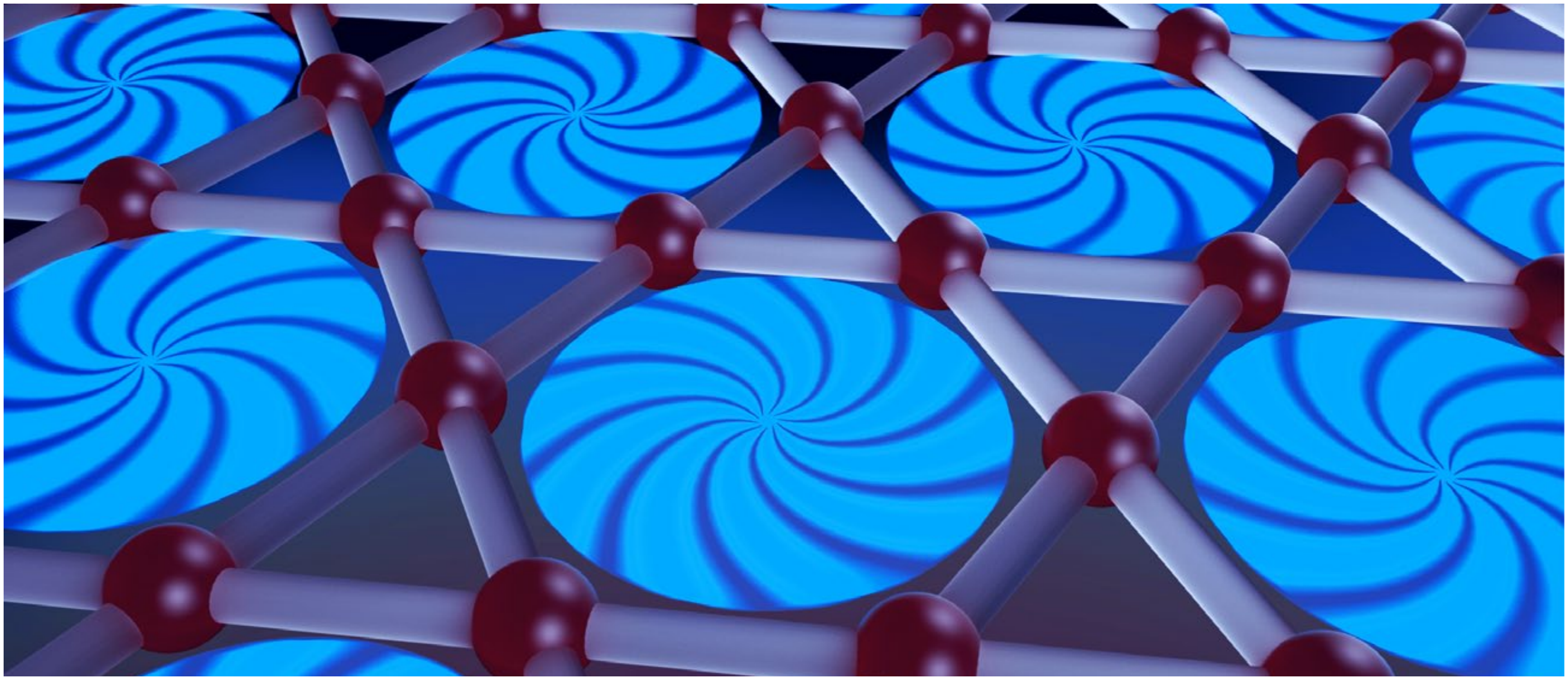


Stephen Wilson (right) and postdoctoral researcher Brenden R. Ortiz, who discovered the new material.

A NEW MATERIAL EXCITES RESEARCHERS AROUND THE WORLD

Created at UCSB's National Science Foundation Quantum Foundry, the material may be a unique kind of superconductor

Since receiving a $25 million grant in 2019 to become the first National Science Foundation (NSF) Quantum Foundry, UC Santa Barbara researchers affiliated with the Foundry, including co-director and materials professor **Stephen Wilson,** have been working to develop materials that can enable quantum information–based technologies for such applications as quantum computing, communications, sensing, and simulation.



Concept illustration shows what makes this superconductor special: its rare kagome lattice, formed by connected triangles in a two-dimensional array, making it a highly favorable testbed for physicists' theories of superconductivity. Illustration by Brian Long

In a new paper, published June 10, 2021 in the journal *Nature Materials*, Wilson and more than twenty co-authors, including key collaborators at Princeton University, describe a new material developed in the Quantum Foundry as a superconductor candidate — a material in which electrical resistance disappears and magnetic fields are expelled from the material — that could be useful in future quantum computation.

As a prelude, last year, a paper published by Wilson's group in the journal *Physical Review Letters* and featured in *Physics* magazine, described a new material, cesium vanadium antimonide (CsV_3Sb_5), that exhibits a surprising mixture of characteristics involving a self-organized patterning of charge intertwined with a superconducting state. The discovery was made by Elings Postdoctoral Fellow **Brenden R. Ortiz** and, as it turns out, Wilson says, those characteristics are shared by a number of related materials, including RbV_3Sb_5 and KV_3Sb_5, the latter (a mixture of potassium, vanadium, and antimony) being the subject of this most recent paper, titled "Discovery of unconventional chiral charge order in kagome superconductor KV_3Sb_5."

Materials in this group of compounds, Wilson notes, "are predicted to host interesting charge density wave physics [that is, their electrons self-organize into a non-uniform pattern across the metal sites in the compound]. The peculiar nature of this self-organized patterning of electrons is the focus of the current work."

This predicted charge density wave state and other exotic physics stem from the network of vanadium (V) ions inside these materials, which form a corner-sharing network of triangles known as a kagome lattice. KV_3Sb_5 was discovered to be a rare metal built from kagome lattice planes, one that also superconducts. Some of the material's other characteristics led researchers to speculate that charges in it may form tiny loops of current that create local magnetic fields.

> "You can imagine the charge moving around in a little loop.... Such a state would be a new electronic state of matter and would have important consequences for the underlying unconventional superconductivity."

Materials scientists and physicists have long predicted that a material could be made that would exhibit a type of charge density wave order that breaks what is called *time reversal symmetry.* "That means that it has a magnetic moment, or a field, associated with it," Wilson says. "You can imagine that there are certain patterns on the kagome lattice where the charge is moving around in a little loop. That loop is like a current loop, and it will give you a magnetic field. Such a state would be a new electronic state of matter and would have important consequences for the underlying unconventional superconductivity."

The role of Wilson's group in the Foundry was to make the material and characterize its bulk properties. The Princeton team then used high-resolution scanning tunnelling microscopy (STM) to identify what they believe are the signatures of such a state, which, Wilson says "are also hypothesized to exist in other anomalous superconductors, such as those that superconduct at high temperature, though it has not been definitively shown."

STM works by scanning a very sharp metal wire tip over a surface. By bringing the tip extremely close to the surface and applying an electrical voltage to the tip or to the sample, the surface can be imaged down to the scale of resolving individual atoms and where the electrons group. In the paper, the researchers describe seeing and analyzing a pattern of order in the electronic charge, which changes as a magnetic field is applied. This coupling to an external magnetic field suggests a charge density wave state that creates its own magnetic field.

This is exactly the kind of work for which the Quantum Foundry was established. "The Foundry's contribution is important," Wilson says. "It has played a leading role in developing these materials, and Foundry researchers discovered superconductivity in them and then found signatures indicating that they may possess a charge density wave. Now, the materials are being studied worldwide, because they have various aspects that are of interest to many different communities."

Wilson explains further: "They are of interest, for instance, to people in quantum information as potential topological superconductors; they are of interest to people who study new physics in topological metals, because they potentially host interesting correlation effects, defined as the electrons' interacting with one another, and that is potentially what provides the genesis of this charge density wave state. And they're of interest to people who are pursuing high-temperature superconductivity, because they have elements that seem to link them to some of the features seen in those materials, even though KV_3Sb_5 superconducts at a fairly low temperature."

If KV_3Sb_5 turns out to be what it is suspected of being, it could possibly be used to make a topological qubit useful in quantum information applications. For instance, Wilson says, "In making a topological computer, one wants to make qubits whose performance is enhanced by the symmetries in the material, meaning that they don't tend to decohere [decoherence of fleeting entangled quantum states being a major obstacle in quantum computing] and therefore have a diminished need for conventional error correction.

"There are only certain kinds of states you can find that can serve as a topological qubit, and a topological superconductor is expected to host one," he adds. "Such materials are rare. This system may be of interest for that, but it's far from confirmed, and it's hard to confirm whether it is or not. There is a lot left to be done in understanding this new class of superconductors."

cooking up a SUPERCONDUCTOR

The making of a novel, new material

As a physics graduate student at the Colorado School of Mines (CSM), **Brenden R. Ortiz,** now a postdoctoral researcher in the lab of UC Santa Barbara materials professor **Stephen Wilson,** was looking for new materials related to energy efficiency. A mix of intuition and experience led him to believe that mixing the element antimony with the alkali metals on the Periodic Table was a promising way to proceed. Because most materials made from two elements had already been discovered, however, Ortiz decided he would need to combine at least three elements. "Solid-state chemistry is a bit like cooking," he says. "To find something novel, you have to be willing to experiment with new combinations and accept that some of your creations might be failures."

Ortiz eventually conducted numerous experiments, each a unique combination of antimony, one alkali metal, and one transition metal. He put small pieces of each element into a vial, which was shaken in a machine to yield a powder. He then pressed each powder into a small disc, heated it, polished it, and examined it with an electron microscope.

Ortiz deliberately made samples that were "impure" and contained swirls and pockets, like a marbled cake, indicating how and where the elements had mixed. "What you see is a spotted pattern, with regions of white, gray, and black," he says. "It's easy to visually identify the different regions of interest, and once you see them, you can use electron microscopy to identify the ratio of each element in the mixture."

By cross-referencing the elemental ratios extracted from electron microscopy with databases of known compounds, he was able to identify any new compounds he had made. He then had to identify the crystal structure. "At first, you know what the mate-

Brenden R. Ortiz, postdoctoral researcher in Stephen Wilson's materials lab at UCSB, separates newly grown crystals, the result of placing the mixed elements in a steel capsule, heating them to one thousand degrees Celsius, then slowly cooling them to five hundred degrees over a two-week period. Here, he begins the laborious task of using tweezers and solvent to separate the crystals from unwanted residue.

rial is made of, but you don't know how it's put together," he says.

It is possible to perform X-ray diffraction on the powder as a way to see the structure, but that process gives a kind of "fingerprint" of the structure, and, Ortiz says, "If you don't have any matching fingerprints [in a database], it doesn't help you. You still don't know how it's arranged."

Today's powerful computers, however, make it possible to reverse-engineer the fingerprint to provide the actual structure. By having the powders characterized at a national laboratory, he successfully solved the structure of several of the new materials. The crystal structure of one such combination, a mixture of alkali (A), vanadium (V) and antimony (Sb) — AV_3Sb_5 — comprised a distinctive arrangement of six-pointed stars and hexagons. He soon realized that the material was a new manifestation of a *kagome lattice,* which holds special significance for materials scientists and physicists, owing to the unique and varied properties arising from its unusual crystal geometry.

When cooled to temperatures near absolute zero, kagome lattices serve as an ideal testbed for theories related to the fundamentals of quantum mechanics. "The kagome lattice on its own, especially if it's a metal, imparts some special characteristics just by the very nature of the atoms being arranged in that pattern. If it's a kagome *metal,* you're guaranteed to have some weird physics" Ortiz says.

Realizing that the structure was unique and potentially interesting, Ortiz and his collaborators at CSM knew that they would need to grow single crystals of the materials. The data from the powders *implied* certain properties, but the definitive way to identify a structure or measure its properties begins with growing a single crystal. "If you can do that, a single-crystal X-ray diffractometer can then tell you exactly what it is, no questions asked," he says. "You essentially have a full picture of the crystal."

Ortiz describes the process as "essentially growing rock candy," although it did take him a year and a half to develop the specifics. "You dissolve sugar (the solute) in water (the solvent) and heat it as a solution. Then, you slowly cool it down or evaporate off some of the water, and over time the water can't hold as much sugar. The sugar starts to fall out, and you get the crystallized cubes of sugar. I do exactly the same thing; the only difference is that, in my case, I dissolve the cesium vanadium antimonide in a flux, a mixture of cesium and antimony."

He puts the mixture inside a miniature steel "bomb," heats it to a thousand degrees Celsius, and then cools it very slowly, about one degree per hour, down to five hundred degrees. After two weeks, he pulls it out, breaks it open, and gets what looks like a geode with the crystals scattered through it. He then uses liquid and tweezers to extract them.

Ortiz published his discovery in the journal *Physical Review of Materials,* although it initially generated limited interest, and other prestigious journals turned the manuscript down.

Six months later, he joined Wilson's lab as an Eilings Fellow and brought the new material with him, with the approval of Eric Toberer, his PhD advisor at CSM. Ortiz included a description of the material in his fellowship proposal, saying essentially that he had new kagome lattices but didn't know much about them, because CSM did not have the low-temperature equipment essential to inducing the material's most interesting idiosyncratic behavior.

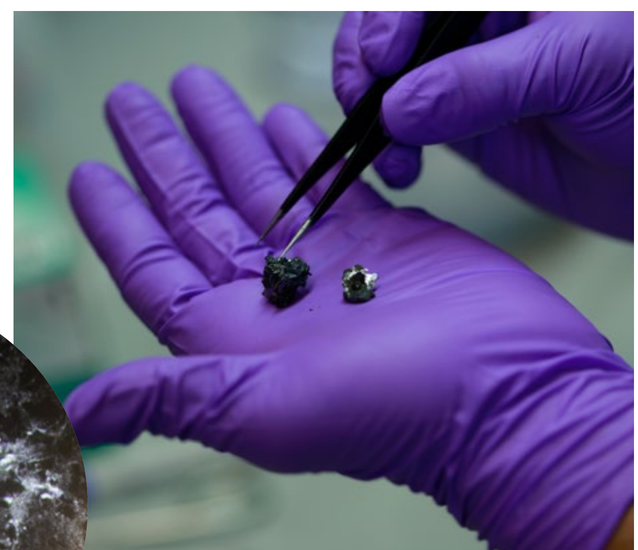
A couple of months after arriving at UCSB, Ortiz was thinking that he had done a lot of measurements on the KV_3Sb_5, the first material he had made, but not on the other two. Then, while performing a suite of measurements, he discovered to his surprise that the cesium compound (CsV_3Sb_5) superconducted. He recalls that, after confirming that superconductivity occurred throughout the crystal, Wilson said, "We need to send it to collaborators to get measurements going as we are publishing, because people go crazy for new superconductors."

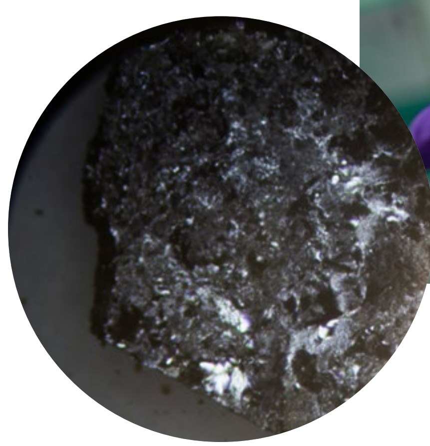
The material was special in another way, too, as one of the few superconducting kagome lattices known to exist in the 2D state. The material is built up by having sheets of lattices stacked on top of each other. In 3D materials, the planes are linked, but in this material, Ortiz notes, "They are separate; they hardly talk to each other, making this a nearly 2D material, and many models and theories are easier to formulate and test in 2D than in 3D."

After no initial interest, the paper has generated a flurry of activity, with nearly one hundred citations since December 2020 and researchers all over the world asking Ortiz for crystals. He is currently growing them as fast as he can. "The theories that could result from this are intriguing," he notes, "in applications from fundamental science to quantum computing, which is why everyone is so interested in it.

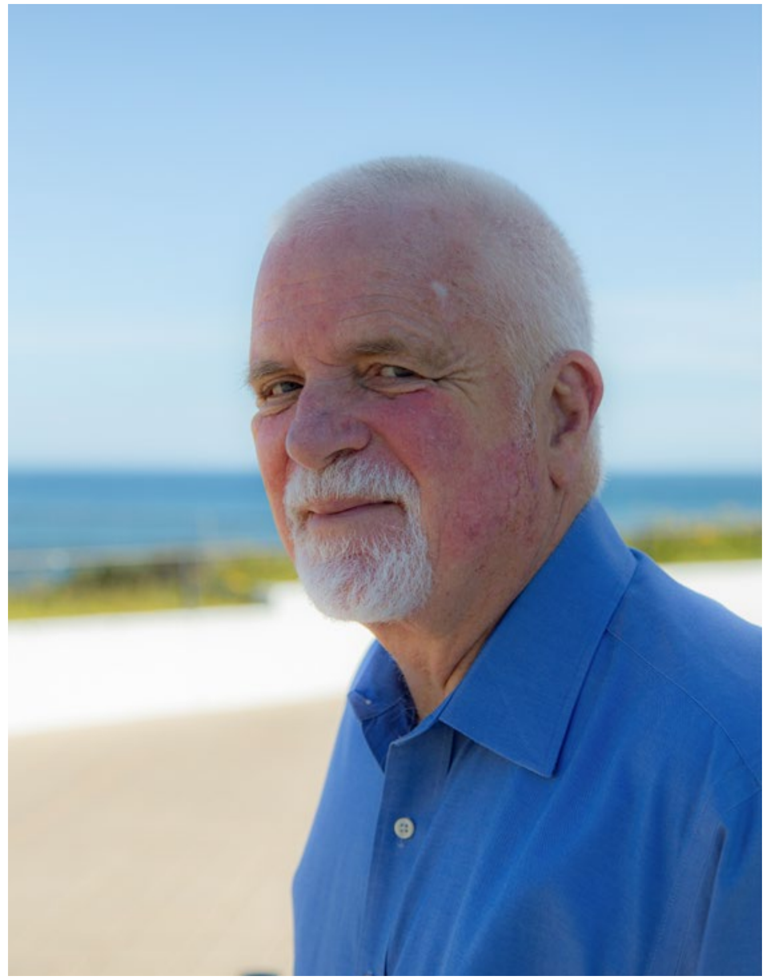
"It's overwhelming how this has blown up," he adds. "The world is learning so quickly that I can no longer keep up with the narrative of my own discovery. It's like you have a kid and you have to let it grow up. The kid is out of my control now. He's out in the world, and he's got a jet. I'm honored when people ask for samples, and I'm ecstatic to collaborate. It's just an honor to have people say, 'We want *your* crystals of *your* material.'"

A superconductor in the palm of his hand: Brenden R. Ortiz (right) displays newly grown crystals (magnified below), that will be sent to researchers around the world for further investigation of their unique properties..





champion of engineering



JIM FRANK: AN ENGINEERING FAMILY'S ***LEGACY OF GIVING***

Low-key is the word **Jim Frank** uses to describe the Raintree Foundation, which was established by his late father, **Harold Frank,** a major donor whose name adorns Harold Frank Hall at UC Santa Barbara. The elder Frank, who died in 2012, was an electrical engineer who graduated from Washington State University and, after working in the U.S. Army Signal Corps during World War II, started a company, Applied Magnetics, which became a leading manufacturer of magnetic recording heads used in computers, and was once the second-largest employer in Santa Barbara County.

Low-key also describes Jim Frank himself, who now runs the foundation with his daughter, Jessica, and Ellicott Million, who was Harold's right-hand person for nearly fifty years. Now retired from CMC, the successful, employee-owned company he started in his garage to provide equipment and training for search-and-rescue teams, Jim says he would have to go into Raintree's financial records to "have any idea" of how much it has donated to UCSB since being established in 1993. Suffice to say, it is a significant amount, enough to have established the family within UCSB's Gold Circle Society, comprising the university's premiere philanthropists.

The Raintree Foundation helps UC Santa Barbara recruit and enrich COE faculty and has endowed the Harold Frank Scholars Fund to inspire student entrepreneurs in the college's Technology Management Department. We caught up with Frank this fall.

Convergence: *Why do you describe the Raintree Foundation as a "low-key" nonprofit?*

Jim Frank: My dad never really looked for recognition as an individual. He was more interested in what he could do to benefit other people, and we continue to follow that philosophy today. There are some major foundations in Santa Barbara that are well known and have well-earned reputations. We're a small foundation and pretty focused.

C: *Your father died in 2012, yet, you continue to provide important support to UCSB. Why is it important to you to support education generally, and the College of Engineering specifically?*

JF: My dad was very intelligent and made good decisions. When he set up the foundation in 1993, he decided what it should support. So, we have that connection and are basically honoring his legacy. Engineering is important to us; it was my dad's heritage, and it is mine. There is a lot going on in the world, and I think that the survival of humans will depend on intelligent decision making, and the best way to ensure good decisions is to educate people. That's why the Raintree Foundation supports education at every level, from young kids in elementary school who are doing a backyard project with the museum, to the Wilderness Youth Project, to students at the highest level of university education.

Further, our support has to do with my father's legacy. His name is on the building there. He was honored by the school, and we want to support that.

C: *Why has the foundation consistently directed its gifts to the College of Engineering's discretionary Dean's Fund, which is used primarily to recruit and retain top faculty?*

JF: We've had multiple discussions with [recently retired dean] **Rod Alferness.** He'd say, "This is what we're doing, this is why we're doing it, and this is how it will help students," and my answer has consistently been, "You're the dean. You're there every day. You're seeing everything. You're in such a better position than I am to figure out where to direct the money." Our support gave him the freedom to do what he thought was best.

C: *Are there any particular aspects of the College of Engineering that resonate strongly with you?*

JF: Whenever I visit the campus, I am just so amazed at what the engineering students today are doing. And I love that there are so many female students, because there were no women at all in my aeronautical engineering program at Cal Poly San Luis Obispo. Seeing that and listening to the students talk — they are over my head almost immediately — and seeing how bright and creative they are makes me feel positive about the future.

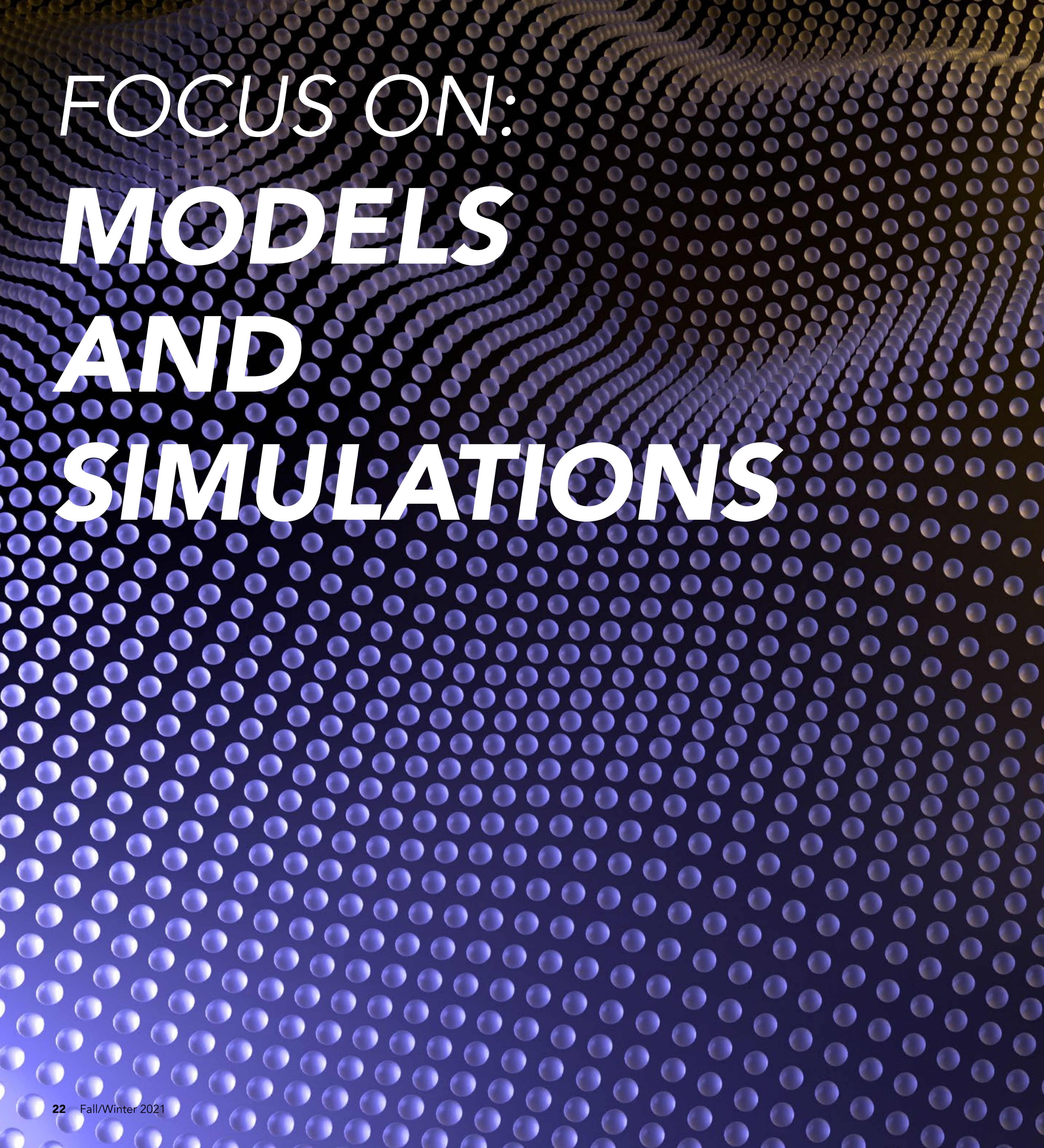
> "There is a lot going on in the world, and I think that the survival of humans will depend on intelligent decision making, and the best way to ensure good decisions is to educate people."

C: *Your father, a German-born first-generation college graduate who attended Washington State University, felt a particular kinship with other first-generation students. Is that focus still reflected in the Raintree Foundation's philanthropy?*

JF: We're maybe not so concerned with the particulars of someone's background as we are with the goal of ensuring that all students get the opportunity to study and pursue a career. We want to provide the resources that can make those opportunities available.

C: *You are an entrepreneur, and your father was, too. Do you think there's anything like a genetic predisposition to entrepreneurship?*

JF: I think it has to do more with role models. For instance, my dad was my role model as an engineer and an entrepreneur. That's what I knew. Someone who doesn't have that role model might not know that the opportunity is there, so we try to give those opportunities to as many students as possible.



FOCUS ON: MODELS AND SIMULATIONS

Our coverage of research in *Convergence* often mentions theories, models, and simulations. But what exactly are those things, and how do they differ from or complement each other? Why are they used, how are they made, and what do they add to the research endeavor?

"I use the term *model* to refer to any approximate description of a material or a process," says materials professor **Chris Van de Walle.** "A theory provides a fundamental description, while a model is meant to create an *idealization* of real behavior to a given accuracy. I think of a simulation as the computer code that is developed and run to implement that model."

Fundamentally, says **Linda Petzold,** professor of mechanical engineering and computer science, "A model is simply a representation of something that is happening."

"My working definition of a model is 'any relationship that helps explain how a system, a device, or some aspect of nature behaves,'" says chemical engineering professor **Mike Doherty.** "That means the math equations you wrote down and the many assumptions that went into writing them."

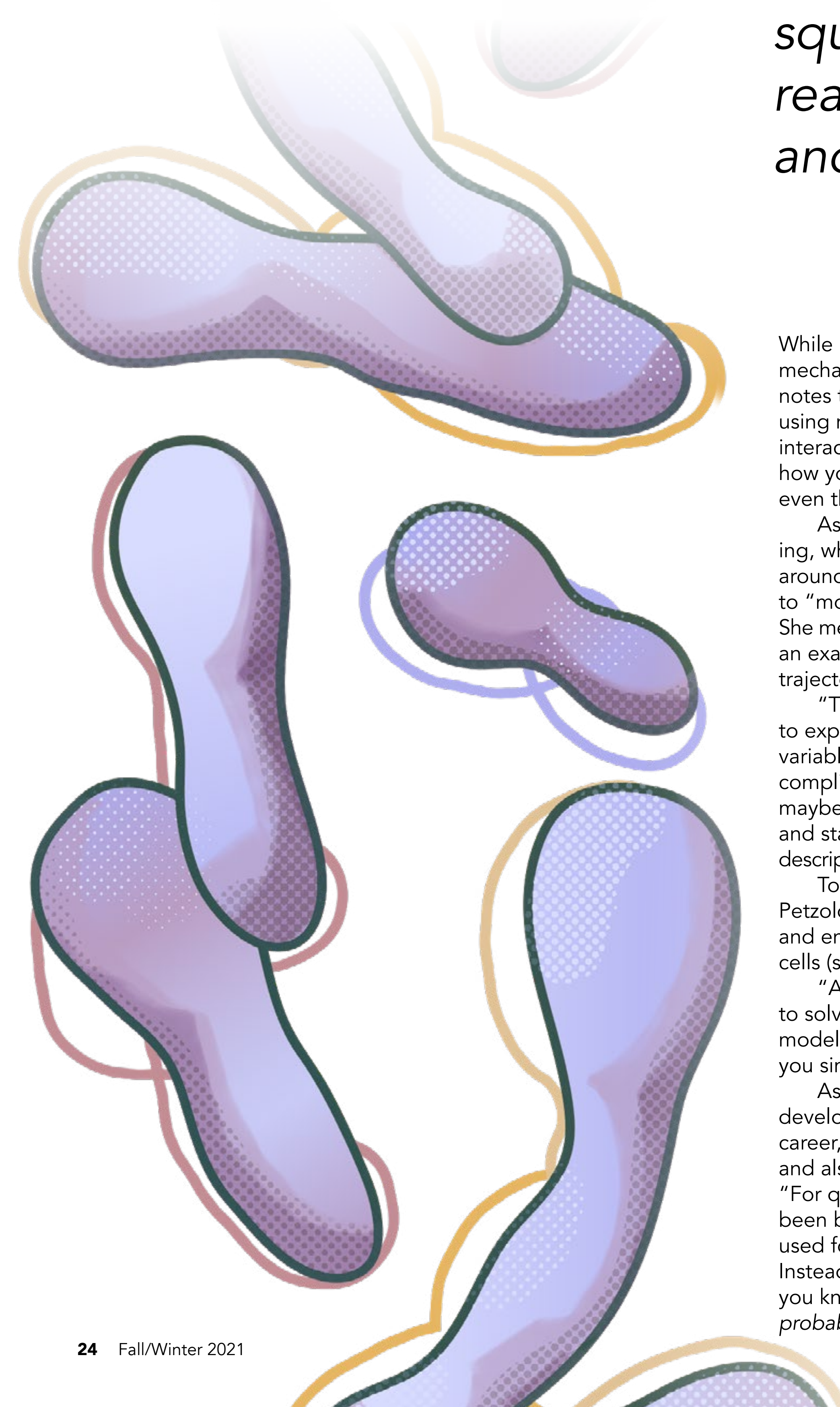
Chemical engineering assistant professor **Sho Takatori** says that his lab develops models "to describe various phenomena in physics, biology, and chemistry. A model is somehow representative of the world out there."

And to **William Smith,** professor in the Department of Molecular, Cellular and Developmental Biology, a model is "an experimentally tractable system that approximates a less tractable, but ultimately more significant, system."

In this issue's section, these five professors, plus postdoctoral researcher **Angela Zhang,** discuss theory, modeling, simulation, and their application in the context of specific projects in the professors' labs. Each offers rich insights, a unique perspective, and unbridled enthusiasm for the pursuit of discovery.

LINDA PETZOLD

Versatility lands her squarely in the twin realms of modeling and simulation



While a model can seem mysterious and esoteric, UC Santa Barbara mechanical engineering and computer science professor **Linda Petzold** notes that all of us are proficient model-makers: "You are making and using models all the time," she says. "You have a model of how you interact with different kinds of people, of how you drive your car, and how you get to the grocery store. You're so used to it that you don't even think about it."

As an applied mathematician, Petzold does mathematical modeling, which, she admits, is quite a bit more complex than the "walking-around-the-world" models she mentions above and allows researchers to "model all sorts of things by using mathematics to describe them." She mentions Newton's second law, F=MA (force = mass x acceleration), as an example of a mathematical model; it allows one to predict, say, the trajectory of a thrown a ball if its initial position and velocity are known.

"Then there is computational modeling, which can be used to express equations representing phenomena having many more variables," she continues. "In the example of throwing a ball, you might complicate the model by adding humidity, wind, or temperature, or maybe you want to know what happens to the ball if it falls into a lake and starts to sink. If you build enough information into the mathematical description, you can expect some predictive power."

To describe a complicated system or process with a model — and Petzold has modeled everything from automotive suspension systems and endangered frogs to migraine headaches and the mating of yeast cells (see below) — she first develops a system of differential equations.

"As we add more complexity," she says, "it becomes impossible to solve the equations exactly. At that point, you build an approximate model and use it to simulate the system on a computer. In other words, you simulate the model."

As a computer scientist, Petzold also works with her group to develop the computational software to run simulations. "Earlier in my career, I built software for simulation of differential equation systems, and also for differential equations subject to constraints," she explains. "For quite a while now, my research group and our collaborators have been building software for discreet stochastic simulation, which is used for systems or phenomena that are characterized by randomness. Instead of having something deterministic, like Newton's law, where you know that doing X will result in Y, stochastic simulation posits the *probability* that something will happen under a certain condition or

> **Who knows why the yeast cell prefers that one over the other one? What motivates this? We wanted our model to replicate that kind of behavior. So, we started thinking, *What would it take for the model to be able to produce that?***

set of conditions. This can involve a lot of computation."

In recent years, Petzold has frequently modeled biological data at the cellular level, an area rife with complexity. "A cell is so complex that nobody can really look at it and say with certainty, 'This is what's going to happen next,'" she says.

One of her recent projects involved modeling the dynamics of yeast mating. "You probably haven't thought much about yeast mating, but yeast can mate!" she quips. "They sense a pheromone from another yeast cell and grow a projection, called a *polarisome,* in that direction."

How Petzold became involved in the project speaks to the often-serendipitous pathways that lead her to specific research. "It seems that every research project begins in a different way," she says. "It can come from anywhere. It can come from someone asking, 'Why doesn't your software do this' And I've thought, *Why would anyone want to do that?* And then I find out and think, *Well, that's really interesting,* and then I might get pulled in that direction for a while. The initial impetus can just as easily come from the mathematics or science side of it, too."

In the case of the yeast cells, the opportunity arose after she took a seat in the front row at a conference, following a talk she gave about her stochastic simulation software. She recalls, "The next speaker, Dr. Tau Mu Yi, then a faculty member at UC Irvine, was sitting next to me and asked me if I had any specific biological problems in mind for our spatial simulation software And I said, 'No, and we really want to find one.' And he said, 'I think I have one.' We talked about it, and that was the beginning of our yeast mating collaboration."

Many biologists Petzold has worked with begin by describing the system of interest via a simple cartoon-style drawing having several panels, similar to a comic strip or an advertising story board. "But these things can get really complicated, and they can have feedback loops in them. There can be processes that have different time scales — fast ones and much slower ones — that all work together," she says. "A mathematical model essentially quantifies the processes illustrated in the cartoon. As it develops, the model can become quite complicated, as there are usually a great many processes and interactions to keep track of, so we simulate it on a computer."

For the yeast-mating model, she says, "We began with fairly simple models and added more processes, as needed, to explain the data. For example, you can begin with a model of the pheromone response, and from there you ask, 'How does it form this structure, the polarisome?' And then, there are observed properties that we wanted the model to mimic; for example, sometimes the cell makes a polarisome spontaneously, apparently without reason, with no mate nearby. We wanted the model to be able to replicate that behavior."

If models sometimes don't give the expected results, they can also give *partial* results, making it necessary to adjust them. "In the yeast project, we knew that it can also happen that two yeast cells are attracted to each other and start growing toward each other. Then, another potential mate arrives from another direction, and one yeast cell may start retracting the polarisome it had made initially and start growing it on the other side toward the new mate," Petzold explains. "Who knows why the yeast cell prefers that one over the other one? What motivates this? We wanted our model to replicate that kind of behavior. So, we started thinking, *What would it take for the model to be able to produce that? And of all these possible unknown reactions, what could be the one that could make this happen without screwing up any of the other capabilities of the model*?

"It takes a team of people to do that; you need mathematicians, computer scientists, engineers, and biologists," she continues. "Finally, we had a quite-plausible model that was supported by experimental data and could reproduce the growth of the polarisome in one and two dimensions.

"But when it came time to extend the results to three dimensions, we met with a surprise: the polarization was not stable — it drifted from location to location — which is not what happens in nature! We postulated, in collaboration with our then–UCSB mechanical engineering colleague **Professor Otger Campàs,** that in nature, stabilization of the polarisome might be achieved through a mechanical feedback. It was a new wrinkle, but it was correct, and after quite a bit of research, we elucidated this feedback and incorporated it into our three-dimensional model, which now responds like a yeast cell."

MICHAEL DOHERTY

When models describe realities that are not yet known

Models often inform experimentation, but experimentation can also validate a model. UC Santa Barbara chemical engineering professor **Michael Doherty,** whose group is known for modeling and simulating chemical engineering processes, is intimately familiar with that terrain. "The most interesting models are those that predict something that no one has ever experienced or seen before," he says. "We've done this probably twice in my career, and we've used experiments specifically to test those models."

But to test a model, you first have to develop one, and before doing that, says Doherty, "The modeler has to decide which type of model is needed. Am I going to build a *deterministic* model, in which all of the quantities are typically averaged quantities, like temperature, expressed as an average of the kinetic energy of all the molecules in the system? Or do I need a *stochastic* model, which explicitly takes into account the random microscopic behavior of molecules in a gas or a liquid? I might make a *steady-state* model, one in which time has no part in how the model is formulated, or a *dynamic* model, in which case time is an intrinsic variable in the system. You need different classes of mathematics and different types of modeling schemes depending on your purpose and the nature of the system. It's a conscious decision."

Whatever type is needed, Doherty says, "You start with the simplest possible model you can. You strip down all of the phenomena to the absolute minimalist set needed. From there, you can build a higher-fidelity model if you feel the need to do it.

"You can make a qualitative model. For example, in the shower, you know qualitatively that if you turn up the flow of the hot water, the shower gets hotter. There's no mathematical model involved, just a qualitative cause-and-effect relationship. For many aspects of modeling, that works fine, but say you want to know exactly how much you should turn up the hot water to reach a certain temperature. Now, you need a mathematical model that does an energy balance and a mass balance and tells you what's required to increase the flow rate to get to the desired temperature. If you want a quantitative model, which you almost always do, you have to develop some mathematical equations and ultimately solve them in order to figure out what's going on."

THE FIRST BREAKTHROUGH

In his first major finding that was confirmed by experimentation, Doherty used modeling to predict the existence of a state called a *reactive azeotrope*, which, he says, "is very important in chemical separations but also something that people previously had no clue about," despite the fact that for two hundred years before it was discovered, that state had limited the effectiveness — and therefore the use — of a complex process in which a chemical separation and a chemical reaction are conducted simultaneously. Under certain circumstances, the separation process would continue for only so long, and then, suddenly, stop; no further separation was possible. "Nobody understood why," Doherty says.

His model posited that the reactive azeotrope existed and that it also stopped the process, and his group wrote papers about it, despite there being "not the slightest scrap of experimental evidence that this was in any way part of reality," he recalls. "It had never been predicted or anticipated, and while some phenomena arising as a result of it had been seen in experiments, no one could explain them."

Year after year, Doherty, now the Mellichamp Chair in Systems Engineering at UCSB, attended meetings where plenty of experimentalists were present. And he would suggest to them that if they would plug key quantities from their experiments into his equations, they would know whether they had found a reactive azeotropic state.

But nobody did, so rather than waiting, he and his colleague Michael Malone decided to do it themselves. "We scrounged up some funding and built the equipment and hired a really great experimentalist, Wei Song, now a technology leader at Shell," he recalls. "And sure enough, we showed experimentally — absolutely and conclusively — that this phenomenon is real. We discovered it in a real mixture with a real reaction and real separations and in 1997 got a very nice paper, titled "The Discovery of a Reactive Azeotrope," published in *NATURE*, which is not a place I publish as an engineer."

With experimental evidence to validate the model, interest grew, and Doherty and Malone, currently Vice Chancellor for Research and Engagement at the University of Massachusetts, Amherst, later wrote about the work in a broader context in their widely read, extensively cited book *Conceptual Design of Distillation Systems.*

> **"Frequently, you want a particular polymorph for a particular application, and the question is, how do you get the one you want and not some other one?"**

THE SECOND ACT

From there, Doherty switched tracks, teaching himself a whole new field, a process he likens to "getting another PhD," which led to his spending the past roughly twenty years focused on crystals. "We and others have devised ways of writing down mathematical models for how molecules are attached to crystal surfaces, and those models can tell us the rate at which they attach, which can tell us the speed at which a crystal face will grow," he explains. "We then perform computer simulations to solve the equations and determine the outcome, given the molecule, its environment, and so on."

Simulations and models are extremely close, highly interdependent, mutually indispensable siblings. "Just writing down a set of equations doesn't typically give me the slightest hint of what those equations are going to tell me about my system or phenomena or natural processes," Doherty says. "You actually have to solve the equations. If you can't, then you've learned nothing. That's where mathematics comes in. Simulation occurs when you have a model for which you cannot find a closed-form mathematical solution, which is most commonly the case, so you have to devise a numerical method that solves it. Typically, the models are so complicated that you could never solve them without a computer."

Recently, one of Doherty's students, **Thomas Farmer** (PhD '18), worked with him to make another important breakthrough, in crystal formation. "It was a model we put together that predicted a very exciting and unusual outcome that no one had discovered before and that could have a big impact on pharmaceutical manufacturing," he says,"perhaps one as profound as the discovery of the reactive azeotrope was in the world of separation and reactions." The discovery led the European Federation of Chemical Engineers to invite Doherty to give the 2021 Euro Danckwerts Memorial Lecture last September.

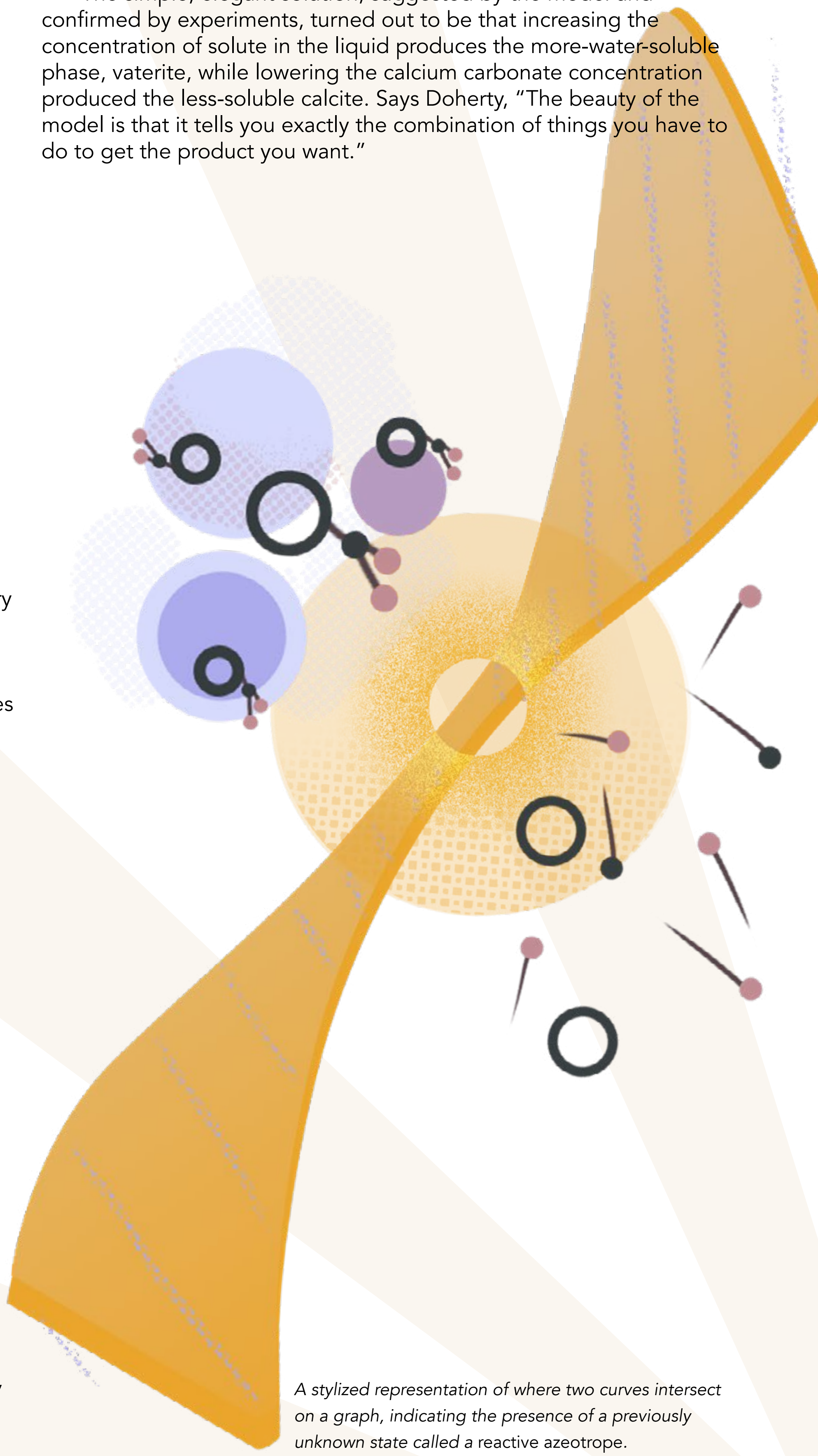
The work is based on the fact that most solids can crystallize in multiple different lattice configurations, or phases, and different phases of the same solid, each of which is called a *polymorph,* have wholly different qualities. The prime example is carbon, which, in its graphite form is soft, gray, opaque, and a good conductor of electricity, but that same carbon under enough pressure gets arranged differently to become diamond, a hard, transparent solid that does not conduct electricity.

"Frequently, you want a particular polymorph for a particular application," Doherty explains. "And the question is, how do you get the one you want and not some other one? We figured out how to do that and published a paper about the findings, which said, essentially, that if you design your system in *this* part of the space, you'll get this output, and if you design your system in *this* part of the design space, you'll get a completely different output. The two outcomes are mutually exclusive."

It is theoretically known and experimentally proven that the most stable polymorph is also the least soluble, and most chemical engineering processes naturally produce the most stable solid. "The problem is that the most stable form is also the least soluble in water, and we're made mostly of water," Doherty says. "So, while a lot of modern pharmaceuticals are effective, you can't get enough of them into you. The companies want a form of the drug that has much higher solubility in water. We were able to achieve better solubility on demand in a stable process that doesn't change or give unexpected, unwanted results even if you run the system for weeks."

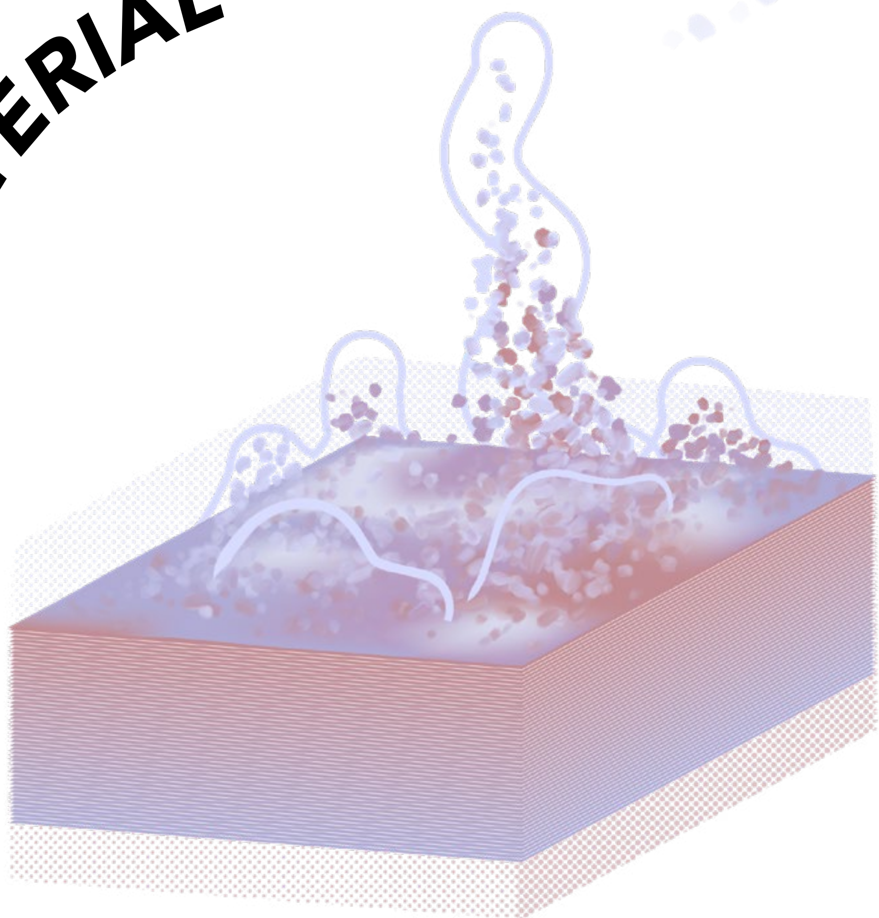
While the model was compelling, once again, experiments were needed to validate it, and this time Doherty decided not to wait. They built an apparatus and, over eighteen months, did the experiments to test the model. They determined how to crystallize their target material, calcium carbonate, into one of the two main forms it takes: calcite, which is the lowest-energy, the most stable, and the least water-soluble form; and vaterite, a very high-energy form, called *metastable,* that is more water-soluble.

The simple, elegant solution, suggested by the model and confirmed by experiments, turned out to be that increasing the concentration of solute in the liquid produces the more-water-soluble phase, vaterite, while lowering the calcium carbonate concentration produced the less-soluble calcite. Says Doherty, "The beauty of the model is that it tells you exactly the combination of things you have to do to get the product you want."



A stylized representation of where two curves intersect on a graph, indicating the presence of a previously unknown state called a reactive azeotrope.

MODELING BACTERIAL "PILE-UPS"

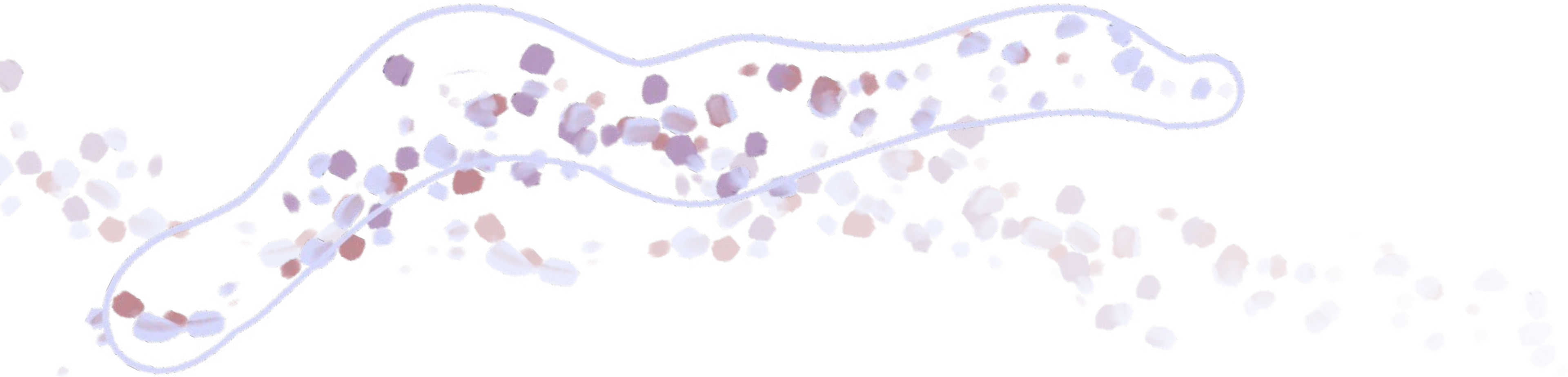


Sho Takatori tracks the swarming behavior of tiny organisms

Like many of us, UC Santa Barbara chemical engineering assistant professor **Sho Takatori** is fascinated by the swarming behavior exhibited by birds, fish, insects, and other organisms. A part of Takatori's research group studies such behavior, not in the sky or the ocean, but under an optical microscope and through models and simulations, to see how it plays out among populations of self-propelled particles such as bacteria. These particles exhibit autonomous motion and are classified in the category of *active matter.*

Such particles often show interesting dynamics, Takatori says, because they are able to communicate with each other as they move. "A fish swimming alone in the ocean might appear to be undulating in a random motion, but if you put it into a school of fish, you see this beautiful swarming pattern. Those patterns emerge because the fish can both move in a directed fashion and communicate with each other. Whenever you have a large collection of constituents that are able to make their own decisions individually, non-trivial patterns can come about. Our group tries

> **"It describes how a colony of bacteria initially organized as a densely packed, two-dimensional monolayer of cells can suddenly transform into a hierarchical three-dimensional stack of cells."**



to understand how that motion of an individual entity or constituent within a material might serve to dictate the overall properties of that system or material."

In one project, Takatori was interested in the swarming and aggregate behaviors of bacteria on surfaces. "A lot of times, they're adsorbed onto a surface, such as a biomedical device or other implant that is put into the body," he says. "We want to understand how colonies form and grow there and on other surfaces, such as soil, rock substrates in the ocean, or the surface of our lungs. Understanding the physics behind the swarming behaviors of such organisms is a rapidly growing field right now."

Projects in Takatori's lab are usually inspired, as he says, "by something really cool that happens in a simulation or an experiment or, if I'm doing a pen-and-paper analytical theory, and the model produces surprising results I would not have expected. I might wonder then if we could realize this experimentally or if a simulation would show that it is really happening. A lot of it is curiosity-driven."

In one recent project, Takatori's group, in collaboration with UC Berkeley chemical engineering professor Kranthi Mandadapu, examined a process that they refer to as *motility-induced buckling.* It describes how a colony of bacteria initially organized as a densely packed, two-dimensional monolayer of cells can suddenly transform into a hierarchical three-dimensional stack of cells. The project involved a combination of experiments, theory, and simulation in a way that required "a lot of careful modeling and understanding the different types of interactions that lead to such a transition," Takatori says.

Takatori sees multiple benefits arising from the varied competencies of his lab group. "Having the experimental side allows us to narrow down the very large parameter space of all the interesting phenomena that can happen and informs better theoretical models," he says. "Experimentalists can also tell us that something we are proposing in the model cannot be done experimentally. Models are useful at guiding the way by narrowing the pathways for experimentation, just as experiments are useful for refining the model."

In the motility study, the researchers began by performing experiments (on other projects, the equations and simulations might precede experiments), which showed that swarming motions exhibited by dense concentrations of bacteria moving around on a 2D surface could cause individual bacteria to pop out to a third dimension. "We observed this under the microscope and felt that it was an important process that could describe various sorts of other phenomena out in nature," Takatori says.

From there, they used a simulation to see if they could reproduce some of the results they observed in the experiment. "Our ultimate goal is to come up with a good pen-and-paper equation or an analytical model of this particular cell growth on a substrate," he says, adding, "If you have a good model, you don't need anything else, but often, we don't have the right, accurate model to begin with for very complex systems, so we need other tools, like computation and simulations, to help us develop better models for those systems."

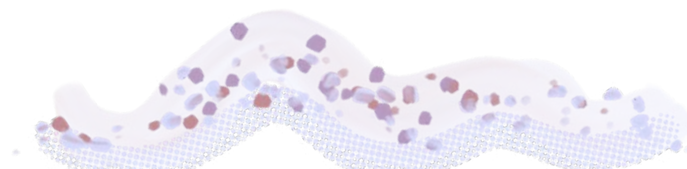
Even simulations can require further modeling. "We might need a model to describe the interactions among the constituents that are represented in the simulation," Takatori says. "For instance, we often do simulations of particles suspended in a fluid, and we need to model how the individual particles communicate with each other. Their communication is quite complex, so we need a model to describe it easily so that we can perform a large-scale simulation of it."

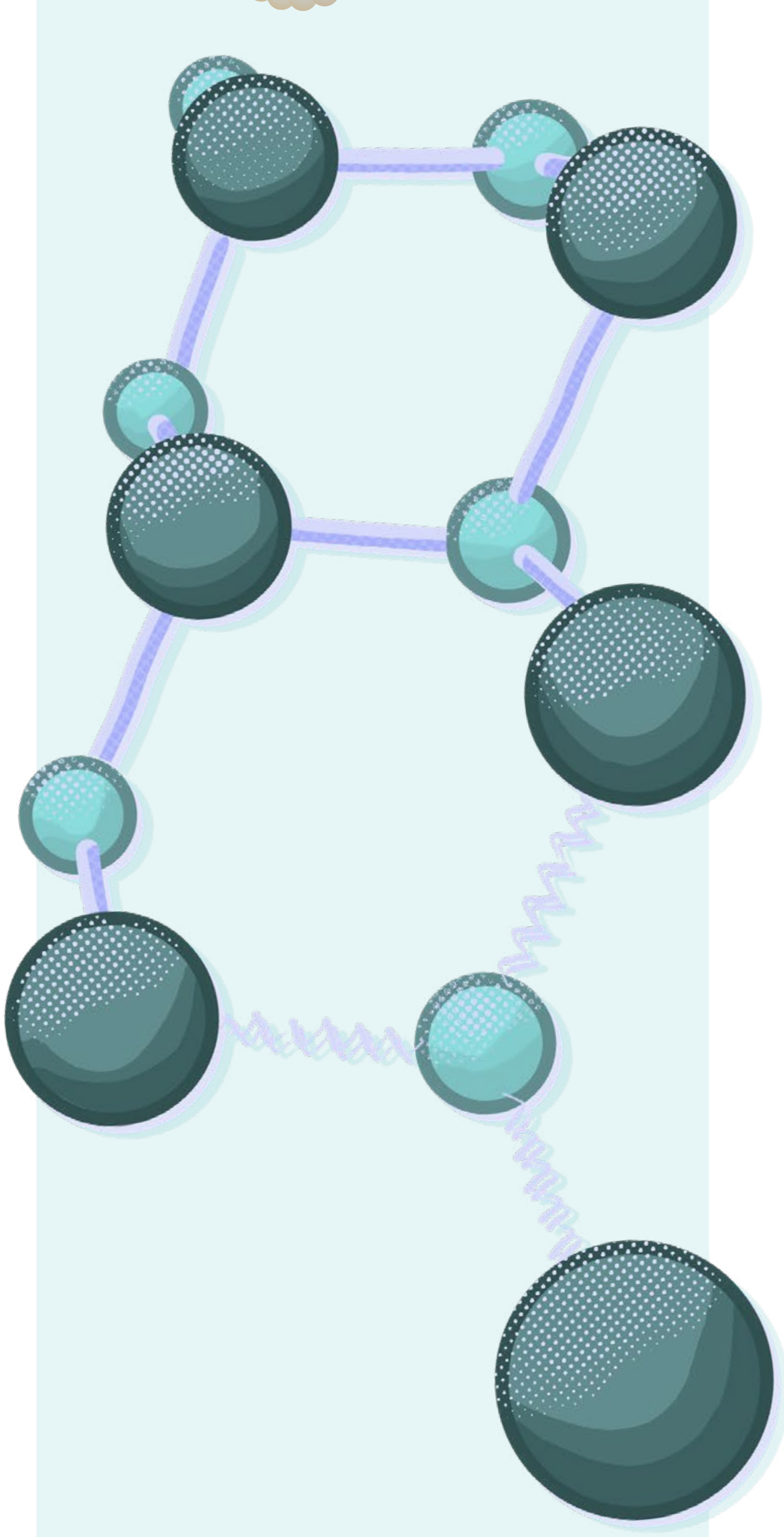
Takatori explains that researchers use different tools from the modeling-simulation-experimentation workflow, and use them in different ways, depending on the scales of time and length they are looking at. For those who study molecular systems, he says, "The simulation might evolve every single solvent molecule and every single hydrogen and carbon molecule. One usually performs a very short simulation, because one is interested in understanding the dynamics that occur on a very short time scale."

On the other hand, he says, "A lot of what our group studies takes place on much larger length and time scales. We're not looking at the motion of an individual water molecule. Rather, we're interested in suspensions of larger, micro-sized particles, like bacteria, suspended in a fluid. Because the bacteria are much larger than the solvent molecules, we can often do what's called *coarse-graining,* which means removing the solvent from the simulation, because the solvent molecules are much smaller than the particles we're interested in.

"If I wanted to do the full simulation that included all the solvent molecules, it would take longer than the academic career of a PhD student. We're focusing on the dynamics of the particles we're interested in as opposed to trying to evolve every single molecule and particle in the system. Computational tricks like coarse-graining can be used to accelerate the simulation dramatically."

He concludes: "Our goal, by combining theory, coarse-grained simulations, and experiments, is to advance a mechanistic understanding of complex fluid systems, such as bacterial films and particle suspension interfaces. Theory, simulations, and experiments each provide a different tool to study these systems across diverse length and time scales."





CHRIS VAN DE WALLE

Modeling in the quantum realm

In 2007, the laboratory group of UC Santa Barbara materials professor **Chris Van de Walle** began working to model *Auger recombination*, a key process in the functioning of semiconductor-based light-emitting diodes (LEDs). Their work was motivated by experimental reports showing a rapid loss of efficiency in LEDs when the current into them reached a certain level. Since efficiency is a key strength of the tiny, long-lasting lights, breaking through this high-current efficiency "droop" was driving research around the world.

Van de Walle explains the process: "In an LED or a laser, we inject electrons and holes — the positively charged counterpart of electrons — and when they meet, they annihilate, producing energy that is emitted in the form of light, a process called *radiative recombination*. But sometimes, when an electron and a hole recombine, no light is emitted; instead, the energy is released in some other way, a so-called *nonradiative* recombination process — Auger recombination — which creates a source of loss, or reduction of efficiency, in the device. Using first-principles calculations, we can calculate the rates at which these processes happen; and these rates then can be fed into a model that predicts the efficiency of a device.

"In principle, the findings about efficiency loss could be explained by Auger recombination, but the majority of the community did not believe this to be true," Van de Walle continues. "Their belief was based on older models that did not take into account vibrations of the crystal lattice of the semiconductor. We thought the vibrations were important."

Making choices is an important part of developing a model, Van de Walle says, and in modeling Auger recombination, his group made a choice — to account for lattice vibration — a choice that would have a profound impact on the entire semiconductor field. It paid off, leading them to discover that, as suspected, in some materials, such as gallium nitride, which is the key material for solid-state light emitters, and the one UCSB Nobel Laureate **Shuji Nakamura** used to invent the world-changing blue LED, "The vibrations make a huge difference. They were the source of a stubborn barrier to efficiency gains at high current!"

The model, developed over a three-year period, provided an abject lesson in the tradeoffs involved in modeling and simulation. "Including the vibrations makes the model a lot more complicated and makes the simulations a lot more expensive [because they require much more computer time to run]," Van de Walle says. "We went through the considerable effort to include the vibrations, and found that the results could beautifully explain the experimentally observed efficiency loss."

Subsequently, he notes, [UCSB materials professors] **Jim Speck** and **Claude Weisbuch** performed detailed, highly original experiments in which they actually observed the "Auger electrons" — electrons that are kicked up to higher energies during Auger recombination. "That clinched it!" Van de Walle recalls. "The findings changed the perception of the role of Auger recombination in gallium nitride.

"Now that we have the model, we can apply it to other materials," he adds. "It has produced very useful insights for materials ranging from lead selenide, used in infrared detectors, to hybrid perovskites, used for novel solar cells. We discovered that Auger recombination in hybrid perovskites is greatly enhanced by a particular feature in the band structure of the material, and that this feature can be tuned my substituting some elements for others in the crystal, for instance, replacing a fraction of the lead atoms with tin atoms. Even in the absence of full-scale simulations, this model can tell the people who synthesize the material how to optimize it!"

There is a good deal of back and forth between the model and simulations, Van de Walle says: "Once the model is developed, we need to run the simulations to generate the data that the model needs. Even though we use established codes [written by groups that are experts at developing them] to solve the key equations, additional software needs to be written to process the output of those simulations for specific materials and calculate the quantities needed for the model.

"Along the way, we need to balance accuracy — and determine what level of accuracy is required — with computational cost; it's always a tradeoff. But once we have demonstrated that the simulations are 'converged,' or have met the desired tolerance requirement, we can produce results that elucidate the physical mechanisms. This, in turn, makes it possible to redesign devices to avoid the efficiency bottlenecks."

And that is where fundamental, first-principles science meets the marketplace.

Van de Walle's group works primarily at the scale of atoms, performing simulations of materials based on fundamental quantum-mechanical calculations. The output of those simulations can be used to do various types of modeling, such as the one his group developed to describe Auger recombination.

> **"Many beginning students in the field have a tendency to just run a lot of simulations, hoping that somehow a result will jump out. It never does. Before running any code, you need to carefully think through the problem and develop a model that will allow you to test hypotheses."**

The mathematics are particularly complex, because, as Van de Walle says, "To model materials at a fundamental level requires very complicated equations that describe the behavior of electrons in materials. That behavior is governed by quantum mechanics — essentially a complicated version of the Schrödinger equation that was proposed almost a century ago to describe particles at the atomic scale. The solutions to that equation allow us to predict almost any property of any material."

Modeling, Van de Walle says, "allows us to develop and test hypotheses about materials behavior, thus guiding experimental growth and characterization efforts." And the first step in developing a model, he notes, is always the same: to think — slowly, deeply, thoroughly — about the problem to be solved. "Many beginning students in this field have a tendency to just run a lot of simulations, hoping that somehow a result will jump out," he says. "It never does. Before running any code, you need to carefully think through the problem and develop a model that will allow you to test hypotheses."

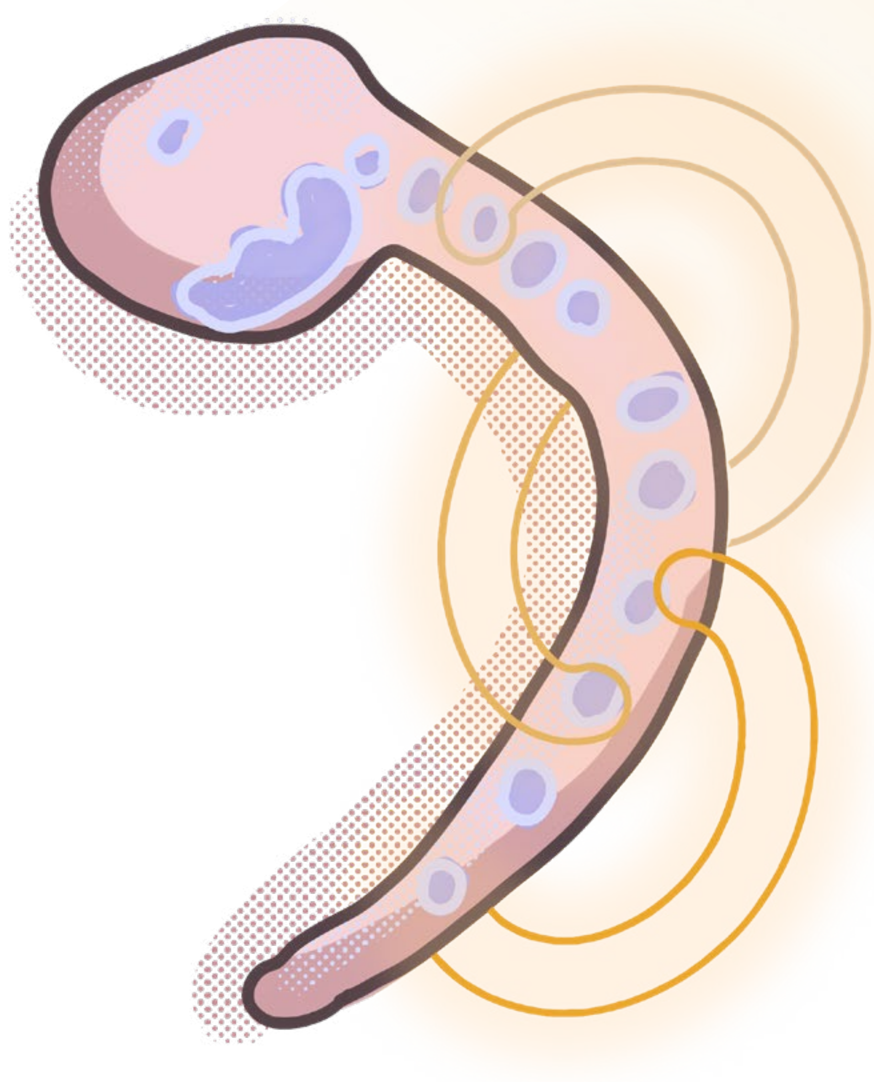
Once a model is developed, Van de Walle adds, "The most important thing is to verify and validate. Verifying means ensuring that the model actually returns what is desired. Validating means comparing the predictions with experimental results for a well-established case. Such benchmarking should also include checking the model's sensitivity to input parameters and establishing over what range of conditions the model is valid. Running computational simulations puts meat on the bones of the models, which is essential for validating the model and for making direct connections with experimentation."

Simulations can serve various purposes. "In some cases, we aim to characterize behavior or performance," says Van de Walle. "For instance, when experimental results are puzzling, simulations can help to provide understanding, as they did in the case of Auger recombination. In other situations, we make predictions that might guide the development of novel materials, or new combinations of materials."

Asked if he finds reward in modeling, Van de Walle does not hesitate. "Absolutely!" he says. "As an engineer, I like solving puzzles, and I like having an impact on how technology develops. It's very gratifying to see the papers that report our key insights being heavily cited. It means that other scientists are actually using those results and benefiting from them."

WILLIAM SMITH

The Ciona, Model Organism



William Smith, a professor in the UC Santa Barbara Department of Molecular, Cellular and Developmental Biology, understands as well as anyone that mapping the neural circuitry of the human brain and tracking the coordinated interactions of our roughly 85 *billion* neurons is a daunting task.

"Ultimately, we'd like to understand how vertebrates, animals like us, work," says Smith, whose research is focused on the nervous system of animals in the chordate phylum of animals, which includes vertebrates. "But we're enormously complicated, and at this point we're very far from a full understanding of our complex nervous system at the individual neuron level; there are just too many neurons."

A better place to start, he thought, would be to model the neural circuitry of a simpler chordate organism, to serve as a surrogate for — a kind of model of — the human neural system. Enter the ocean-dwelling *Ciona*, a primitive chordate that is closely related to vertebrates but has only 177 neurons. As one of few universities to have marine science facilities on its main campus, UCSB is ideally situated for this research.

The work, funded by NIH's Institute of Neurological Disorders & Stroke, began with Smith's collaborators at Dalhousie University in Halifax, Nova Scotia, gathering electron microscopy (EM) images of every neuron in a Ciona larva and then creating a wiring diagram, or *connectome*. Even with so few neurons, the project took many years of work by the Dalhousie team. Their results can be seen as an interaction matrix showing the 6,618 synaptic connections among the 177 neurons. "To do that for the human brain would require a matrix 2.17×10^{17} — or a billion trillion — times bigger than that," Smith says.

Beyond mapping the *Ciona*'s neural circuitry, the researchers wanted to determine which of six key neurotransmitters are present in which neurons. "It's important to know, because that tells us how it will act on its targets. Neurons can be excitatory — they can tell other neurons to have an action potential downstream — or they can be inhibitory," Smith says. "It's not a trivial undertaking."

To begin that work, Smith teamed up with UCSB Electrical and Computer Engineering professor **B. S. Manjunath**, Co-PI on the NIH project and an expert in computer vision and machine learning, and his student **Angela Zhang,** who received her PhD in September 2021, in an interdisciplinary undertaking of the kind that is much valued at UCSB. Zhang began by developing a method for overlaying the EM data onto the light microscopy (LM) data from Smith's lab, bringing the two kinds of information into alignment, or *register,* so that specific organs in the Ciona, seen with LM, could be correlated with specific neurons identified in the EM data.

The light microscopy was conducted using *in situ hybridization,* which involves incubating fixed *Ciona* larvae with fluorescently tagged antisense RNA probes. Each RNA probe differs depending on the type of neurotransmitter marker it is meant to find, and when the probe locates the target, it fluoresces in a color correlated to that neurotransmitter.

The light microscopy allowed Smith's group to do a three-dimensional reconstruction of the actual nervous system, but not at synaptic resolution, which requires electron microscopy. "We can see the outlines of cells here, but not all the little fine synapses," he says, pointing to a photograph of an LM-generated image.

"Maybe we know the nucleus location of a cell in both sets of data. We have the shape information of this cluster of cells from the EM and of another cluster of cells from the light microscopy," Zhang says. "I have to use computation to rotate and stretch and kind of move the cells in one set of data so that it overlays well with the other set. If we get the alignment right, we can see how a cell in the EM data corresponds to one in the LM data."

The registered data can then be correlated with the location of neurons to deduce which neurotransmitters might be present at specific synapses. "We got pretty good matches for certain parts of the brain, such as the photoreceptors," Zhang says. "We could match the location of the neurons in the two sets of data."

Smith's team could then use logic and their own eyes to go further, for example, identifying specific neuron types. "We know from the EM data that there is a cluster of cells located by itself, between the head and the tail, and that it is emitting only one type of neurotransmitter, GABA [the inhibitory neurotransmitter gamma-aminobutyric acid], for example, because the probe is lighting up with the color associated only with GABA."

Things were less resolved in other locations. "They'd see something that looked kind of like a hand and fluoresced in many different colors," Zhang explains. "They knew the location of the cell and its nucleus from the EM data, but the intermingled colors of fluorescence prevented them from knowing what was going on. But, by combining many samples, we were able to make predictions with high confidence for most neurons."

Smith says that by allowing his team to model what kinds of signals are sent between neurons, Zhang's initial work "led to some new and interesting models about how the nervous system in this animal works," for example, that many of the behaviors in *Ciona* are evoked by disinhibition, or one inhibitory neurotransmitter inhibiting the (inhibitory) influence of another inhibitory transmitter, thereby allowing an action to occur.

After converging the LM and EM data, he adds, "Angela would come up with a hypothesis, saying maybe, 'I think these cells are inhibitory and connect with other cells that also appear to be inhibitory,' and then we'd do various behavioral and pharmacological experiments that would allow us to say, 'Yes, that really is how it works.' It's modeling, where we're working together."

"Angela would come up with a hypothesis, saying maybe, 'I think these cells are inhibitory and connect with other cells that appear to be inhibitory,' and then we'd do various behavioral and pharmacological experiments and be able to say, 'Yes, that really is how it works.' It's modeling, and we're working together."

Next, Zhang built a deep-learning model to try to complete the work of correlating specific cells with their neurotransmitter types. The in situ hybridization had made it possible to identify with confidence some neurons and the various neurotransmitters they make. She used those confirmed data points to train the model, providing it with examples of known excitatory and inhibitory synapses. She thought, *What if we used the EM data to look at the individual synapses and see if there are physical differences in their structures that can indicate whether it is an excitatory or inhibitory synapse?*

One challenge, Zhang says, was that, unlike many engineering problems, where the final answer is known and the task is to train an ML model to get the right answer, "With science, you don't actually know what the truth is; you're trying to figure it out."

The result, she says, is that "The model is able to learn, but we don't know what it is learning. Is it learning that a particular set of photoreceptors has a certain quirk, so it groups them together? Or is it learning something universal to all excitatory *Ciona* synapses? And can we trust the results of the model? We can't know now without more experiments, and I'm definitely not an advocate of trusting models blindly."

As Smith likes to say, "All models are wrong. Some are useful." Time will tell.

NEW GRANTS

Development of an Agile Free-Electron-Laser-Powered Pulsed Electron Magnetic Resonance Spectrometer

Mark Sherwin (PHY), Raphaële Clément (MAT), Songi Han (ChemE, Chem) — NSF, $2.16 million, 3 years:

High-field electron magnetic resonance (EMR) is needed to achieve breakthroughs in disciplines ranging from biology to quantum information science. Magnetic resonance imaging (MRI) spectrometers deployed in hospitals use powerful pulses of electromagnetic radiation at frequencies well below 1 GHz to excite and detect the magnetic moments of protons in large magnetic fields. Because the magnetic moments of electrons are nearly 700 times larger than those of protons, high-field EMR spectrometers require powerful pulses of electromagnetic radiation having frequencies above 100 GHz. Generating such pulses is extremely difficult; as a result, the capabilities of high-field EMR spectrometers lag far behind those of MRI and other nuclear MR spectrometers. Researchers will build an agile free-electron-laser-powered EMR spectrometer designed to enable unprecedented studies of the basic properties of materials seen as candidates for new classes of quantum sensors; fast, energy-efficient alternatives to electronics; and exotic quantum mechanical states of matter.

During the 2020-'21 academic year, the College of Engineering had: **324** ***proposals awarded***

Rheology-enhanced Chemo-Catalytic Upcycling of Polyolefins

Rachel Segalman (ChemE), Mahdi Abu-Omar (ChemE, Chem), Songi Han (ChemE, Chem), Susannah Scott (ChemE, Chem) — Dept. of Energy, (up to) $2.5 million, 3 years

The world faces an enormous plastic-pollution problem, which recycling cannot solve. In this project, the researchers seek to use shear forces in novel ways to facilitate breaking carbon-carbon and carbon-hydrogen bonds in long, complex polymeric molecules, making it possible to upcycle the carbon-based molecules (rather than simply recycling the same polymers) which can be used as feedstock for new polymers. Developing a successful technique would be an important step in addressing the plastic-pollution problem.

Mitigation of Clogging in Drip-Irrigation Emitters: A Hydrodynamic Approach

Alban Sauret (ME) — US-Israel Binational Agricultural Research and Development Fund (BARD), $309,000, 3 years

Drip irrigation supports sustainable agriculture by reducing water consumption by up to 70 percent and reducing water scarcity, which is expected to affect nearly six billion people worldwide by 2050. Clogging, however, whether by contaminants such as grit or by biofilms growing within the emitter, reduces drip-irrigation efficiency, and clog mitigation adds complexity and cost to irrigation systems. Further, long-term use of herbicides to hinder biological clogging raises environmental concerns. Sauret and colleagues will use advanced in-situ imaging techniques to understand how clogging occurs in the emitter, and then take a hydrodynamic approach to developing and prototyping new geometries for clog-resistant drip emitters.

At any moment, hundreds of research projects are under way at UC Santa Barbara, while many dozens more are receiving funding or ramping up. Here are some of the many newly funded projects in the College of Engineering.

Integration Large: Democratizing Networking Research in the Era of AI/ML

Arpit Gupta (CS), Elizabeth Belding (CS), Trinabh Gupta (CS) — NSF, $1 million, 2 years

Emerging "self-driving networks" enable administrators of campus networks to automate most network-management tasks, ensuring reliable performance amid disruptions and requiring minimal interventions from network administrators. However, making significant contributions to a self-driving network requires developing tools based on artificial intelligence and machine learning and demonstrating that they work in practice. Unfortunately, in contrast to their counterparts in industry, most academic researchers have neither access to the proper data for developing learning-based tools nor properly instrumented testbeds for road-testing the resulting tools in realistic settings. Researchers in this project will investigate how to use campus networks to overcome barriers to self-driving network research. The project promises to be transformative not only for the network community as a whole but also for a range of campus-network stakeholders.

$91.7 M

awarded in total to the COE during the 2020-'21 academic year

Scalable and Quantitative Verification for Neural Network Analysis and Design

Tevfik Bultan (CS), Yufei Ding (CS) — NSF, $750,000, 4 years

Neural Networks (NNs) have been applied successfully in many areas, including computer vision, speech recognition, and natural language processing. However, the increasing adoption of NNs in safety-critical and socially sensitive domains, such as self-driving cars, robotics, computer security, criminal justice, and medical diagnosis, gives rise to a pressing need for verification techniques that can guarantee the dependability and safety of NN applications. The team intends to develop a holistic formal-verification framework that will provide a systematic and principled approach for developing dependable and safe NNs.

New End-to-End System for a Practical and Accessible Internet of Things (IoT)

Chandra Krintz (CS), Giovanni Vigna (CS), Rich Wolski (CS) — NSF, $1.2 million, 3 years

The project is aimed at determining how to securely program, deploy, and manage IoT systems and applications, making it possible to perform advanced data analysis in place and, therefore, to enhance human decision-making; detect, diagnose, and remediate problems without human intervention; and automate operations throughout our economy. The researchers will develop a portable, multi-tier (sensors, edge, cloud) platform, called Detroit, that supports "write-once-run-anywhere" programming for IoT devices and is aimed at democratizing key processes in order to realize the positive societal transformation and shared economic impact that the IoT promises.

Largest sponsors of awards received by COE faculty in 2020-'21:

$20.7 M
Department of Defense

$18.5 M
National Science Foundation

$11.3 M
Department of Energy

Wicking in Gel-coated Tubes

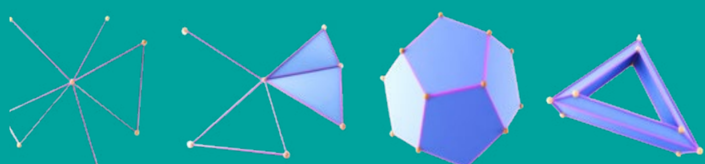
Emilie Dressaire (ME) — NSF, $646,875, 3 years

Surfactant replacement therapies rely on plugs of liquid to carry drugs into the lungs to treat respiratory distress syndrome. The administered liquid plugs travel through airways lined with mucus, a gel that traps inhaled contaminants. The deposition of liquid in the airways is often held responsible for therapeutic failures, yet the influence of the mucus lining on drug delivery is not yet understood. Experiments will be conducted onboard the International Space Station and on Earth to establish the role of a gel lining in the transport of a liquid plug. The team will examine and explain how the gel's mechanical properties affect the liquid delivery in gravity and microgravity conditions. The aim of the project is to develop a comprehensive understanding of free and forced liquid imbibition through gel-coated tubes.

Symmetry-Guided Machine Learning for the Discovery of Topological Phononic Materials

Susanne Stemmer (MAT), Bolin Liao (ME) — NSF, $1.04 million, 4 years

Fundamental understanding and control of heat-conduction processes in materials are important for energy infrastructure, electronic devices, and renewable-energy generation systems. The researchers will focus on a novel property of phonons — vibrations of atoms that carry heat in materials, in a process called *topology* — which may allow new phenomena, including more efficient transport of heat waves on material surfaces. The research team will search for materials hosting these special heat carriers, synthesize and characterize candidate materials, and use the results to refine the search algorithm. A public database of materials will be created. This research will not only advance the fundamental understanding of how topology affects heat conduction in real materials, but also provide new routes to realizing unusual functionalities, such as heat conductors that can be switched on and off.



Examples of cell complexes, courtesy of collaborator Mustafa Hajij, an assistant professor of mathematics and computer science at Santa Clara University.

A Unifying Deep Learning Framework Using Cell Complex Neural Networks

Nina Miolane (ECE) — NSF, $334,780, 3 years

Deep learning has fostered the development of many new transformative technologies that originated with rapid advancements in the fields of computer vision and natural language processing, that is, the processing of images and texts. Yet, a wide range of data is not best represented by a grid of pixels or a sequence of words. For example, (biomolecular) shapes and (social) networks are data types exhibiting local and global geometric properties that might not be efficiently leveraged by existing deep-learning architectures. Hence, there is a need to rigorously understand and expand the data types to which deep-learning methods can be applied. This research project considers the more abstract "cell complex" data type, and is aimed at quantifying the potential of "cell complex networks" in deep learning. Applications range from computational biology and medicine, social science, and art, to a better understanding of deep learning itself. Miolane will collaborate with Mustafa Hajij, an assistant professor of mathematics and computer science at Santa Clara University.

Development of an Ultrafast, Ultrasensitive, High-resolution Direct Electron Detector for Next-Generation Electron Back-scattered Diffraction of Metallic and Beam-sensitive Materials

Daniel Gionola (MAT), Michael Chabinyc (MAT), Tresa Pollock (MAT), B. S. Manjunath (ECE), Raphaële Clément (MAT) — NSF, $578,000, 2 years

Electron back-scattered diffraction (EBSD) is a powerful, widely used characterization technique for mapping and analyzing phases in materials. The advent of direct electron detection, which circumvents inefficient conversion between electrons and photons, has revolutionized the field of transmission electron microscopy, but its use in scanning electron microscopes (SEMs) is in its infancy. In this project, researchers will develop an ultrafast, ultrasensitive direct electron EBSD instrument for the widely accessible SEM platform, providing a rich opportunity for materials research currently hindered by electron beam damage and temporal limitations of detectors. The development project improves on the state-of-the-art EBSD acquisition speed and enhances sensitivity through a new sensor design, unlocking the most vexing challenges in the rapid 3D characterization of additively manufactured materials and emerging dose-sensitive materials.

The researchers plan to develop a new direct electron sensor design to address the key challenges faced when using present-day instruments, like the one shown here.

Direct-force Measurements and Analysis of Intrinsically Disordered Proteins

Omar Saleh (MAT) — NSF, $835,000, 4 years

A major goal of this project is to find the key molecular-scale features that control the behavior of disordered proteins, a class of proteins found in all living organisms and named for their unique trait of being both dynamic and floppy. Saleh and his collaborators in Israel will investigate the overall incidence of these anomalous effects across biologically occurring disordered proteins, and study the molecular determinants that cause the behavior. The research has the potential to broadly impact our basic understanding of the molecular processes of life, while also disseminating a specialized experimental technique that is expected to have wide utility in the quantitative study of biological molecules.

Living Biotic-Abiotic Materials with Temporally Programmable Actuation

Megan Valentine (ME) — NSF, $360,000, 4 years

A team of five comprising physicists, biologists, and engineers intends to design and create a new class of self-directed, programmable, reconfigurable materials inspired by cells and capable of producing force and motion. Their approach will capitalize on two important design principles of living organisms, to wit: 1) cells are composite in nature to meet numerous functional demands, and 2) decision-making and timing are achieved through biomolecular circuitry.

This effort will couple synthetic hydrogels to living layers of active polymer composites infused with cellular timing circuits to produce next-generation materials that self-actuate programmable cycles of work and motion. The proof-of-concept design will be a gap-closing micro-actuator that closes upon exposure to light and then autonomously re-opens at times and locations programmed into the embedded cell circuits. The goals in terms of material development, combined with customized high-throughput characterization and publicly shared property-formulation libraries, will empower the broader Materials Genome Initiative community to manufacture and deploy such disruptive materials of the future.

UCSB ALUMNA PLAYS CRITICAL ROLE IN **DEVELOPING PFIZER-BIONTECH COVID-19 VACCINE**

Nearly 250 million doses of the Pfizer-BioNTech COVID-19 vaccine have been administered in the United States since the Food and Drug Administration (FDA) issued an Emergency Use Administration (EUA) in December 2020 to help curtail the pandemic. The vaccine, now called Comirnaty, became the first FDA-approved COVID-19 vaccine for patients 16 years and older on August 23 of this year. The recommendation came after a months-long, multinational placebo-controlled trial showed results that met the agency's high standards for safety, effectiveness, and manufacturing quality. Results from the clinical trial demonstrated that the vaccine was 91 percent effective in preventing COVID-19 disease. A key member of the vaccine development effort at Pfizer was **Nikki Schonenbach**, who received her PhD in chemical engineering from UC Santa Barbara in 2017.

"There were many, many motivations to work on this project; the highest priority was simply the rapid spread and devastating effects COVID-19 had on so many lives," said Schonenbach, who was a key member of the in-vitro transcription (IVT) process development team. "This was my opportunity to help. As a whole, this entire well-functioning team both challenged and supported the members in their knowledge development. Every member was critical."

Comirnaty contains messenger RNA (mRNA), a kind of genetic material that is used by the body to make a mimic of one of the proteins in the virus that causes COVID-19. The result of a person's receiving the vaccine is that their immune system will, ultimately, react defensively to the virus that causes COVID-19. The mRNA is present in the body for a short time and does not become incorporated into or alter an individual's genetic material in any way.

"Part of the beauty of mRNA as a therapeutic is that there are so many opportunities for treatment areas," Schonenbach said. "In the vaccine space, as we have demonstrated with COVID-19, we can scale up and manufacture a vaccine faster than ever before in response to a global pandemic. Unlike traditional vaccines, an mRNA vaccine does not contain a viable virus at any point in the manufacturing process, so there is no chance of catching the virus from the vaccine that is meant to protect you."

Schonenbach designed experiments, analyzed data, and presented the results to the wider team. She earned the unofficial title of "Lab Captain" and led experiments at the laboratory scale that were critical to the scale-up and robustness of the characterization process. Her supervisor at Pfizer, Khurram Sunasara, described Schonenbach as "one of the key thought leaders in the mRNA space," who played a critical role in the COVID vaccine program and will do so in future mRNA programs. As a result of her efforts during the vaccine development process, she was promoted to principal scientist.

"I am honored beyond words to be a part of this team," she said. "The time I have spent at Pfizer has been the time of my life, and I feel so lucky to have been able to get involved and stay involved with our efforts to develop mRNA therapeutics. We have pushed the envelope for mRNA vaccines a great deal in the past year, but there is still so much to learn and develop in vaccines and other therapeutic spaces."

Schonenbach was co-advised at UCSB by chemical engineering professors **Michelle O'Malley** and **Songi Han**. Her research focused on characterizing pharmaceutically relevant membrane protein complexes to link changes in structure and dynamics to function. She describes much of her work in graduate school as "RNA-adjacent," as she did not work with RNA prior to Pfizer.

"Several things I learned and was proficient in became of tremendous use at Pfizer," she said, citing her significant experience with different types of cloning techniques, molecular biology, and cell culture work, as well as handling proteins that are sensitive to degradation. "I had mastered techniques at UCSB that were helpful in working with RNA, which is sensitive to degradation if handled improperly. My experience also helped me to implement lab protocols for our team to follow in the COVID-19 development labs at Pfizer."

Schonenbach hopes that current and future students see the endless opportunities that are available to them from a UCSB education.

"UCSB has excellent educators and principal investigators who conduct research across a broad range of engineering, chemistry, and physics that is invaluable to the real world," she said. "I am far from the only alumna making an impact, or the only graduate working on the COVID-19 vaccine."

Nikki Schonenbach (PhD Chemical Engineering, '17), played a key role in developing the Pfizer COVID vaccine.

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The philanthropy of individuals like you helps to ensure that breakthroughs in science and engineering remain the order of the day across our beautiful UC Santa Barbara campus. Large gifts, small gifts, estate gifts — they all matter, because each advances academic excellence and leading-edge research that, together, help pave the way to a better tomorrow. Please consider making a difference by making your gift today!

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