### CHEMICAL AND BIOLOGICAL ENGINEERING



We're making research strides, safely

#### Chair's Message



#### Hello from Madison!

We are excited to welcome our incoming freshmen, our new graduate students as well as our

returning students as we start the fall semester. Certainly, these are challenging and unusual times; faculty and staff have been working hard throughout the summer to prepare for the necessary changes to instruction due to COVID-19. Some of our classes will be offered remotely, others in-person, and some with a mix of remote and in-person activities. Protective masks and face shields are distributed, Plexiglass barriers have been installed and we are all practicing protocols to keep everyone healthy and safe.

CBE's first experience with fully remote teaching took place with our iconic Summer Lab. Once the decision was made this spring to teach remotely, faculty and instructors creatively reworked experiments so students could learn and develop their skills through "informals" right in their own homes. Supplies were sourced, purchased and sorted, and boxes of "goodies" were quickly assembled. Students living in Madison picked up their lab kits in person, while other kits were shipped across the nation and even across the sea. Students stayed connected and cheered each other on by posting photos and videos of their experiments on Instagram. Details about our online Summer Lab experiences are in this issue.

On campus, we have been busy with wholesale remodeling of lab spaces for our new assistant professors, Matt Gebbie and Marcel Schreier. Matt's research focuses on interface science, soft materials, electrochemistry and sustainable energy. Marcel's work targets electrified interfaces, electrochemical energy storage and electrocatalysis. Their graduate students are now busily setting up instrumentation and conducting experiments in their beautiful new labs.

After the campus shutdown in late March, research activities were re-introduced in early July, with close attention to face

mask wearing, cleaning protocols and physical distancing. Graduate students and postdocs are now happy to be back in the lab. Progress towards degrees has been maintained as preliminary exams, fourth-year progress report meetings and thesis defenses are all held remotely. Our graduate student group ChEGS is holding many virtual social events to keep students connected with opportunities for fun and relaxation.

This fall issue features some of the timely and significant research our faculty has been undertaking in response to COVID-19. We announced the establishment of a new research center devoted to plastic recycling, and we described how a stochastic model for utility plants can be used to plan for extreme events. You can also read about our highly successful venture in offering a virtual summer research experience for undergraduates, the awarding of the prestigious Steenbock Professorship in Engineering to Professor Michael Graham and other highlights.

On a somber note, we report the sad news that Professor Jennifer Reed passed away in July after a long illness. Jennie was a wonderful colleague, a devoted mentor to her students and a good friend. Jennie's passing is a tragic loss for the university and department. More about Jennie's life and accomplishments, and an undergraduate research award to honor her, are in this newsletter.

As we settle into the fall semester, I am planning to set up virtual events to connect with alumni and keep you up to date on our department activities. Stay tuned for this information. Meanwhile, if you have any news you'd like to share with us, please reach us at che@che.wisc.edu.

Our hope is that you, your family and loved ones stay healthy and safe during this time.

On, Wisconsin!

Regina M. Murphy, PhD

Remmy

R. Byron Bird Department Chair Kreuz-Bascom Professor regina.murphy@wisc.edu • (608) 262-1587

## IMPACT

A historic \$32 million commitment from The Grainger Foundation of Lake Forest, Illinois, will propel the College of Engineering on a growth trajectory.

Recently, the college announced plans to increase its enrollment by 1,000 undergraduates students, along with an initiative to create the physical infrastructure to support that growth.

With \$20 million, the pledge funds the Strategic Targeted Achievement Recognition (STAR) initiative for undergraduates. The scholarship program is aimed at recruiting the best students in the country and includes matching options for named scholarships to amplify the commitment's impact.

The pledge also fully endows or creates a total of seven Grainger professorships to support high-achieving faculty leaders and establishes the Grainger Dean of the College of Engineering. Ian Robertson, who has led the college since 2013, will be first to hold the named deanship.

Read more:

go.wisc.edu/grainger-engr-32M-gift

Contact Amber McLoughlin, amber.mcloughlin@supportuw.org, to learn more about the matching opportunity.







### **MELTING POINT**

## CBE FACULTY HOPE TO CLOSE THE LOOP ON PLASTIC RECYCLING

Many of us fastidiously clean and sort our yogurt containers, milk jugs and mountains of other plastic waste each week, getting that packaging ready for the recycling bin.

Yet in the end, much of that effort has been wasted: Of the 8,300 million metric tons of plastics produced between 1950 and 2015, only 9 percent was actually recycled. That's because recycling plastic is difficult, and there is currently no economical way to "upcycle" plastic back into items like water bottles or food packaging.

But Richard L. Antoine Professor George Huber is hoping new methods he is developing can help close the loop on recycling, and the new \$10 million U.S. Department of Energy-funded Center for Chemical Upcycling of Plastic Waste based at UW-Madison will make the university a hub for plastic recycling research.

In his recent work, Huber and his team have pyrolyzed plastic, essentially reacting it in low oxygen conditions to produce a liquid oil. They then analyzed the liquid and gas products after pyrolysis with the goal of separating the products into usable chemicals which can be reused as feedstocks for making new polymers.

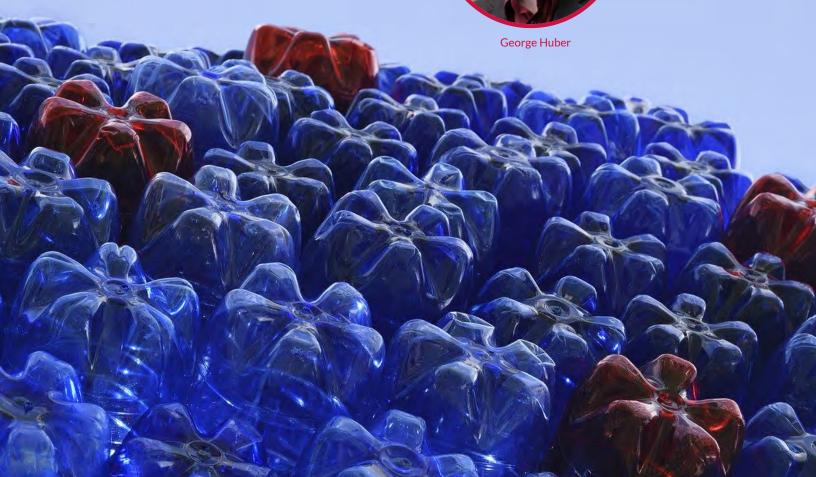
"We're trying to provide more molecular-level information about the chemicals that you can make from pyrolysis," Huber says. "That gives us ideas about how we can more efficiently go back to the original plastics."

In the near future, he believes, pyrolysis could lead to true closed-loop plastic recycling. Eventually, it will be possible to pyrolyze large bales of mixed plastics and separate the resulting liquid into their various chemical components. Those could then be reprocessed into various virgin plastic polymers, which could be reused over and over again, similar to aluminum cans.

Huber won't be closing the loop alone. As director of the new multi-university Center on Chemical Upcycling of Waste Plastics, he'll be collaborating with researchers and industry partners across the world as well as drawing on the expertise of many CBE colleagues. Conway Assistant Professor Reid Van Lehn will focus on STRAP processing, a technique for recycling multilayer plastic films; Baldovin-DaPra Associate Professor Victor Zavala will analyze system economics, the plastics recycling lifecycle and logistics; Paul A. Elfers Professor Manos Mavrikakis will use modeling tools to understand the molecular chemistry occurring in plastic recycling; John and Dorothy Vozza Professor Ive Hermans will help develop new catalysts for conversion of plastic oils into the original monomers; Distinguished Faculty Associate Andrew Greenberg will lead the center's educational and outreach activities; and Research Professor William Banholzer will serve as chairperson of CUWP's industrial board.

"This is a team effort that brings together many different people with a range of expertise in chemical engineering, mechanical engineering, and

chemistry to tackle the grand challenges of developing new technology that more efficiently recycles plastic waste," Huber says. "We want UW-Madison to become the global leader in plastic recycling."



#### **ENERGY STAR**

### New control approach helps campuses cope with uncertainty



Victor Zavala

The central utilities plant is the industrial heart of a university campus, distributing the electricity, steam, hot water and chilled water needed to run air conditioning systems and research facilities to multiple buildings.

Keeping a plant like that running, however, is enough to boggle the sharpest minds.

Managers must predict future energy needs from all the buildings and decide how much water, natural gas and electricity to buy.

Even tougher to manage are unforeseen fluctuations and events, like a spike in electricity prices or an unexpected cold snap.

Most current control systems don't take these types of uncertainties into account. That's why Ranjeet Kumar, a spring 2020 PhD graduate, and Baldovin-DaPra Associate Professor Victor Zavala designed a new stochastic model predictive control system for central utility plants that takes into account potential disruptions or extreme events.

To understand how to optimize the control system, Kumar modeled the utilities plant of a typical university campus derived from data collected by his industrial collaborator, Milwaukee-based Johnson Controls, which develops control systems for large utility

plants. He then ran simulations to find optimal strategies to maximize efficiency and minimize cost while mitigating energy demands and market uncertainties.

There could be a big benefit to their new method. By incorporating uncertainty into the control system, the stochastic model was able to save about 7.5% on utility costs, which in the case of a large university utility system translates into hundreds of thousands of dollars per year.

The new control system isn't just for universities; large manufacturers and chemical plants that must also balance energy costs and demand could also benefit from the stochastic approach.

Zavala says this research is a great example of industrial cooperation. "One of the things that I like about this particular project is that it shows how industry and academia can benefit from cooperating," he says. "It's nice to highlight the synergy; our collaborator proposed a real-world problem that current control technology cannot solve and it gave us an interesting problem to research. I think it would be nice to keep pursuing those types of collaborations."

## Yin and Graham receive NSF grants to study coronaviruses

Vilas Distinguished Achievement Professor John Yin has received a National Science Foundation Rapid Response Research (RAPID) grant and, along with Steenbock Professor of Engineering and Harvey D. Spangler Professor Michael Graham, an Early-Concept Grant for Exploratory Research (EAGER) to work on projects related to human coronaviruses.

For the RAPID project, Yin and his team will take an ecological view of these viruses to better understand how they enter cells, spread and cause varying immune responses in different individuals.

Most models of diseases like COVID-19 are based on purified virus stock. But in nature, many viruses are not particularly pure. RNA viruses, which include coronaviruses,



John Yin

are sloppy when they replicate themselves, resulting in lots of partial viruses, mutations and other "junk" particles. These are also known as defective

interfering particles and can no longer replicate and spread themselves. They can, however, tie up resources and make it more difficult for an active virus to spread from cell to cell.

Yin and his colleagues plan to find out if these defective interfering particles, documented previously in mouse coronaviruses, exist in human coronaviruses as well. If that's the case, their next step may be to examine how viruses spread as a mixture of active and defective virus strains and how those particles interact with one another and with their host cells.

The EAGER grant will support the development of a new kind of testing for antiviral drugs. In the current gold-standard test, a plaque assay, researchers release a virus onto a dish of cells overlaid with a layer of semi-solid agar to force the virus to spread only to neighboring cells. But Yin, along with former graduate student Ying Zhu, found that by replacing the agar with a thin layer of flowing liquid medium, they could reduce testing time from three to five days to just a day or two and increase the sensitivity.

During this project, Yin will collaborate with Graham to determine the best conditions for testing drugs that may be effective against COVID-19.



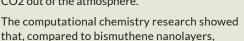
Michael Graham

#### **SEEING GREEN**

## Computational chemistry leads to eco-friendly technology advances

Some of the most exciting advancements in modern chemistry don't require test tubes, bioreactors or even lab coats. In two recent projects Paul A. Elfers Professor Manos Mavrikakis and postdoctoral researcher Roberto Schimmenti collaborated with a multidisciplinary team of researchers, using their computational chemistry expertise to advance emerging green technologies.

In the first paper in the journal *Nature Communications*, the team, including recent PhD graduate Ahmed Elnabawy, analyzed freestanding bismuthene synthesized by researchers at the Changchun Institute of Applied Chemistry in China. The 2D material, only one atom thick, has high potential as a catalyst in carbon capture technology, which traps and converts carbon dioxide emissions into useful chemicals, an important advance to keep CO2 out of the atmosphere.





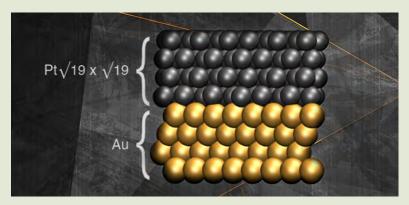
Manos Mavrikakis



Roberto Schimmenti

freestanding bismuthene acted as a superior electrocatalyst for converting carbon dioxide into formate, which has applications as a hydrogen carrier for energy-related technologies.

"The best part of this was the collaboration between experimental and computational work," says Schimmenti. "Atomic-scale insights derived from quantum mechanics guide the materials synthesis community toward making materials with improved catalytic properties."



The second paper, in the journal *Nature Materials*, discusses electro-catalysts which are essential in the development of proton-exchange membrane fuel cells. Fuel cells produce chemical energy in a manner similar to batteries, but they keep working as long as they receive new fuel, often hydrogen. These type of fuel cells could replace batteries in cars, laptops and many other devices in the near future.

One problem with the technology, however, is that the platinum cathodes performing the oxygen reduction reaction in the cells lose platinum over time through dissolution. Collaborators characterized dissolution rates experimentally, whereas Mavrikakis and Schimmenti came up with atomic-scale models that explained how a thin film of gold diminished the dissolution of platinum.

"This increases electrode stability by about 30 times more than scientists have reported in other studies," Schimmenti says. "It basically paves the way for practical and long-term utilization of platinum in fuel cells."

## Building bridges between graduate students and faculty in CBE

Ellen Murray, a sixth-year PhD student in the lab of Paul A. Elfers Professor Manos Mavrikakis, decided to pursue chemical engineering with a belief that it was a way to make a difference in the world.

But Murray isn't just interested in the impact she can make through her research (which involves first-principles modeling to evaluate and design better electrocatalysts and electronic materials, including deposition techniques for producing graphene nanoribbons).

Over the last few years, she's advised the department as an advocate for diversity and women in science. "I hope my research is just a small step in making the world a better place and I think making a better department is part of it," she says.

During her second year at UW-Madison, Murray stepped up when the department asked her to join a committee dedicated to recruiting and supporting women in chemical and biological engineering. Since then, she's expanded her involvement in diversity issues, serving as a representative to the graduate student advisory council where she's worked on issues related to international students, students of color and LGBTQ students.



Ellen Murray

The work has taught her to step back and listen to everyone's experience, and to let them know that people are interested in helping to find solutions to their challenges.

"I feel like everything always comes

down to trying to find more effective ways of communicating the different experiences that everyone has in the department," she says.

Murray says things have definitely changed during her time at UW-Madison. The number of female graduate students in CBE is way up. More and more graduate students are active on the graduate student committee, providing more varied perspectives. And faculty and graduate student representatives meet several times a semester to discuss diversity issues.

"I think if we as a department continue to talk about these sorts of issues and make sure the way we feel about diversity issues is public knowledge, that will help move the needle and help us get to a place where we're more representative," she says.



#### **GOING THE DISTANCE**

#### CBE's Summer Lab doesn't miss a beat in virtual setting

For many students participating in summer lab, it's their chance to put together everything they've learned over the last few years.

But as the reality of the COVID-19 pandemic set in during spring 2020, students and faculty began to wonder if they would be able to pull off the chemical engineering "rite of passage" that has run every summer since 1948.

To adapt, the summer lab team decided it would focus its virtual lab sessions on something almost everyone has: a kitchen.

CBE faculty and staff filled up more than 100 cardboard boxes with goodies for students' kitchen laboratories, including thermocouples, a scale, a pH meter, a total dissolved solids meter, activated charcoal, sand, coffee filters and other items that students might need.

Working in teams, students designed and performed a variety of experiments. Many chose food-science based exercises, working with cookies and cupcakes, sweet potatoes, orange juice, coffee and other items they could grab or order from the grocery store.

"What was really cool is that our students did some really good science," says Faculty

Associate Jim Miller, director of the second session of 2020 summer lab. "There were a number of different, inventive and scientifically rich experiments."

One team built a sophisticated heat exchanger using plastic bottles and PVC tubing included in their box. Others examined heat transport by baking sweet potatoes or analyzed properties of cookies, ice cream and salt.

For the formal experiments, students were presented real data sets from previous summer lab sessions. In all, students report working the same long, intense hours as previous in-person summer labs.

"I thought the professors knocked it out of the park under the online conditions presented to them. They were always available and willing to meet with students to help us with formal and informal labs," says Maggie Pozorski, who participated in the second session of 2020.

Sahana Walter, who participated in the first session, also thinks it was worthwhile. "I think we got a different set of skills than previous graduating classes," she says. "But that's the heart of engineering. Not everything in life is ideal and you have to make do with the resources you're given."

# REU program brings a diverse group of students to campus, digitally, in summer 2020

Duck into any almost any science building on the UW-Madison campus and you'll find laboratories stuffed with busy graduate and undergraduate students. While working on research projects is a big part of the experience at Madison, it's not the case at many small and community colleges, technical schools and even at some larger universities.

That's one reason for Research Experiences for Undergraduates (REU) programs. Each summer, a group of diverse, highly-qualified college sophomores and juniors visit campus to work full time in a lab for 10 weeks while also attending professional development

and STEM seminars. At the end of the session, students present a poster based on their research

In summer 2020, however, the Integrated Chemistry, Chemical Engineering, and Materials Research Experience for Undergraduates program made some big changes to pivot to distance education.

"What we decided to do was focus on professional development and community building, as well as giving them research skills through group research projects," says Distinguished Faculty Associate Andrew Greenberg, director of the REU.

Participants joined one of three research tracks, each facilitated by a graduate student who coordinated the research activities under the mentorship of an experienced faculty member.

Greenberg and his team also significantly increased the professional development curriculum, covering topics including how to read scientific literature, writing NSF fellowship applications and how to look for grad schools.

While he hopes the distance REU experience, which concluded in late-July 2020, was valuable for the participants, Greenberg

says he understands that it can't completely replace time spent in an actual research laboratory.

Still, participants say the experience was worthwhile. "In terms of professional development, the REU program was incredibly helpful," says Jorge Elvis Umana, a senior at the University of Kansas studying chemistry who will soon apply to

graduate school. "Overall, the experience went beyond my expectations and I enjoyed nearly every moment of the REU."



Jorge Elvis Umana



Undergraduates Alex Yost and Abigail Lawrence are recipients of 2020-2021 Wisconsin Idea Fellowships, which support public service projects. Yost is working with Engineers Without Borders to install water treatment equipment in Camarones, Ecuador. Lawrence is part of a team developing a machine to produce biomass briquettes for fuel to help reduce deforestation in Kenya.



Recent PhD graduate Sanjan Gupta is the recipient of an Undergraduate Research Scholars program Exceptional Mentorship Award, which recognizes his work mentoring first- and second-year undergraduates.



Matt Gebbie has been named Conway Assistant Professor and Marcel Schreier is now Richard H. Soit Assistant Professor. Gebbie's research focuses on ionic liquids, which can be used to convert carbon dioxide into fuel and other chemicals and has the potential to replace flammable liquids and acids inside batteries. Schreier studies methods for using electrical energy streams to power chemical transformations.



David Lynn has earned one of 10 Kellet Mid-Career Awards from UW-Madison. Lynn and his research group develop new "soft" organic materials with potential applications in advanced drug delivery, environmental sensing and microorganism control.



CBE graduate alumnus Ole Hassager has won the 2020 Bingham Medal from the Society of Rheology, the highest honor in the field. Hassager is a professor of chemical engineering at the Technical University of Denmark in Copenhagen. He earned his PhD at UW-Madison in 1973, studying under R. Byron Bird, a previous winner of the Bingham Medal.



Remembering Chemical and Biological Engineering Professor Jennifer Reed

On July 5, 2020, Karen and William Monfre Professor Jennifer Reed passed away at age 41 after a protracted struggle with cancer. Reed's passing is a tragic loss for the university and devastating for the colleagues, students, friends and family members who loved and respected her.

After earning her PhD at the University of California-San Diego, Reed joined the department in 2007. Her work focused on modeling microbial metabolism and regulation, quickly earning her many honors, including a National Science Foundation CAREER award, an early career award from the U.S. Department of Energy and the prestigious NSF Presidential Early Career Award for Science and Engineering (PECASE).

She was also a major contributor to the Great Lakes Bioenergy Research Center, a cross-disciplinary center working on the development of sustainable biofuels.

Jay and Cynthia Ihlenfeld Professor Brian Pfleger worked closely with Reed, collaborating on many research projects.

"She was hardworking, creative, brilliant, kind and patient. But most importantly, she was just fiercely strong," he says. "If she wanted to do something, no matter what the obstacle, she was going to get through it and accomplish that goal."

Reed wasn't all about work. She was something of an oenophile and had a passion for cars, liking nothing more than taking her vintage Porsche out for a spin.

Her biggest impact, however, may be on the students she taught and mentored during her career, which earned her several teaching awards.

"Jennie was a gifted teacher who simultaneously challenged and supported her students in the classroom, and an extraordinarily caring mentor to the graduate and undergraduate students in her research group," says R. Byron Bird Department Chair Regina Murphy. "Even in the face of her declining health, Jennie's greatest concern was for the continued progress and success of her students."

Contribute to the Jennifer L. Reed Memorial Undergraduate Research Award at www.supportuw.org/giveto/reedresearchaward



After 30 years in the department, Milton J. and A. Maude Shoemaker and Beckwith-Bascom Professor Thomas Kuech has retired. Kuech, a member of the National Academy

of Engineering and fellow of the American Association for the Advancement of Science, served as department chair twice and has published nearly 500 journal articles covering a broad range of topics in chemical engineering and materials science, including impurity incorporation, ordering, and substrate engineering. He is also a leading innovator in metalorganic chemical vapor deposition, a process used to create complex semiconductors.

But Kuech's contributions go beyond his technical expertise. He held a professorship in the Department of Physics at Nanjing University in China and has served as a visiting fellow at Hong Kong University of Science and Technology. He has also been interested in improving the educational experience of undergraduates, which he's worked toward with the college and department. In retirement, Kuech will continue his research and serve as program director in the National Science Foundation's Division of Civil, Mechanical and Manufacturing Innovation.

#### www.engr.wisc.edu/cbe

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#### Graham Receives Steenbock Professorship

Michael Graham has received the university's prestigious Steenbock Professorship in Engineering.

Graham's research uses theory and computation to study problems in fluid dynamics, rheology and transport phenomena, focusing on microscale flows and complex fluids as well as nonlinear dynamics in turbulent flows. Most recently, he has focused on applying machine learning and data science tools to problems in fluid dynamics.

Graham says he is still determining how he will use his Steenbock funding, but he's confident that it will give him the space to investigate new ideas. "This will allow me to poke around in new directions, which has been really valuable to me in the past," he says.