

# CHEMICAL AND BIOLOGICAL ENGINEERING

YANNE V

# DRIVING INNOVATION

CBE graduate students are taking research in exciting new directions



# **Greetings from Madison!**

Fall is always a vibrant time of year as we welcome new and returning students to campus. This semester, we welcome 35 new graduate students, bringing us up to 114 future PhDs in chemical and biological engineering. In addition, 124 freshman undergraduates will join us for fall 2023.

Our newsletter cover features one of our newest labs: The Krishna Sustainable Catalysis Research Lab led by Duane and Dorothy Bluemke Assistant Professor Siddarth Krishna. The Krishna research group focuses on catalytic technologies that address urgent sustainability challenges, such as producing fuels and chemicals from renewable carbon sources with a lower carbon dioxide footprint, and mitigating emissions that harm human health and climate.

We have made two new and exciting faculty hires: Quentin Dudley and Mai Ngo. These new assistant professors bring great strength to the biological engineering aspects of CBE. Quentin joins us in January 2024. He deploys a unique combination of tools in plant synthetic biology, metabolic engineering and cell-free systems to produce value-added chemicals. Mai, who joins the department in August 2024, brings a proficiency in tissue engineering, cell engineering, mammalian synthetic biology, biomaterials and cell-cell communication to address engineering challenges related to cancer therapy.

In other news, two of our young faculty were awarded named assistant professorships. Please join me in congratulating Rose Cersonsky and Whitney Loo as Conway Assistant Professors. The named professorships will assist in the growth of their research and teaching enterprises.

I look forward to welcoming two of our CBE alumni back to campus this fall to receive College of Engineering distinguished honors: Julie Cameron (BSChE '86), CEO of Excel Scientific, is our department's 2023 Distinguished Achievement Award winner. Julie receives this distinction as a chemical engineer and executive who built and managed myriad product categories with complex chemistries and developed new opportunities for those products across a global marketplace. Brian Gettelfinger (PhDChE '09), digital transformation director for Procter & Gamble, will receive the 2023 Early Career Achievement Award. Brian is honored as a chemical engineer who leverages data science and business intelligence in developing successful consumer products and transforming work processes.

There is one more alumni event before the end of the calendar year! Please join us in December for the last town hall meeting for 2023. More information will follow in late November.

I am pleased to report great progress in the building of our instructional and bio laboratories. We are in the final building phases, and continue to look for partners as we finish up the lab starting in the fall. For more information on partnership opportunities, please see the sidebar on this page.

It's a great time to be a Badger chemical and biological engineer! Thank you for staying connected with the department through our newsletter and our town hall meetings. As always, if there is news and information you'd like to share, please e-mail me at che@che.wisc.edu.

On, Wisconsin!

#### Eric Shusta

Howard Curler Distinguished Professor and R. Byron Bird Department Chair (608) 262-1092 eshusta@wisc.edu

#### **Renovation update**

Shortly before the beginning of our fall 2023 semester, the renovation of B103, CBE's new instructional space in Engineering Hall, was almost complete! The space will be ready to host its first transport labs in spring 2024 and will be ready for the first sessions of Summer Lab beginning in May 2024. Opportunities to contribute to the project are still available.

Naming opportunities for equipment remain, starting at \$50,000. Donors who contribute \$1,000 will be recognized in a physical display in the renovated lab-but we appreciate contributions of any size. All donors will be recognized in a digital display in the newly renovated space.





To learn more or make a gift, contact: Mike Holland Director of Development mike.holland@supportuw.org (608) 440-1178

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Cover photo: Susann Ely.



"Synthetic biology really captured my imagination because it's this evolving discipline. We try to make biology, which is inherently complex, a little messy, and optimized by millions of years of evolution, into a rational engineering discipline."

#### FOCUS ON NEW FACULTY

# Quentin Dudley is engineering plants to produce medicine, fuels and more

Most of today's pharmaceuticals and chemicals are produced from petroleum products or refined from natural materials, often using energy-intensive and costly methods. But as it turns out, we're surrounded by fast, efficient bioreactors that can do the same work.

Plants.

That's why Quentin Dudley, who will join CBE as an assistant professor in January 2024, is engineering plants to produce biomolecules that could be used in medicines, biofuels, plastics, agriculture and many other applications.

"Synthetic biology really captured my imagination because it's this evolving discipline," he says. "We try to make biology, which is inherently complex, a little messy, and optimized by millions of years of evolution, into a rational engineering discipline."

Dudley, who grew up in southwestern Minnesota, earned his bachelor's degree at the University of Nebraska-Lincoln before pursuing his PhD at Northwestern University. There, he helped develop a new approach for prototyping enzyme pathways for metabolic engineering. Conventionally, biological engineers use varieties of microbes such as well-studied E. coli bacteria to synthesize enzymes and useful molecules. However, that means keeping the cells alive, which can be costly and time-consuming. Dudley and his team found a way to use just the bacterial "guts" to produce the enzymes in a much faster process called cell-free protein synthesis.

During his graduate studies, Dudley realized that most metabolic engineering uses sugar as a substrate. That sugar primarily comes from plants. "That inspired me to pivot into doing a postdoc fellowship where I explicitly looked at the plant side of the equation," he says. "Plants are some of nature's most sophisticated chemists. I thought we could take the microbial fermentation step out of the loop and make the compounds we want directly within the plant. That's easier said than done."

Over four years at the Earlham Institute and John Innes Centre in Norwich, United Kingdom, Dudley worked on developing tools for engineering plants to produce valuable bioactive metabolites. One project included producing strictosidine, a precursor to anticancer compounds, in tobacco plants.

He also spent a year leading the analytical chemistry team at the plant synthetic biology company Calyxt, which gave him insights into the industrial side of synthetic biology. For the last year, he's been a field strategist for the nonprofit research organization Speculative Technologies, identifying risky but promising research areas in metabolic engineering for philanthropic investment.

At UW-Madison, Dudley will continue his work in plant synthetic biology. He says he plans to use the cell-free synthesis techniques developed during his PhD to pioneer highthroughput prototyping techniques to speed up the plant engineering process.

The university is a great place for his lab, Dudley says, not only because of its excellent chemical and biological engineering department, but also because of its agricultural roots. "I wanted to be at a university where all of my tinkering in plants could be backstopped by a university full of experts in botany, horticulture and agronomy—so that as we are developing the basic tools, I have the collaborators and community to actually take this into an agroeconomic system," he says. "Wisconsin is a great blend: a strong department with a commitment to synthetic biology and data-driven research, but also just an incredible wealth of equipment, facilities and collaborators in an agricultural space."



# With innovation and determination, grad students drive new plastics recycling applications

Almost everything we buy from the grocery store is packaged in multilayer plastic, with each layer serving a function, such as moisture-proofing or gas-permeability.

While that makes the packaging great at preserving food, it also makes it incredibly difficult to recycle. That's why several labs in CBE are now collaborating on STRAP research through the Department of Energyfunded Center for Chemical Upcycling of Waste Plastics, with graduate students and postdoctoral researchers bringing STRAP much closer to a commercial reality. In STRAP, developed at UW-Madison, individual layers of plastic are dissolved and recovered one by one using a series of solvents.

Panzheng Zhou, a PhD student working in the lab of Hunt-Hougen Associate Professor Reid Van Lehn, PhD students Kevin Sánchez-Rivera, Charles Granger and postdoctoral researchers Jiuling Yu, Euncheol Ra and Tianwei Yan from the lab of Richard L. Antoine Professor George Huber, postdoctoral researcher Aurora Munguía-López from the lab of Baldovin-DaPra Professor Victor Zavala, and PhD student Ugo Ikegwu, co-advised by Van Lehn and Zavala, have all collaborated on several recent projects.

Zhou worked on ways to match the right solvent to the right plastic layer. "We

need to find a suitable solvent system that dissolves our target plastic, but not the other components," Zhou says. "This is challenging because the number of potential solvents is very large."

He developed computational methods to predict the solubility of common polymers found in plastic packaging when exposed to solvents. Zhou created tools that make thermodynamic calculations for eight common polymers, or plastics, exposed to about 1,000 solvents at various temperatures. "With these tools, we could help select solvents that could do the recycling job and suggest the operational temperature of the process," he says.

Led by Yu, a team of researchers looked into STRAP as a way to combat face mask waste. During the height of the COVID-19 pandemic, the world was using 129 billion disposable face masks per month, creating a huge new stream of waste. These masks are made of several layers of plastics, including different types of polypropylene, while the ear loops are made of nylon, polyurethane and polyethylene terephthalate. Because of this mix of plastics, the masks are considered non-recyclable.

The researchers shredded the masks and used a solvent to remove the polypropylene

from the mix. This allowed them to recover about 90% of the plastic resin by weight. They then used a chemical to remove the blue color from the resin, leaving behind high-quality polypropylene with properties and color close to virgin resin.

Sánchez-Rivera, Munguía-López, Zhou and Yu also demonstrated how STRAP can be used to recycle printed multilayer films. Inks are one of the major hurdles for STRAP, since they can complicate the recycling process.

The team first used gamma-valerolactone, a chemical derived from agricultural waste through an environmentally friendly chemical production method, to remove polyurethanebased inks from food packaging. Once the ink was gone, the team could apply STRAP to dissolve each layer of plastic using a specific solvent and reduce the packaging to virgin resins.

According to economic analysis of the process, it is possible to use STRAP to recycle 6,000 tons of printed multilayer packaging per year, with lower emissions than producing virgin plastic.

These latest projects show that, with the right tuning, STRAP could eventually be applied to post-consumer plastic—the enormous amounts of packaging we currently toss in the garbage.



A new understanding of catalysis developed by Manos Mavrikakis and Lang Xu could help tune industrial processes and lead to massive energy savings. Photo: Joel Hallberg.

# Mavrikakis develops new atomic-scale understanding of catalysis

In breakthrough computational chemistry research, Manos Mavrikakis, the Ernest Micek Distinguished Chair, James A. Dumesic Professor, and Vilas Distinguished Achievement Professor, and his colleagues have developed a new model of how catalytic reactions work.

This understanding will allow engineers and chemists to develop more efficient catalysts and tune industrial processes potentially with enormous energy savings, given that 90% of the products we encounter in our lives are produced, at least partially, via catalysis. In fact, just three catalytic reactions—steam-methane reforming to produce hydrogen, ammonia synthesis to produce fertilizer, and methanol synthesis use close to 10% of the world's energy.

In their research, Mavrikakis, postdoctoral researchers Lang Xu and Konstantinos G. Papanikolaou, and graduate student Lisa Je developed and used powerful modeling techniques to simulate catalytic reactions at the atomic scale. For this study, they looked at reactions involving transition metal catalysts in nanoparticle form.

According to the current rigid-surface model of catalysis, the tightly packed atoms of transition metal catalysts provide a 2D surface that chemical reactants adhere to and participate in reactions. When enough pressure and heat or electricity is applied, the bonds between atoms in the chemical reactants break, allowing the fragments to recombine into new chemical products. "The prevailing assumption is that these metal atoms are strongly bonded to each other and simply provide 'landing spots' for reactants. What everybody has assumed is that metal-metal bonds remain intact during the reactions they catalyze," says Mavrikakis. "So here, for the first time, we asked the question, 'Could the energy to break bonds in reactants be of similar amounts to the energy needed to disrupt bonds within the catalyst?'"

According to Mavrikakis's modeling, the answer is yes. The energy provided for many catalytic processes to take place is enough to break bonds and allow single metal atoms (known as adatoms) to pop loose and start traveling on the surface of the catalyst. These adatoms combine into clusters, which serve as sites on the catalyst where chemical reactions can take place much easier than the original rigid surface of the catalyst.

Using a set of special calculations, the team looked at industrially important interactions of eight transition metal catalysts and 18 reactants, identifying energy levels and temperatures likely to form such small metal clusters, as well as the number of atoms in each cluster, which can also dramatically affect reaction rates. Experimental collaborators at the University of California-Berkley confirmed the models.

Mavrikakis says the new framework challenges the foundation of how researchers understand catalysis and how it takes place.

# Making computational research more welcoming for women



In a recent paper in *npj Computational Materials*, Conway Assistant Professor Rose Cersonsky highlighted the barriers women in computational research face and offered suggestions

for making the field more equitable.

While overt discrimination is not as common as it used to be, women in research face implicit bias (unconscious assumptions about the abilities and roles of women scientists), certain behavioral expectations, as well as assumptions about caregiving responsibilities and a lack of role models and visibility for women in science.

The cumulative effect of these issues, which are often interrelated, is an environment in which women in computational materials research, and many other fields, receive fewer citations, fewer grants and awards, fewer networking opportunities, disproportionate workloads and evaluations, and recommendations that comment on their gender and family commitments instead of solely focusing on their work.

To begin addressing these issues, Cersonsky and her co-authors give many suggestions, including developing ways to reform funding and research metrics to help address unconscious bias, developing stronger mentoring programs within the community, finding ways to diversify speakers and presenters, and finding ways to address caregiving that do not stigmatize parents who need flexibility.

"The goal of this work is that hopefully people interested in these issues don't need to look up all these papers themselves," says Cersonsky. "It gives them the resources, the data, the citations, and the articles with which to empower themselves and to fight for improved equitable practices."

## How tweaking cyanobacteria can help keep phosphorous out of our lakes

Excessive heat this summer wasn't just a problem for beachgoers and crops; it also triggered major algae blooms in lakes and rivers in Wisconsin and across the nation. But heat wasn't actually the main culprit in these blooms; the problem was nutrients such as phosphorous, which enters lakes and waterways in runoff, much of which comes from the farmers who apply manure to fields as fertilizer.

When algae take up this phosphorous, it can lead to major algae blooms. Not only do those blooms foul waterways, they also consume oxygen, killing fish and other creatures, and sometimes cause toxic strains of algae to run rampant and sicken people and animals.

In a project led by Baldovin-DaPra Professor Victor Zavala, a team of UW-Madison researchers is developing an alternative system that cuts back on nutrient pollution. By collecting manure and using biological engineering to transform it into a more balanced biofertilizer, they aim to reduce phosphorous—and nasty algae blooms—in our waterways.

"Instead of letting the cyanobacteria grow in the lakes," says Karen and William Monfre Professor Brian Pfleger, "let's grow them in a place where we can control it. Then let's find uses for that material."

The team is designing a system in which manure is first collected and processed to produce concentrated streams of nitrogen and phosphorous. The resulting inorganic nutrients are then fed to specially tuned cyanobacteria in a bioreactor. The cyanobacteria, which Pfleger has developed over the last two years, concentrate nitrogen, phosphorous and other nutrients at different ratios in their cells. Afterward, they're harvested and processed into a well-balanced biofertilizer.

The cyanobacteria are only one part of an overall system. Zavala is modeling pathways to make the whole process technically and economically feasible. That means working with farmers to understand how to efficiently collect and transport manure, determine where to site the manure processing equipment and algae bioreactor, and figure out what types of fertilizer derived from the cyanobacteria would be most useful.





Using chemical processes to recover olefins—a type of simple hydrocarbon—then upcycling them into high-value chemicals like industrial alcohols could reduce petroleum dependence and keep plastics out of the environment. Photo: Joel Hallberg.

# Chemical recycling process adds big value to 'junk' plastic waste

The world is flooded with plastic waste, with few options for recycling much of that material. One emerging method is pyrolysis, in which plastics are heated to high temperatures in an oxygen-free environment. The result is pyrolysis oil, a liquid mix of various compounds. Pyrolysis oil contains large amounts of olefins—a class of simple hydrocarbons that are the central building blocks of today's chemicals and polymers, including various types of polyesters, surfactants, alcohols and carboxylic acids.

With a new technique, however, a research team led by Richarld L. Antoine Professor George Huber, postdoctoral researcher Houqian Li and PhD student Jiayang Wu have developed a method of converting that pyrolysis oil into high-value chemicals. The team estimates its methods could reduce greenhouse gas emissions from the conventional production of these industrial chemicals by roughly 60 percent.

In current energy-intensive processes like steam cracking, chemical manufacturers produce olefins by subjecting petroleum to extreme high heat and pressure. In their new process, the UW-Madison team recovers olefins in the pyrolysis oil and then uses them in a much less energy-intensive chemical process called homogenous hydroformylation catalysis. The process converts olefins into aldehydes, which can then be further reduced into important industrial alcohols.

The recycling industry could adopt the process soon; in recent years, at least 10 large chemical companies have built or announced plans for facilities to produce pyrolysis oils from waste plastics. "Currently, these companies don't have a really good approach to upgrade the pyrolysis oil," says Li. "In this case, we can get high-value alcohols worth \$1,200 to \$6,000 per ton from waste plastics, which are only worth about \$100 per ton. In addition, this process uses existing technology and techniques. It's relatively easy to scale up."

The next step for the team is to tune the process and better understand what recycled plastics and catalyst combinations produce which final chemical products. "There are so many different products and so many routes we can pursue with this platform technology," says Huber. "There's a huge market for the products we're making. I think it really could change the plastic recycling industry."

### **Department News**



Assistant Professor Styliana Avraamidou received the International Society of Global Optimization Young Researcher Award in July 2023.



Assistant Professors Rose Cersonsky and Whitney Loo each were named Conway Assistant Professors to support the early

stages of their research careers. Cersonsky was also selected as one of "35 under 35" tackling challenges in materials research by the journal *Matter*.



Duane and Dorothy Bluemke Assistant Professor Siddarth Krishna received a doctoral new investigator research award from the ACS Petroleum Research Fund in late 2022 for

a project called "Zeolite structural effects on dynamic multi-site interactions in selective heterogeneous olefin oxidation catalysis."



Karen and William Monfre Professor Brian Pfleger received a Vilas Distinguished Achievement Professorship from UW-Madison, which recognizes distinguished scholarship as well

as standout efforts in teaching and service.



Milton J. and A. Maude Shoemaker Professor Sean Palecek received a UW-Madison Kellett Mid-Career Award, which honors faculty for the quality, significance and productivity of

their research.

Several faculty are participating in UW-Madison Research Forward-funded projects.



Richard H. Soit Assistant Professor Marcel Schreier is leading a Research Forward project, "Enabling technologies for industrial electrochemical synthesis." Assistant Professor Styliana Avraamidou is co-Pl.

Victor Zavala, Baldovin-DaPra Professor, is principal investigator on a project called "Accelerating the discovery of electrolyte systems for safe and sustainable energy storage." Conway



Assistant Professors Rose Cersonsky and Matthew Gebbie as well as Hunt-Hougen Associate Professor Reid Van Lehn will serve as co-Pls.

## **Student News**

PhD student Ryan Cashen was named a Langmuir Award finalist at the ACS Colloids and Surface Science Symposium, which recognizes excellence in research, scientific communication and oral presentation.

PhD student Raka Dastidar was chosen for a Richard J. Kokes travel award to attend the North American Catalysis Society meeting in Providence, Rhode Island, in June 2023.

PhD student Beichen Lu was chosen to attend the Next Generation Electrochemistry Workshop, which selects up to 40 advanced graduate students and postdocs to participate in an intense weeklong summer workshop that explores advanced topics in electrochemistry at the University of Illinois, Chicago.

PhD student Hrishikesh Tupkar was selected for the highly competitive National Defense Science and Engineering Graduate Fellowship Program.

#### PhD students Carlos Huang-Zhu, Megan Kelly and Elvis Umana and undergraduate Rung Shih were selected for National Science Foundation Graduate Research Fellowships. The prestigious award provides three years of financial support for graduate studies.



#### Greenberg honored for science engagement

Distinguished Faculty Associate Andrew Greenberg was one of two inaugural recipients of the UW-Madison Bassam Z. Shakhashiri Public Science Engagement Award in March 2023. The award recognizes those who have shown excellence in engaging the public in their work in STEAM research.

The new award is named for Bassam Z. Shakhashiri, professor emeritus of chemistry and the William T. Evjue Distinguished Chair for the Wisconsin Idea, in honor of his "Science is Fun" philosophy and long-term commitment to science education and public engagement.

Greenberg previously served as the associate director of the Institute for Chemical Education (ICE) from 2010 to 2021. In that role, he co-directed the education and outreach efforts of the UW-Madison Nanoscale Science and Engineering Center and helped lead the outreach efforts of ICE.

He designed and currently teaches *Chemical Engineering in the Community*, an outreachfocused course to help undergraduate and graduate students learn to communicate STEM research being conducted in CBE. He leads the education and outreach efforts for multiple NSF projects and for the DOE-funded Center for the Chemical Upcycling of Waste Plastics. He also serves as the education and outreach advisory board member for the NSF National Nanotechnology Coordinated Infrastructure, a national consortium of 16 university nanotechnology cleanroom facilities.

"It is an honor to be selected as a recipient of this award," Greenberg says. "UW-Madison is at the epicenter of STEAM engagement. Faculty and staff at UW-Madison believe in the Wisconsin Idea and the importance of sharing the university and its work beyond campus boundaries." The Department of Energy renewed two biotechnology research centers in which CBE faculty participate. The Great Lakes Bioenergy Research Center, led by UW-Madison in partnership with Michigan State University, received a five-year extension and will receive up to \$147.5 million in funding. Karen and William Monfre Professor Brian Pfleger and Hunt-Hougen Associate Professor Reid Van Lehn serve as co-investigators for the center. GLBRC works on foundational research developing the cost-effective conversion of non-food plants into low-carbon replacements for jet fuel, diesel and other fossil fuels.

Pfleger and Richard L. Antoine Professor George Huber are investigators with the Center for Advanced Bioenergy and Bioproducts Innovation (CABBI), led by the University of Illinois, Urbana-Champaign, which also received a five-year extension. CABBI integrates advances in agronomics, genomics and synthetic and computational biology to increase the value of energy crops, using a "plants as factories" approach to grow fuels and chemicals in plant stems.



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### Ireland hosts its first session of Summer Lab

In May 2023, 12 students traveled to Limerick, Ireland, to participate in CBE's first Summer Lab session on the Emerald Isle.

While the flight only took a few hours, the journey was much longer; in spring 2020, CBE was all set to offer its first Irish Summer Lab session when the COVID-19 pandemic put those plans on hold. In fact, all Summer Lab overseas sessions were suspended indefinitely.

But in 2022, the program began edging back into the international scene, restarting the longstanding overseas session in Oviedo, Spain. This year, the program was ready to finally launch the Limerick session.

Professor Thatcher Root, Summer Lab director, says that Limerick Summer Lab is a unique experience and takes advantage of local resources. "The pharmaceutical industry is quite strong in Ireland and their department is aligned with that," he says. "So, we're hoping our students will get a chance to learn more about pharmaceuticals than they might here."

Rafael Chavez, who led the inaugural session, says that students enjoyed the experience. "The University of Limerick is one of the top universities in Ireland," he says. "The students have less of a culture shock than in other countries because English is the main language spoken there."

They also had a plenty of chances to get out of the lab. "The cultural experiences are very rich in Ireland," says Chavez. "The folk music, dances, sports and rich history of the country, as well as the amazing panoramas in the mountains, the coastline and countryside, provide wonderful opportunities to explore and enrich our cultural awareness."

