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CHEMICAL & ENGINEERING NEWS

JANUARY 8, 2018

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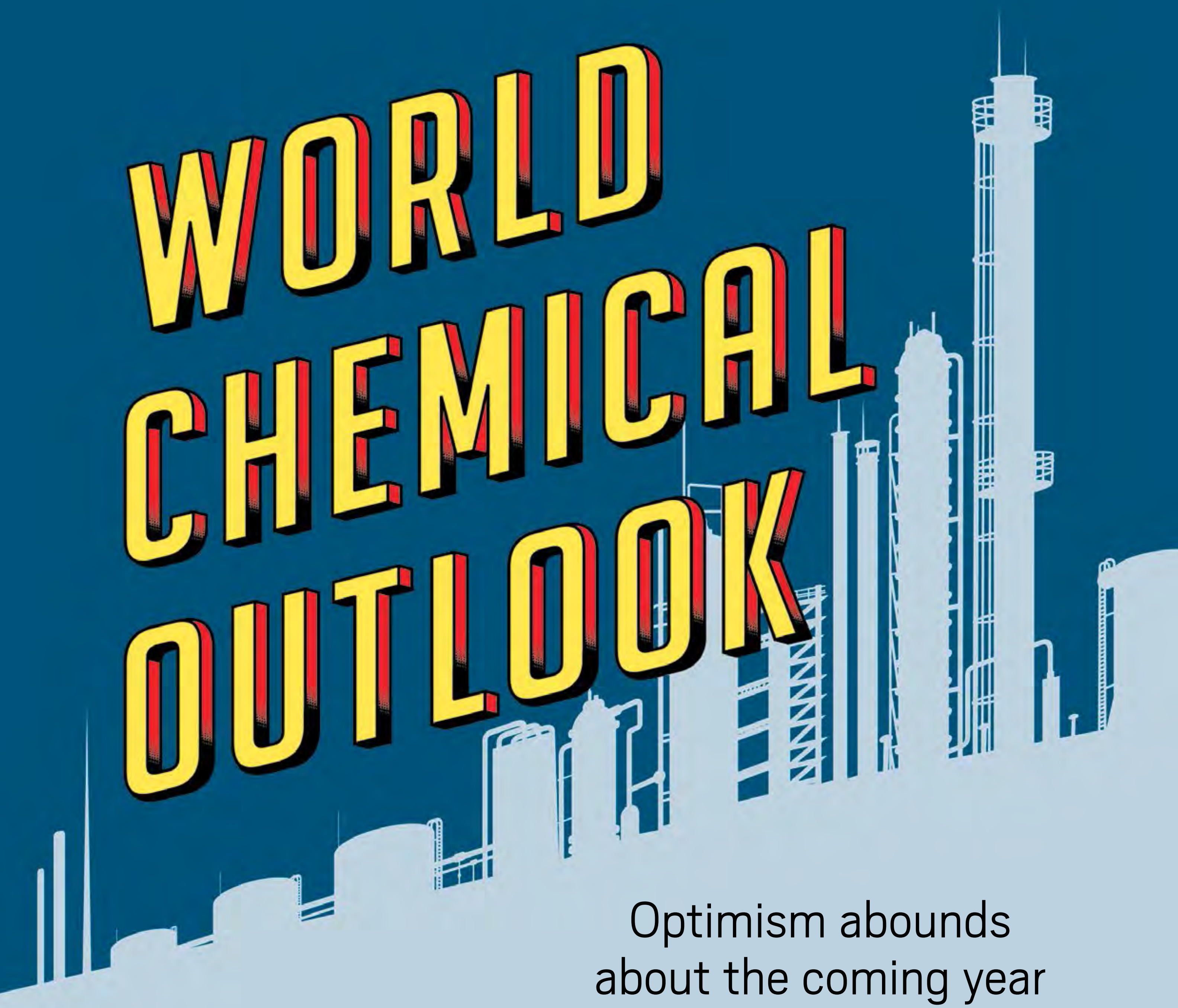

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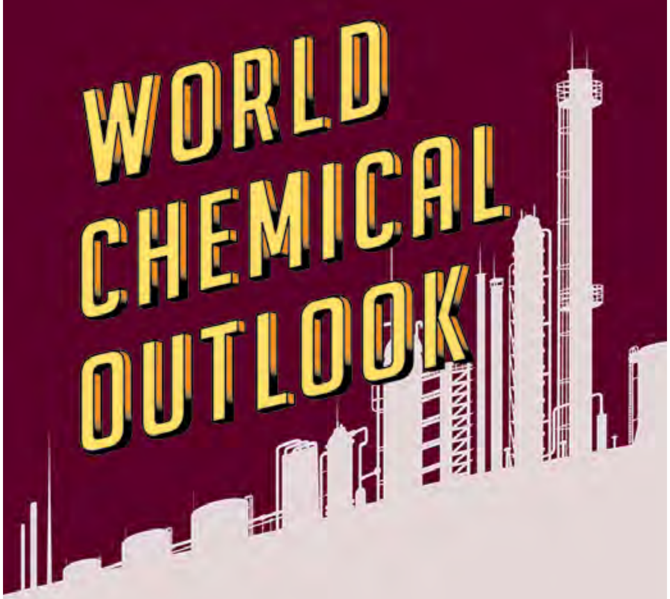

Illustration by Will Ludwig/ C&EN/Shutterstock

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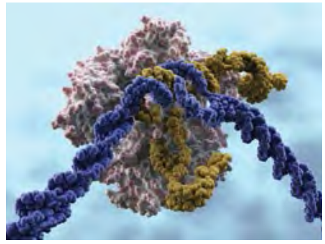

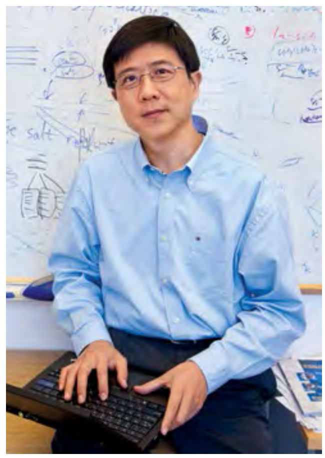

Quote of the week

"If everything works well, a lithium-sulfur battery can store five times as much energy by mass as current lithium-ion batteries."

—**Yuegang Zhang,** professor, Tsinghua University **Page 20**

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Editorial

Happy New Year!

I hope that 2017 was a successful year for all in the chemical sciences and that 2018 comes loaded with opportunities to develop and thrive in the global scientific community.

I'd like to thank you for your continued support of C&EN throughout 2017. It was a very good, if busy, year for us, with lots of activity and many changes to how we have traditionally done things. I'd like you, as readers of C&EN, to be aware of some of what those changes are—in some cases you won't even have noticed them—and understand why they are important. I'd also like to let you know what we have coming up.

We started 2017 with the launch of C&EN Global Enterprise. This new product offers access to a digital version of C&EN's weekly print magazine to thousands of institutions around the world. If your institution has a subscription to ACS journals (ask your librarian), it is likely that you have access to C&EN Global Enterprise. Please do recommend this subscription to C&EN's weekly selection of news and features to colleagues and students who may not yet be ACS members.

Then in May we introduced a new version of C&EN's members-only digital edition. This is the electronic version of the print magazine that we send to members who ask to receive C&EN in their inboxes rather than their mailboxes. This new version is more aesthetically pleasing and has improved functionality and security, which limits the likelihood of unauthorized distribution of our content.

During the summer we undertook an ambitious restructuring of our production processes. This is one of those changes you won't have even noticed. If I can compare it to anything, I'd say that it is like changing a tire while you are still driving your car. Without getting into too much detail, our goal was to replace our print-centric production process with one worthy of a modern, multiplatform media operation. And we achieved that: We are now equipped to publish more content more quickly and efficiently to all our channels.

These new technology and product offerings have been transformative for C&EN. But one fundamental aspect of these activities was that they allowed us to boost the culture of innovation that already existed in the team. In addition to reaching and delighting the widest possible audience, which continues to be priority number one, we want C&EN to remain a vibrant and modern news operation, situated at the cutting edge of publishing technology, and to create exceptional journalism. Last year was a turning point in that sense: Editorial leadership and innovation became our mantra, and there is no turning back.

In this spirit, we have started the year taking measures to make our content more discoverable, more engaging, and more valuable to you. We have just debuted an A/B headline testing tool on cen.acs.org, meaning we'll be able to test multiple headlines for a story and statistically measure which one best captures your attention. Soon we'll also introduce machine learning to power recommended-reading lists on the site. And at the end of February, look for C&EN's first podcast, aptly named "Stereo Chemistry." It aims to be an extension of the reporting that we already do elsewhere but add the voices of our reporters and individuals involved in the stories. You'll be able to find it wherever you get your podcasts, whether via iTunes or voice assistants like Amazon's Alexa. So stay tuned!

This launch will be followed by the redesign of cen.acs.org around the time of the ACS national meeting in New Orleans. Prepare for a better mobile experience, improved navigation, and a vibrant and dynamic look and feel. And this is just the beginning, with better search, personalized features, and so much more to come later on in the year.

Bring on the new year!

Editor-in-chief
@BibianaCampos

Views expressed on this page are those of the author and not necessarily those of ACS.

Concentrates

Chemistry news from the week

Highlights

SUSTAINABILITY

China restricts imports of plastic trash

Move upsets recycling programs worldwide but may lead to better waste management

A Chinese government policy aimed at curbing imports of postconsumer plastic waste went into effect Jan. 1, leaving recyclers in the U.S. and elsewhere without a market for much of their plastic waste and causing material to pile up.

U.S. localities, particularly on the West Coast, have for many years shipped plastics collected in recycling programs to China. Low wages make China an ideal place for the labor-intensive sorting of plastic waste.

According to the U.S. Census Bureau and the U.S. International Trade Commission, China imported 776,000 metric tons of reclaimed plastic and 13 million metric tons of recycled paper from the U.S. in 2016. The total value was $2.3 billion.

China officially notified the World Trade Organization last summer that it would restrict the import of 24 types of waste. It explained that dirty and hazardous substances mixed with plastic and other waste pose a risk to health and the environment.

"This is going to be a huge shock," says Douglas Woodring, the Hong Kong-based managing director of Ocean Recovery Alliance, a group that advocates for improved management of waste plastic. "Not many governments are currently equipped to deal with the huge backup this will create in their waste handling systems."

Recyclers have been trying to prepare for the new rules, which build on an existing import control policy in China called National Sword, for the past few months. By October 2017, imports of waste polyethylene by Hong Kong, a major shipping point, were down by two-thirds compared with a year earlier.

Although the rules don't ban the import of recycled plastics outright, they severely limit the practice by keeping the level of contaminants such as food residue and metals to no more than 0.5%.

"The proposed contamination standard is not practical to achieve, even at the most state-of-the-art facilities in North America," Jeff Murray, international president of the Solid Waste Association of North America, said last month.

Alli Kingfisher, Washington state's recycling coordinator, says materials recovery facilities, which process recyclables from municipalities, are trying to meet the new contamination threshold, hoping to get their plastics into China. But even though they are adding staff, throughput is slowing down, resulting in a pileup.

"They are still collecting as much material as normal, but the facilities are trying to improve quality," she tells C&EN. "They just aren't able to move as much material through."

Some municipalities, particularly in rural parts of the state, have modified residential collection or even halted plastics recycling. However, she says, "most are trying to hold firm."

In Oregon, the pileup has prompted a dozen collectors and processors to ask the state's Department of Environmental Quality (DEQ) to let them dispose of recyclables in landfills, according to Julie Miller, a DEQ materials management official. "DEQ concurs that landfilling these materials on a temporary basis is an unfortunate but needed option," she says.

In October, DEQ issued a bulletin instructing Oregonians to limit the amount of contamination in recycling streams. "Residents are encouraged to continue recycling, but to stop 'wishful recycling,' which is putting an item into a recycling container that doesn't belong, wishing it will be recycled," the agency said.

Despite the short-term repercussions, environmental activists see the new regulations as a long-term win for sustainability. Greenpeace officials in Asia say they will "force many countries to tackle the 'out of sight, out of mind' attitude we've developed towards waste."

Exporting to China has distracted from sustainable waste management, Woodring argues. "The traders got in the way and provided an easy answer to the plastic waste problem," he says.—JEAN-FRANÇOIS TREMBLAY & ALEX TULLO

The Chinese government is severely restricting imports of recycled plastics.

CREDIT: AP

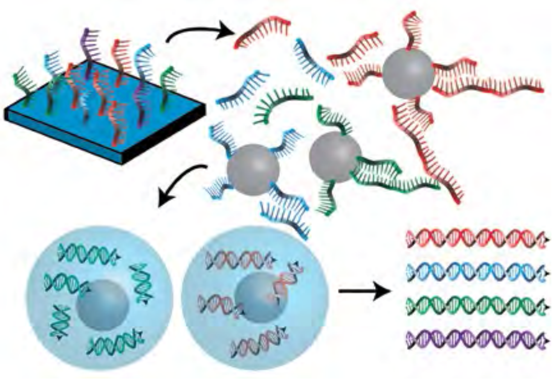
SYNTHETIC BIOLOGY

Stepping up gene synthesis

Emulsions allow multiple genes to be assembled simultaneously from pools of oligonucleotides

Microarray synthesis of DNA oligonucleotides costs a fraction of a penny per base. But such methods can't make pieces longer than about 200 bases. And stitching those oligonucleotide fragments into gene-length sequences typically must be done one strand at a time, losing the multiplex advantage of the array synthesis.

A team led by Calin Plesa, Angus M. Sidore, and Sri Kosuri of UCLA now reports a method called DropSynth that synthesizes multiple genes in parallel from a pool of microarray-generated oligonucleotides (*Science* 2018, DOI: 10.1126/science.aao5167).



Oligonucleotides synthesized on microarrays are captured by barcoded microbeads and enclosed in emulsion droplets, where they are assembled into gene-length sequences.

The researchers design the oligonucleotides so that each piece needed for a particular gene has the same "barcode," or identifying stretch of gene sequence. They then use microbeads tagged with a sequence complementary to that barcode to pull those oligonucleotides out of an oligonucleotide pool.

"Each microbead probably has millions of copies of the barcode," Kosuri says. That means that each microbead will have many copies of each fragment in the gene.

The UCLA team processes the microbeads in a water-in-oil emulsion, with one bead in each emulsion droplet. "The way we generate the emulsion is actually pretty simple," Kosuri says. "You just take an oil and your oligo mixture and vortex it for 30 seconds. You don't need any specialized equipment."

Once in the emulsion, enzymes clip the oligonucleotides from the microbeads. The pieces are assembled into the gene by a method called polymerase cycling assembly, and the resulting genes are recovered from the emulsion. The genes are placed on plasmids containing an assembly barcode. The researchers used next-gen sequencing methods to sequence the assembled genes, using the assembly barcodes to flag genes that were stitched together properly.

The main benefit of the multiplexing approach, Kosuri says, is that a gene pool is now accessible for approximately the same price as an oligonucleotide pool. "We're not adding much to the cost by doing an emulsion assembly," he says.

The method's drawback is that the resulting gene library is "messy," Kosuri says. The efficiency of making any particular gene product is only about 5%.

"I don't think this is going to be the new way that a gene synthesis company might do synthesis, because most users want an exact sequence," Kosuri says. But he does expect DropSynth will allow individual labs to make large libraries of genes. "Say you want to design 1,000 proteins by gene design; you couldn't really synthesize that without lots of money."

"As a field, cost-effective methods for synthesizing DNA—particularly gene-sized DNA fragments—have really lagged behind methods for sequencing DNA. This has been a bottleneck for many areas, but in particular for the field of protein design," says Jay Shendure of the University of Washington. "If this method proves robust, it represents a major advance and will facilitate protein design and many other goals."—CELIA ARNAUD

BIOLOGICAL CHEMISTRY

Food additive boosts pathogen

In the early 2000s, epidemic strains of the bacterium *Clostridium difficile*, which can cause life-threatening diarrhea, began to emerge in the U.S., Canada, and several European countries, and have since spread around the world. But why two virulent types of the bacterium, known as RT027 and RT078, became so prevalent so quickly has been a mystery. Now, researchers led by Robert A. Britton at Baylor College of Medicine believe they have identified a chemical culprit: the disaccharide trehalose.

Britton's team found that both RT027 and RT078 thrive on small amounts of trehalose, a sweetener that retains water and is added to pasta, ice cream, and ground beef. In RT027, a single amino acid change in one protein makes it possible for the bacterium to grow on low levels of trehalose. The researchers also found that improved trehalose metabolism in RT027 leads to higher levels of a *C. difficile* toxin. Independently, RT078 has acquired four different genes that enhance its ability to consume and metabolize the disaccharide (*Nature* 2018, DOI: 10.1038/nature25178).

Scientists had known about RT027 and RT078 long before the outbreaks in the early 2000s, but because of production costs, trehalose was not used as a food additive before that time. A novel enzymatic method for making the disaccharide from starch brought its cost down from around $700 per kg to about $3.00 per kg, and trehalose received approval as a food additive in the U.S. in 2000 and in Europe in 2001.

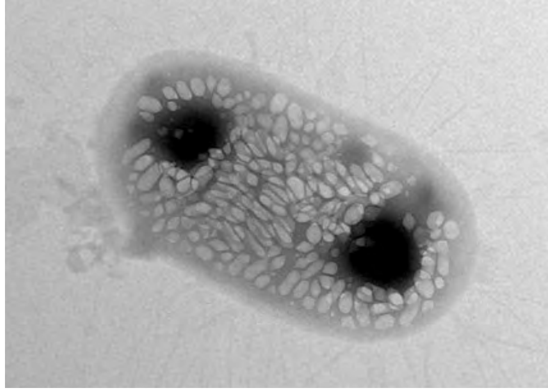
The resulting addition of trehalose to people's diets, the authors believe, has contributed to the deadly *C. difficile* epidemics.—BETHANY HALFORD

CREDIT: COURTESY OF CALIN PLESA & SRIRAM KOSURI

IMAGING

Sound-bouncing bubbles image bacteria in mice

Gas vesicles allow ultrasound tracking of microbes at greater depths than before



Micrograph of an *E. coli* bacterium (about 2 µm long) genetically engineered to express ultrasound-reflecting gas vesicles (light-color structures).

Scientists have engineered bacteria to target tumors to deliver cancer drugs or to travel to the gut to fight off pathogenic strains. To improve such possible microbial treatments, researchers would like to know where the engineered microbes actually go in the body. Currently, the most popular method is to get bacteria to express fluorescent proteins and then track the microbes through their bioluminescence. But bioluminescence imaging works at maximum depths of only a few millimeters below the body's surface, and the technique's resolution degrades quickly with depth.

Mikhail G. Shapiro of Caltech and coworkers have now developed a new ultrasound imaging technique that improves maximum imaging depth to more than 10 cm and substantially enhances spatial resolution (*Nature* 2018, DOI: 10.1038/nature25021).

The inspiration for the technique came from photosynthetic microorganisms that produce protein nanostructures filled with dissolved cellular gases to help them float, allowing the cells to soak up sunlight at the water's surface. The Caltech team discovered that these bubbles also bounce sound waves back to a source. Ultrasound imaging works by detecting sound waves reflected by objects inside the body.

The researchers designed a set of genes from different photosynthetic bacteria and archaea that would allow other bacteria like *Escherichia coli* to produce their own gas bubbles. These bubbles would allow scientists to use ultrasound imaging to spot the microbes in the body.

When the researchers introduced the genes into *E. coli*, the bacteria produced about 100 sound-bouncing vesicles per cell. The vesicles trap a mixture of gases present in the cells, such as oxygen, nitrogen, and carbon dioxide. Slightly changing one of the genes leads to bubbles that respond to sound waves in distinct ways. The researchers exploited such a variation to use ultrasound imaging to distinguish two types of bacteria simultaneously.

Reporter genes for ultrasound is a totally unexpected concept that nobody else in the ultrasound field envisioned before, says Olivier Couture, an expert on ultrasound imaging at the National Center for Scientific Research (CNRS) in Paris. "For animal or even human studies, ultrasound imaging could now observe [products of] reporter genes in bacteria deep inside the body, a vast improvement for the field. Reporter genes are so important in light imaging that we can only dream of what they can do for ultrasound imaging."

Shapiro and coworkers demonstrated the technique by introducing engineered bacteria into the digestive systems of mice. The researchers used an inexpensive ultrasound emitter and detector to image the bacteria in the mouse colon a few millimeters below the skin at about 10 times better spatial resolution than they could with bioluminescence. Ultrasound showed what part of the colon the bacteria occupied, whereas bioluminescence could tell the microbes were in the colon but couldn't localize them further. The researchers also used the approach to track tumor-homing bacteria in mice with cancer.

Caltech has filed patent applications on the technology. "We are now working on imaging bacteria in various diagnostic or therapeutic contexts," Shapiro says, noting that his group also hopes to develop ultrasound reporter genes for mammalian cells, such as in immune cells to track immunotherapy in patients.—STU BORMAN

TISSUE ENGINEERING

Scalable method to make tissue scaffold material

To help restore damaged bone, researchers are developing polymer scaffolds that can be implanted in the body to support the growth of new tissue. Poly(propylene fumarate), or PPF, is one of the few materials available for tissue engineering that is both compatible with three-dimensional printing and can be completely absorbed by the body. But applications for this material have been limited by a lack of production methods suitable for commercial-scale 3-D printing, says Matthew L. Becker of the University of Akron.

Becker's team developed a scalable method to make PPF that involves a ring-opening copolymerization and a functionalized primary alcohol initiator. Using magnesium 2,6-di-*tert*-butyl-4-methylphenoxide as a catalyst, the researchers synthesize poly(propylene maleate), which then isomerizes to produce PPF (*J. Am. Chem. Soc.* 2017, DOI: 10.1021/jacs.7b09978).

Importantly, PPF produced using this method possesses reactive end groups, which engineers could use to attach molecules like peptides that help cells adhere and spread across the surface of a 3-D-printed scaffold. The end groups even survive the harsh conditions of stereolithography—a 3-D printing method that uses light to cure polymer layers—allowing the scaffold's surface to be modified post-printing. The researchers confirmed this property by attaching peptides to small printed PPF discs and observing the growth of mouse cells on the surface.

Unlike traditional step-growth polymerization methods, this new one enables researchers to influence how fast the material degrades in the body by tailoring the polymer's chain length, Becker says.

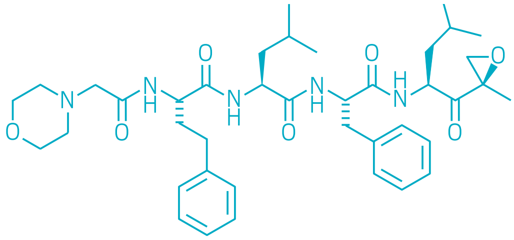
The PPF synthesis technology has been licensed to medical materials company 21MedTech, which Becker cofounded.—KERRI JANSEN

CREDIT: ANUPAMA LAKSHMANAN/CALTECH

ONCOLOGY

Carfilzomib linked to higher cardiovascular risks

Cancer drug increases risk of cardiac problems twofold



Carfilzomib

Multiple myeloma is an incurable type of blood cell cancer. Two decades ago, people diagnosed with the disease lived for about 3–4 years. Now, thanks to new drugs including the protease inhibitor carfilzomib, those affected can survive for 10–20 years. However, since its approval by the U.S. Food & Drug Administration in 2012, people taking carfilzomib have experienced cardiac side effects, as noted on the drug's labeling, but the risk of developing these conditions hasn't been well defined.

A new analysis of data from two dozen carfilzomib clinical trials has determined the incidence of adverse cadiac events such as heart failure, high blood pressure, reduced blood flow, and irregular heartbeat (*JAMA Oncol.* 2017, DOI: 101001/jamaoncol.2017.4519).

The researchers, led by Adam Waxman of the University of Pennsylvania, found that 18% of carfilzomib-treated patients experienced at least one of these events, with 8% experiencing severe to life-threatening events. In three of the large, randomized trials, compared to people with myeloma not taking the drug, those taking carfilzomib were twice as likely to suffer from a cardiac event.

Treating patients with severe diseases like multiple myeloma requires a constant balance between risks and benefits, says C. Ola Landgren, an oncologist at Memorial Sloan Kettering Cancer Center, and unfortunately, all current treatments for the disease are associated with serious side effects such as pain, numbness, and organ failure. He points out that survival data were not presented in the new analysis as they were in two recent large clinical trials showing that people receiving combination treatments including carfilzomib lived up to eight months longer than those treated with other drugs.

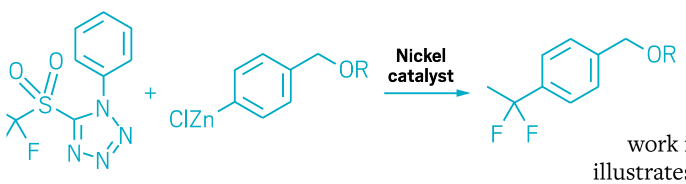
Carfilzomib's high efficacy cannot be understated, Waxman says. He hopes the study will help inform patient-doctor discussions and push them to look for early signs of cardiac conditions. Some of these cardiovasular conditions may be reversible if patients stop taking the drug, and others like hypertension can be managed with medication.—TIEN NGUYEN

CATALYSIS

Sulfones expand the reach of radical cross-couplings

New reagents offer streamlined synthesis of valuable fluorinated products

Cross-coupling reactions, wherein a catalyst brings together molecular partners to forge a new bond, are powerful transformations that are among the most used tools in synthesis. For decades, researchers have mined this area of chemistry, developing methods for a litany of coupling partners. Now chemists have found a novel, and valuable, pairing.



= *tert*-Butyldimethylsilyl

A team of researchers led by Phil Baran at Scripps Research Institute, California, has introduced alkylsulfones as coupling partners for radical cross-coupling reactions, providing access to fluorinated structures that would be cumbersome to make with typical alkyl coupling partners (ChemRxiv 2017, DOI: 10.26434/chemrxiv.5715106.v1). Whereas classic cross-couplings conjoin two aryl partners, this type of cross-coupling is particularly well-suited for threading together aryl and alkyl partners.

With the help of a nickel catalyst and bipyridine ligand, the reaction couples arylzinc compounds with special alkylsulfone reagents. The researchers demonstrated the scope of the reaction with more than 60 examples containing a variety of substitution patterns and by synthesizing biologically relevant molecules to highlight the shortened synthetic routes enabled by the technique.

Notably, the sulfone reagents let researchers directly install fluorine atoms at the alkyl coupling site, whereas previously chemists would have had to run difficult deoxyfluorination reactions to make the requisite fluorinated coupling partner, says Scott Denmark of the University of Illinois, Urbana-Champaign. "The unique reactivity of the *N*-phenyltriazolylsulfones is surpassed only by their practicality as bench stable and odorless, crystalline compounds," he says.

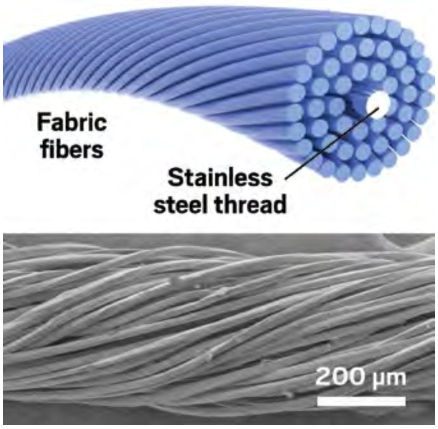
"There is no doubt that this work is going to be game-changing and illustrates that there is still much to do in the field of cross-coupling," say Cathleen Crudden of Queen's University in Ontario and Masakazu Nambo of the Institute of Transformative Bio-Molecules at Nagoya University.

The authors declined to speak with C&EN except to confirm the scientific accuracy of our reporting as per the embargo policies of the journal where they have submitted their manuscript.—TIEN NGUYEN

ENERGY STORAGE

Spinning a triboelectric yarn

To Georgia Tech's Zhong Lin Wang, our daily fidgeting, or even tossing and turning in bed at night, is a possible source of renewable energy. Wang's group has made yarn composed of fabric fibers wrapped around a 50-µm-diameter stainless steel thread that can be woven into brightly colored, washable textiles that generate energy from motion (*ACS Nano* 2017, DOI: 10.1021/acsnano.7b07534). Sewn into clothing, the textiles could harvest enough energy from walking and everyday activities to charge



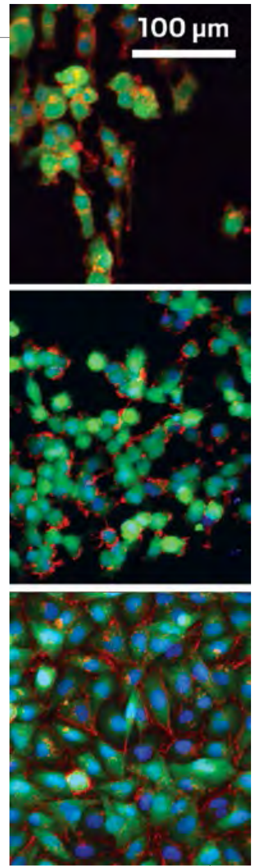
Common textile materials such as cotton and wool can be wrapped around a thin, conductive steel wire to make a power-generating yarn.

cell phones and wearable electronics. The yarn is powered by the triboelectric effect, in which static electricity builds up from the friction between two different materials. When the materials move close together, electrons jump from one to the other. When they move back apart, those electrons flow into either a capacitor to store the charge or a circuit to generate power. As the yarn is stretched and released, the outer layer of fabric fibers—made from polyester, cotton, silk, or wool—moves closer to the stainless steel core, then away again, generating a small electric current. The researchers report that a sock with a textile patch charged a capacitor to 1 V after about 19 seconds of walking. The yarn works at up to 90% humidity, so it can survive heavy sweating. It also withstood 120 cycles through a washing machine, but it's line dry only.—KATHERINE BOURZAC, special to C&EN

3-D PRINTING

Print processing improves popular polymers

Current fabrication methods limit poly(dimethylsiloxane) (PDMS)—a popular material for biomedical applications—to simple device geometries. Veli Ozbolat of Çukurova University, Ibrahim T. Ozbolat of Penn State, and coworkers have found that three-dimensional printing enables fabrication of more complex shapes and at the same time improves the mechanical and cell adhesion properties of PDMS devices compared with standard PDMS casting methods (*ACS Biomater. Sci. Eng.* 2017, DOI: 10.1021/acsbiomaterials.7b00646). The researchers blended two PDMS elastomers to make 3-D-printing inks with desired properties. They then used those blends to print and cast various samples. The samples made by 3-D printing were stronger, stiffer, and less porous than the ones made by casting. The researchers also found that cells adhere better to 3-D-printed PDMS devices than to ones made by casting and that coating the printed surface with the extracellular matrix protein fibronectin further improves cell adhesion. They additionally used infrared spectroscopy of the devices to show that printing doesn't alter the surface chemistry, leading them to attribute the improved cell adhesion to surface roughness imparted by the printing process.—CELIA ARNAUD

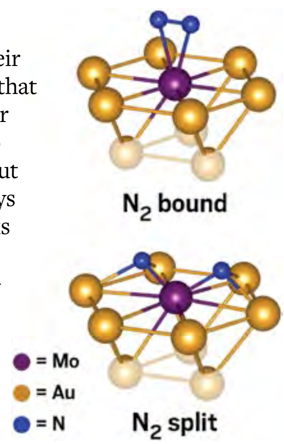


Cells adhere better to 3-D-printed PDMS surfaces, without fibronectin (center) and with fibronectin (bottom), than they do to conventionally cast PDMS surfaces (top).

COMPUTATIONAL CHEMISTRY

Lowering the heat for splitting nitrogen

The world relies on the Haber-Bosch process to reduce atmospheric nitrogen to ammonia to make fertilizer, pharmaceuticals, and other industrially important chemicals. But the process requires high temperature and thereby consumes a tremendous amount of energy—about 1% of the world's electricity every year. A new light-activated catalyst could dramatically reduce the temperature needed to drive the reaction, according to computer simulations (*Sci. Adv.* 2017, DOI: 10.1126/sciadv.aao4710). John Mark P. Martirez and Emily A. Carter at Princeton University have proposed that a gold-molybdenum catalyst could split dinitrogen's triple bond at room temperature using visible light. That dissociation step is the primary limit on the Haber-Bosch process's reaction rate. Their catalyst relies on a phenomenon called surface plasmon resonance, in which the valence electrons on a nanoparticle—made of molybdenum-doped gold in this case—oscillate in unison when excited by a photon. Harnessed correctly, that excitation energy could push the nitrogen dissociation reaction over its high activation energy barrier, Carter says. The researchers evaluated the dissociation reaction for nitrogen in different excited states that are accessible at gold nanoparticle plasmon frequencies (models shown). Their calculations suggest that the catalyst can lower the energy needed to split nitrogen by about 80 to 90%. Carter says plans are in the works to collaborate with Naomi Halas and Peter Nordlander of Rice University to test the predictions.—SAM LEMONICK



CREDIT: *ACS BIOMATER. SCI. ENG.* (MICROGRAPHS); *ACS NANO* (TEXTILES); ADAPTED FROM *SCI. ADV.* (MODELS)

DRUG DISCOVERY

Expansion Therapeutics launches to target RNA

Add Expansion Therapeutics to the growing list of biotech companies developing small molecules that target RNA—the messenger molecule between DNA and proteins. The start-up launched last week with $55.3 million in series A funding.

Disney

Most small-molecule drugs bind to proteins and chemists have shunned targeting RNA for years, due to its floppy structure and the difficulty of designing drugs that selectively target one RNA sequence.

But Matthew Disney, a chemist at Scripps Research Institute in Florida, has been pushing to develop RNA-binding drugs for more than a decade. RNA folds and loops back on itself, creating a three-dimensional structure that small molecules can bind to. "That's something that's still not appreciated," Disney says. To realize the concept, he is launching Expansion Therapeutics along with Kevin M. Forrest, who will serve as the firm's CEO.

The start-up's first focus will be treatments for expansion repeat disorders, a group of about 30 genetic diseases marked by abnormally repetitive strings of genetic code. One such disease, myotonic dystrophy type 1 (DM1), is caused by a repeating CUG sequence in RNA, which is toxic to muscle, heart, and nerve cells.

Disney's lab developed compounds that are able to selectively target the long CUG repeats that cause DM1, while ignoring the CUG bases found in other RNA strands. One version of the potential drug binds CUG repeats to inhibit their toxic actions. Another version binds and cleaves the RNA into pieces.

The company also has earlier-stage programs for discovering compounds that target RNAs related to other diseases. One technique to do this uses a "library versus library" screen that pairs RNA segments with small molecules to find structures that bind regions of folded RNA.—RYAN CROSS

FOOD INGREDIENTS

U.K. firm achieves nitrite-free bacon

There's good news for people whose New Year's resolution is to eat more bacon. This week, the British sausage maker Finnebrogue will introduce bacon rashers made without added nitrites, which have been linked to cancer.

The new English breakfast component will be available only to shoppers in the U.K., who consume, on average, more than 3 kg of bacon per year. Finnebrogue says its Naked Bacon is made with natural fruit and spice extracts.

The firm spent 10 years and $19 million to develop the recipe with the Spanish food ingredients firm Prosur. It claims that the product has beaten the competition in taste tests.

Traditionally, bacon is made in a curing process that uses nitrites or nitrates to preserve it and give it a distinctive flavor, texture, and pink color. During cooking, the additive reacts with secondary amines in the meat to form cancer-causing nitrosamines. The World Health Organization classifies processed meat as carcinogenic because studies show it increases the risk of colorectal cancer when eaten routinely.

Some U.S. brands of so-called natural or uncured bacon rely on natural sources of nitrates such as celery juice or spinach extract, which still form nitrosamines. But that practice is banned in the European Union, Finnebrogue points out. Unlike the U.S. bacon, Finnebrogue's is labeled as "made without nitrites."

"To have a bacon produced naturally, that doesn't require such chemicals to be added or formed during processing, is a very welcome development," says Chris Elliott, chair of the Institute for Global Food Security at Queen's University Belfast.—MELODY BOMGARDNER

DRUG DISCOVERY

Pfizer, Arvinas sign protein degradation pact

Pfizer is the latest company to get in on the swell of interest in small molecules that send problematic proteins to the cellular trash bin. The big pharma firm and Arvinas have established a multi-year protein degradation drug discovery pact worth up to $830 million.

Arvinas launched in 2013 based on technology developed in the labs of Yale University chemist Craig Crews. While conventional small molecules are typically designed to turn off or attenuate the activity of a protein, Crews came up with compounds that cause an unwanted protein to be disposed of altogether.

His bifunctional compounds, called protein-targeting chimeric molecules (Protacs), feature a protein-binding domain and a ubiquitin ligase domain. The idea is to bring a ubiquitin ligase close enough to the protein for it to be tagged for the proteasome, the cell's trash compactor. The Protac then moves on to the next protein.

Pfizer will use Arvinas' technology to work on proteins relevant in multiple diseases. Under the pact, the biotech firm will design molecules and Pfizer will handle their clinical development.

Pfizer joins a cluster of big firms that in the past two years have invested in protein degradation technology. Arvinas also has deals with Merck & Co. and Genentech. Another firm developing protein degraders, C4 Therapeutics, has lucrative pacts with Roche and Calico, Alphabet's life sciences arm.

Novartis, meanwhile, is working on degraders through a collaboration with the University of California, Berkeley, and Boehringer Ingelheim has a protein degradation pact with the University of Dundee.—LISA JARVIS

CREDIT: SCRIPPS RESEARCH INSTITUTE (DISNEY); SHUTTERSTOCK (BACON)

START-UPS

▶ Evonik invests in Danish peroxide firm

Evonik Industries has acquired a minority stake in HPNow, a start-up based in Copenhagen that has developed technology for on-site production of hydrogen peroxide using only water, air, and electric current. HPNow will use the money from Evonik to scale up its technology. Evonik has an annual hydrogen peroxide production capacity of almost 1 million metric tons. "We're an ideal match for HPNow," Evonik says.—ALEX SCOTT

POLLUTION

▶ Dow tackles ocean plastic waste

Dow Chemical is participating in initiatives in Japan and Indonesia aimed at reducing plastic waste in oceans. Working with Tokyo University of Science and the Japan Plastics Industry Federation, and using special video surveillance equipment, Dow has been monitoring the amount of plastic waste flowing through Japan's Edogawa and Ohori Rivers. The program is part of a $2.8 million pledge Dow made to help solve marine plastic waste problems. Separately, Dow is collaborating with Bandung Institute of Technology and Indonesian industry associations to develop roads made with recycled plastic. One trial last year made a 1.8-km road with 3.5 metric tons of plastic waste mixed into the asphalt. —ALEX TULLO

MERGERS & ACQUISITIONS

▶ Frutarom makes it a dozen

The acquisitive Israeli flavors and fragrances maker Frutarom Industries rounded out 2017 with the purchase of Brazil's Bremil Indústria and Poland's Fabryka Substancji Zapachowych Pollena-Aroma, its 11th and 12th acquisitions of the year. Frutarom paid $31 million for a 51% interest in the Brazilian firm, a maker of savory flavors that has annual sales of about $47 million. It paid nearly $9 million for the Polish company, a maker of ingredients for aromatherapy and cosmetics with annual sales of $5 million.—MARC REISCH

INVESTMENT

AkzoNobel to create Dutch innovation park

AkzoNobel is going ahead with plans to convert its R&D and hydrogen peroxide production site in Deventer, the Netherlands, into an innovation park for developers of high-energy chemistry. The move follows the signing of a seven-year agreement by the government of Deventer and the province of Overijssel (of which Deventer is a part) to invest more than $30 million to transform the site. The complex already has space for a small number of technology firms. By the end of 2025, AkzoNobel plans to be able to accommodate 300 people from technology companies, 50 staffers involved in training and education, and 315 of its own research staff. About 270 of AkzoNobel's R&D employees currently work at the site, which boasts safety labs, analytical labs, and pilot facilities for scaling up production. AkzoNobel anticipates that knowledge exchange with the site's future tenants will help it accelerate introduction of its own technologies. Two technology start-ups have already moved to the park. One, Exxfire, focuses on products for fire prevention. The other, Ahrma Holding, develops sensor-equipped shipping pallets.—ALEX SCOTT

BIOBASED CHEMICALS

▶ Clariant, Global Bioenergies sign pact for biobased isobutene

Swiss specialty chemical firm Clariant and French industrial biotech company Global Bioenergies have developed a biobased polymer used to modify rheology in cosmetic creams and lotions. The polymer is made from sugar-derived isobutene, and more than half its carbon is from renewable sources. The two companies say they are working to scale up production at Global Bioenergies' demonstration plant in Leuna, Germany.—MELODY BOMGARDNER

This plant in Leuna, Germany, is producing biobased isobutene for cosmetics applications.

CREDIT: GLOBAL BIOENERGIES

INSTRUMENTATION

▶ Thermo Fisher buys Phenom-World

Thermo Fisher Scientific has acquired Phenom-World, a small Dutch maker of desktop scanning electron microscopes (SEMs). Financial details were not disclosed. Thermo Fisher says the deal expands its line of entry-level and desktop SEMs for materials science, industrial, life sciences, and electronics customers. Thermo Fisher became a significant force in electron microscopy in 2016 when it bought Oregon-based FEI for $4.2 billion.—MARC REISCH

PHARMACEUTICAL CHEMICALS

▶ Navin expands fluorine chemistry site

Navin Fluorine will spend $18 million to expand operations at its site in Dewas, India. The investment will support the manufacture of complex chemicals and fluorinated intermediates used in the pharmaceutical industry in India and abroad, the company says. Navin says it is proceeding with the investment in anticipation of orders for intermediates from customers developing new drugs.—JEAN-FRANÇOIS TREMBLAY

GENE THERAPY

▶ First gene therapy costs $850,000

The first gene therapy to treat genetic disease approved by the U.S. Food & Drug Administration will cost $850,000. Luxturna, from Spark Therapeutics, is designed to partially restore vision in people with a rare form of inherited blindness. The one-time treatment was expected to cost $1 million or more. Spark will offer rebates to insurance companies if patients do not improve in short- or long-term tests of light sensitivity. Spark is also in talks with the Centers for Medicare & Medicaid Services about letting government or commercial drug payers foot the bill in installments.—RYAN CROSS

PHARMACEUTICALS

▶ Mallinckrodt to buy Sucampo for $1.2 billion

Mallinckrodt has agreed to acquire Sucampo Pharmaceuticals, a Rockville, Md.-based drugmaker, for $1.2 billion. With the deal, Mallinckrodt will pick up two approved drugs: Amitiza, a treatment for various bowel diseases with 2016 sales of $456 million, and Rescula, a treatment for ocular hypertension and glaucoma with annual sales of about $9 million. Mallinckrodt CEO Mark Trudeau says the deal also bolsters the company's rare disease drug pipeline with VTS-270, in development for Niemann-Pick disease type C1, and CPP-1X/sulindac, in development for familial adenomatous polyposis.—RICK MULLIN

GENE THERAPY

▶ Pfizer and Sangamo enter gene therapy deal

Drug giant Pfizer will partner with Sangamo Therapeutics to develop a gene therapy for the neurodegenerative disorders amyotrophic lateral sclerosis and frontotemporal lobar degeneration. The therapy will use a zinc finger protein to bind a region of mutant DNA implicated in familial versions of the diseases. When the zinc finger is present, a second protein attached to it shuts down expression of the disease-causing gene. Sangamo will receive $12 million up front and potential milestones of up to $150 million.—RYAN CROSS

OUTSOURCING

▶ European contractors land deals in the U.S.

Siegfried will manufacture for Keryx at this facility in Pennsville, N.J.

Two European manufacturers of active pharmaceutical ingredients have signed supply contracts with U.S. biotech firms. France's Novasep was selected by Tetraphase Pharmaceuticals to manufacture eravacycline, an antibiotic in Phase III development for life-threatening infections. Novasep has supplied early-stage clinical quantities since 2014. Meanwhile, the Swiss contractor Siegfried will supply Keryx Biopharmaceuticals with ferric citrate, the active ingredient in the iron deficiency drug Auryxia. Keryx announced a similar agreement last month with the Canadian firm BioVectra.—RICK MULLIN

BIOTECHNOLOGY

▶ BioNTech raises $270 million

BioNTech, a German company developing mRNA-based therapies, raised a healthy $270 million in its series A funding, led by Redmile Group. The firm's mRNA therapies include vaccines for infectious diseases, cancer immunotherapy vaccines, and mRNA to make therapeutic proteins in the body. BioNTech has also added small-molecule and CAR T-cell cancer immunotherapy programs to its pipeline. BioNTech was founded in 2008 by scientists from Johannes Gutenberg University Mainz. Since then it has established pacts with firms such as Bayer Animal Health, Eli Lilly & Co., Genentech, Genmab, and Sanofi.—RYAN CROSS

Business Roundup

▶ **Agrium** and PotashCorp have completed their merger, creating the fertilizer maker Nutrien. The firm can make up to 25 million metric tons of potassium, phosphate, and nitrogen fertilizers annually.

▶ **Ineos** has made a final decision to build a 120,000-metric-ton-per-year poly(α-olefin) plant in Chocolate Bayou, Texas. The facility, which will mainly serve lubricant markets, is expected to start up during the third quarter of 2019.

▶ **BASF** and Sinopec will double neopentyl glycol capacity at their joint-venture plant in Nanjing, China, to 80,000 metric tons per year. The plant started production in 2015.

▶ **Thin Film Electronics** has sold intellectual property covering printed rewritable memory labels to Xerox. The two firms inked a partnership to produce the smart labels in 2014. Thin Film will receive an up-front payment plus royalties.

▶ **Nippon Shokubai**, PTT, and Mitsui & Co. will study construction of an alcohol ethoxylate surfactants plant at the Hemaraj Eastern Industrial Estate in Rayong, Thailand. PTT produces ethylene oxide, a raw material, at the site.

▶ **Gevo** will cut 40% of the workforce at its headquarters in Englewood, Colo. The biobased chemicals company seeks to improve its cash flow so it can expand its isobutyl alcohol plant in Luverne, Minn.

▶ **Yield10 Bioscience**, a plant science spin-off from biobased polymer firm Metabolix, has raised $14.5 million in a public sale of shares. Yield10 seeks to alter gene activity and carbon flow in oilseeds and rice to improve yields.

▶ **Boehringer Ingelheim** is more than doubling the size of its corporate venture fund to $300 million. The extra money will go toward early-stage companies focused on regenerative medicine, infectious diseases, and immuno-oncology. The cash will also help Boehringer expand its portfolio in the U.S.

CREDIT: SIEGFRIED

A cloud of chlorine gas rose above an MGP distillery in Kansas in 2016 after workers mistakenly added sulfuric acid to a tank of sodium hypochlorite.

BIOLOGICAL CHEMISTRY

▶ NIH allows gain-of-function research on pathogens

The U.S. National Institutes of Health has resumed funding research on how pathogens that cause diseases like influenza and SARS become more deadly, the agency announced last month. Funding was halted three years ago under the Obama administration after a series of safety failures at biosecurity labs raised concern that the research could fall into the wrong hands. With the renewed funding comes a more stringent review process that will weigh the risks and benefits of any research on potentially pandemic pathogens. "I am confident that the thoughtful review process laid out [in the plan] will help to facilitate the safe, secure, and responsible conduct of this type of research in a manner that maximizes the benefits to public health," NIH Director Francis Collins says. The new review process will apply to research on any pathogen that is highly transmissible and likely to cause significant illness or death in humans.—ANDREA WIDENER

INDUSTRIAL SAFETY

Mix-up led to chlorine release at Kansas distillery

The U.S. Chemical Safety Board is recommending changes to chemical transfer procedures and better transfer equipment, including automated and remote shutoff systems, following an accident that released chlorine and sent 140 people to medical centers in Atchison, Kan. The accident occurred in October 2016 when workers inadvertently unloaded sulfuric acid from a tanker truck into a fixed tank of sodium hypochlorite at a distillery owned by liquor and wheat products supplier MGP, CSB says in a report and video. Fill pipelines for the sulfuric acid and sodium hypochlorite tanks looked identical, were only 0.5 meters apart, and were not clearly marked, CSB notes. As a result, 15,141 L of sulfuric acid entered the hypochlorite tank, releasing a toxic cloud of chlorine and other chemicals. CSB says industry figures show similar unloading operations can involve large quantities of chemicals with serious consequences—every 8.4 seconds, 36.2 million metric tons of chemical products were delivered in the U.S. last year. "Facilities need to work collaboratively with chemical distributors to conduct a risk assessment and develop and agree upon unloading procedures," CSB investigator Lucy Tyler says. The board says regulatory gaps did not lead to the accident.—JEFF JOHNSON, special to C&EN

POLLUTION

▶ Three U.S. carbon black makers to clean up emissions

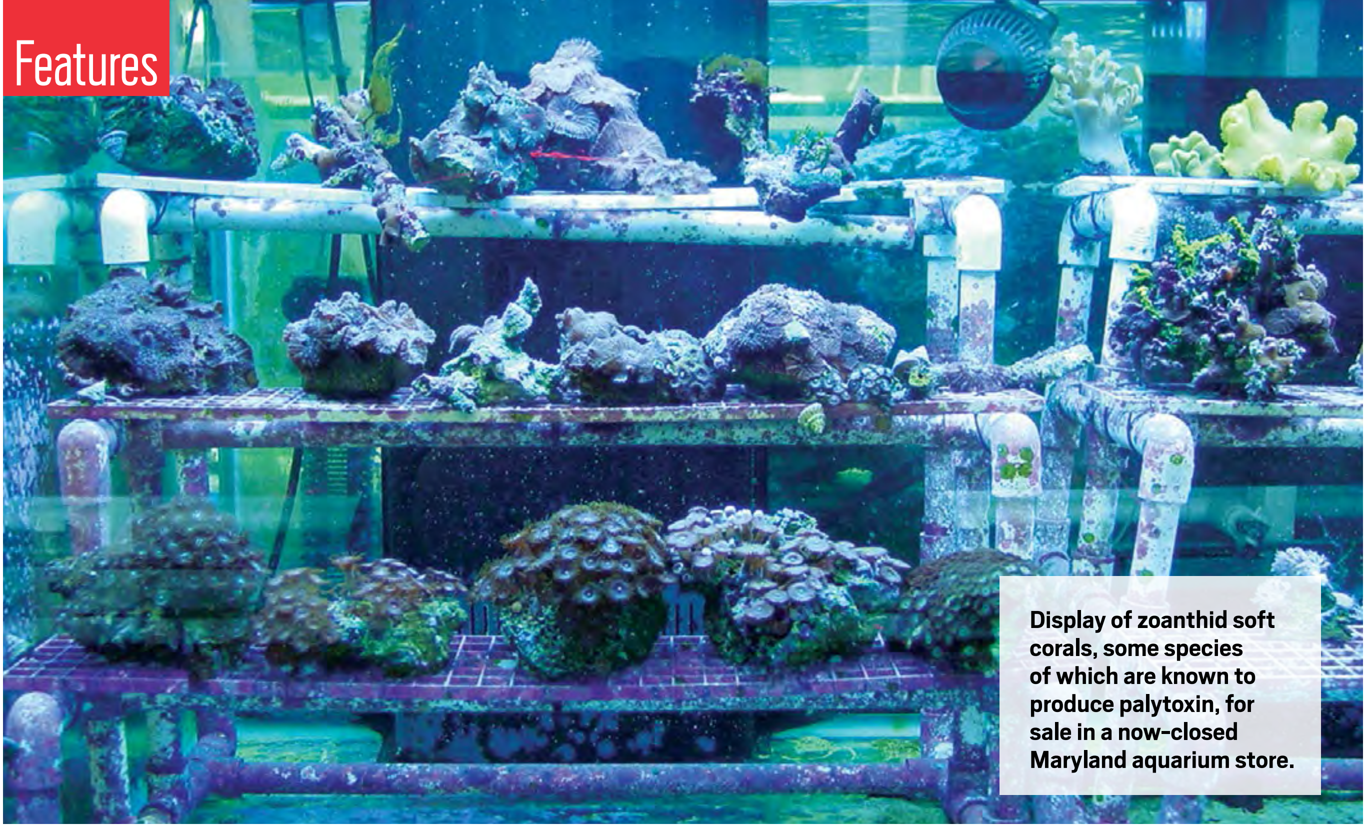
Three U.S. producers of carbon black will collectively pay nearly $2.5 million to settle alleged air pollution violations, the Environmental Protection Agency announced late last month. EPA says the companies failed to obtain needed Clean Air Act permits and did not install required technology to control sulfur dioxide, nitrogen oxides, and particulate matter. For alleged violations at plants in Louisiana and Texas, Sid Richardson Carbon & Energy will pay civil penalties of $999,000 and spend $490,000 to reduce its particulate emissions, its consent decree says. Orion Engineered Carbons will pay a civil penalty of $800,000 and spend $550,000 on installation of pollution control technology at its facilities in Louisiana, Ohio, and Texas, according to its consent decree. Some of Orion's payments will be covered by an agreement that the company has with Evonik, from which Orion bought four facilities in 2011. Columbian Chemicals will pay a civil penalty of $650,000 and spend $375,000 to reduce particulate matter emissions at plants in Louisiana and Kansas, its consent deal says.—CHERYL HOGUE

PHARMACEUTICALS

▶ India's drug security threatened by reliance on imports

Concern is growing among Indian government officials about pharmaceutical companies' dependence on low-cost bulk drug imports, especially antibiotics from China, to meet escalating demand for pharmaceuticals at home and for export. Although India is a key supplier of formulated generic medicines to the world market, it imports bulk active pharmaceutical ingredients from China, the U.S., Germany, Italy, and Singapore. Indian companies can manufacture the compounds in needed quantities, but the compounds can be imported at lower cost, India's minister of state for chemicals and fertilizers, Mansukh L. Mandaviya, told Parliament on Dec. 19. India's draft Pharmaceutical Policy 2017, unveiled by the government in August, says India's dependence on imported drug raw materials and intermediates "has a direct bearing on the drug security of the nation as a whole." To make India's pharmaceutical industry more competitive on cost, companies are seeking corporate tax breaks, cheaper electricity, flexible and simple environmental regulations, faster drug approvals, and antidumping duties on products that are abundant in India.—K. V. VENKATASUBRAMANIAN, special to C&EN

CREDIT: CHEMICAL SAFETY BOARD



Display of zoanthid soft corals, some species of which are known to produce palytoxin, for sale in a now-closed Maryland aquarium store.

CREDIT: JONATHAN DEEDS

TOXICOLOGY

Palytoxin: The danger hidden in tropical aquariums

The massive molecule has been poisoning home aquarium owners

EMMA HIOLSKI, C&EN WASHINGTON

Nature's deadliest chemicals often come in beautiful packages. Take, for instance, the batrachotoxin harbored in the vibrant skins of poison dart frogs, or the cardiac glycosides permeating the glossy green leaves and delicate pink petals of the oleander plant.

Palytoxin, which causes severe respiratory reactions, is no different. The massive molecule comes wrapped in the deceptively alluring package of an anemone-like creature related to coral. An undulating fringe beckons from the edges of flat, green, sunburst discs, hiding the deadly substance within.

In May 2017, a family of seven living near Adelaide, Australia, went to the hospital after one member of the household cleaned the family's tropical saltwater aquarium. The person reportedly removed and scrubbed some rocks or corals from the tank, presumably to remove unwanted, unattractive growths. This cleanup triggered the release of aerosolized palytoxin that caused everyone to struggle to breathe.

These kinds of poisoning incidents are rare, but they are occurring more frequently now that improvements to home aquarium technology have made the care of beautiful and exotic fish, corals, and anemones easier. As more hobbyists are able to master the highly specific water quality, nutrient, and heat requirements needed to keep the tropical critters in good health, the chances of encountering a toxic species—and needing an emergency hospital visit—have edged upward.

A recent survey of the U.S. National Poison Data System revealed at least 171 cases in which people called poison control centers with reports of inhaling or coming into skin contact with palytoxin between 2000 and 2014 (*Environ. Toxicol. Pharmacol.* 2017, DOI: 10.1016/j.etap.2017.08.010). This boils down to nearly a dozen calls per year in the U.S. alone. Most of the incidents—86%—occurred at residences, leading the researchers who conducted the survey to suspect home aquariums as the source.

Still, home aquariums and coral reefs are not the only places where palytoxin lurks. Some species of single-celled, planktonic algae also produce the toxic natural product. Blooms of these algae in the Mediterranean Sea have been known to disperse palytoxin and palytoxin isomers in marine aerosols. Such an event sent more than 200 beach-going tourists along the coast of Italy near Genoa to the hospital in 2005, with about 10% requiring intensive care.

To prevent these harrowing, albeit nonlethal, incidents, scientists and health care professionals alike want to better identify and detect palytoxin and to continue raising awareness of the toxin, especially among home aquarists.

The Mount Everest of chemistry

The history of palytoxin is tied to a Hawaiian legend. Ancient warriors killed a fearsome shark god and scattered his ashes into a tide pool. So deadly was this god that applying "seaweed" from this pool to spear points ensured the death of the warriors' enemies.

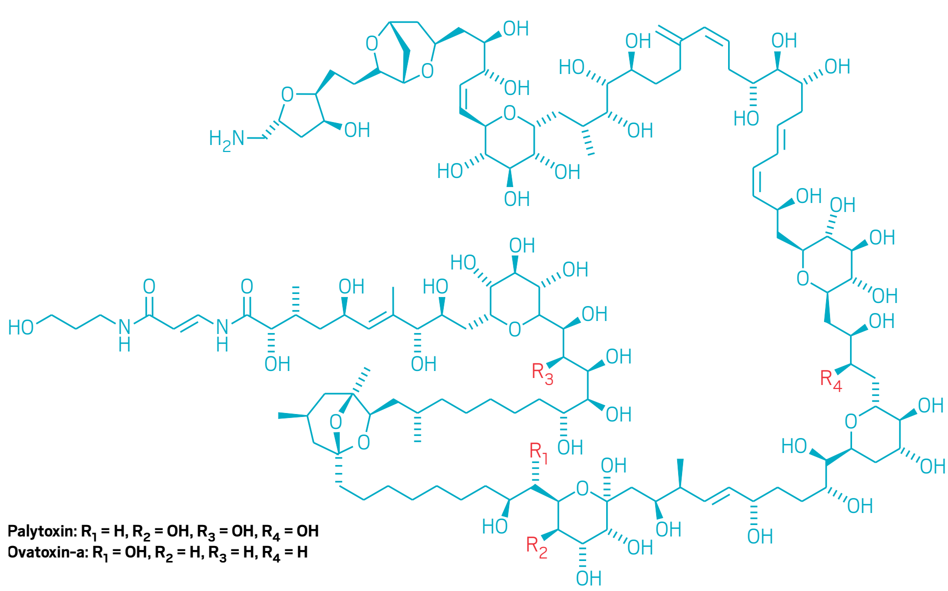
In 1961, a biologist at the Hawaii Institute of Marine Biology came across a mention of this deadly seaweed in a Hawaiian-English dictionary. After learning of the legend, and after a long search, he and a colleague located the tide pool on the island of Maui. There, they discovered an extremely potent toxin produced by a species of zoanthid—a reef-dwelling organism related to corals and resembling a cluster of miniature anemones. The species was later named *Palythoa toxica*.

The discovery of the zoanthid launched a saga of molecular discovery. For a decade, scientists tried to isolate palytoxin, then they labored to elucidate the compound's structure—a feat that took until 1982 to accomplish. Finally, in 1994, a team led by Yoshito Kishi of Harvard University reported a total synthesis of the molecule—more than three decades after its discovery in the tide pool (*J. Am. Chem. Soc.*, DOI: 10.1021/ja00103a065). The team initially synthesized eight pieces of the molecule separately, linking them to form palytoxin carboxylic acid (*J. Am. Chem. Soc.* 1989, DOI: 10.1021/ja00201a038). Then they converted the structure to its final form.

What took so long? Palytoxin is gargantuan, weighing in at 2,680 daltons, and it has a backbone 115 carbon atoms long. It is the longest continuous carbon chain that's been found in nature outside a protein. Containing 64 dissymmetric carbons and six olefinic bonds, palytoxin could have more than 10^{21} possible isomers. A 1989 C&EN story dubbed palytoxin the Mount Everest of chemistry for the monumental effort required to understand and synthesize the devilishly complex molecule.

Despite humans needing more than 30 years to figure out how to cobble palytoxin's components together, a variety of aquatic organisms seem to do so readily. Aside from the subset of toxic *Palythoa* zoanthids, some species of the phytoplankton genus *Ostreopsis* as well as a type of cyanobacteria also synthesize and release compounds from the palytoxin family.

These palytoxin isomers share the same carbon chain structure but have slight variations in the methyl and hydroxyl groups dotted along their backbones. For example, the toxin responsible for the



Palytoxin: R_1 = H, R_2 = OH, R_3 = OH, R_4 = OH
Ovatoxin-a: R_1 = OH, R_2 = H, R_3 = H, R_4 = H

2005 seaside poisoning in Italy, ovatoxin-a, differs from palytoxin in four spots. It's produced by *Ostreopsis* cf. *ovata*. Ostreocins are also toxic isomers of palytoxin and are produced by *Ostreopsis siamensis*. The full suite of these palytoxin-like compounds has yet to be uncovered, and scientists are still working to determine which isomers pose the greatest danger.

"Deadly with an asterisk"

Although scientists still don't know exactly how marine creatures synthesize palytoxin, they do know that it exerts its poisonous effects by binding to sodium pumps on the surface of all cell types in the body. Normally, these pumps push sodium ions out of cells and pull potassium ions in to maintain a healthy balance, or homeostasis. Palytoxin jams the pumps into an open position, flooding cells with sodium and calcium, which ultimately leads to cellular damage and death.

When inhaled, palytoxin acts fast, rapidly constricting blood vessels and triggering asthma- or flulike symptoms. But change a few functional groups on the monster molecule, and it can lose much of its devastating punch.

Modifications at a single chiral center are enough to reduce toxicity, says Aurelia Tubaro, a toxicologist at the University of Trieste. Tubaro began studying palytoxin after the 2005 seaside incident near Genoa. A team of Italian scientists identified ovatoxin-a as the compound responsible and demonstrated that both it and the algae cells producing it could have caused the poisonings by becoming aerosolized (*Environ. Sci. Technol.* 2014, DOI: 10.1021/es405617d). Though palytoxin is 100 times as potent as ovatoxin-a, the isomer can still reach harmful levels in seawater during an algal bloom, Tubaro says.

Despite its extreme toxicity to cells—concentrations as low as 20 pM can injure about half the cells in a petri dish—palytoxin's effects on people are often less harmful in comparison because they encounter the molecule primarily through inhalation or skin contact, says Lauren T. Murphy, a medical resident at Cooper University Health Care in New Jersey. Murphy was the lead author on the 2017 survey of palytoxin-related calls to U.S. poison centers. For palytoxin to exert its characteristic cellular lethality, it must be introduced directly into the bloodstream, a highly unlikely scenario, she says. So, she says, it's "deadly with an asterisk."

Usually, aquarium owners come into contact with palytoxin when cleaning rocks or corals or when transferring them into or out of tanks. A common way to clean rocks—to get rid of nuisance polyps and make space for prettier ones—is by boiling them in water. If a toxic zoanthid is present, palytoxin rises with the steam.

Exposure to the aerosol triggers symptoms that can initially be confused with allergies or the flu: difficulty breathing, runny nose and eyes, and fever. But palytoxin also elevates blood pressure and heart rate and causes tingling sensations in the fingers, toes, and lips. Some aquarium owners exposed to palytoxin have also reported a strong metallic taste in their mouths. Handling live rocks and corals also creates tiny cuts in people's skin, and the presence of palytoxin can lead to skin ulcers or inflammation.

Jonathan R. Deeds, a research biologist with the U.S. Food & Drug Administration, has become the go-to scientist for U.S. agencies—and in some cases international agencies—seeking to confirm the chemical culprit of suspected aquarium palytoxin poisonings. When a request for analysis comes in, he tests water and zoanthid samples from home saltwater aquariums. “It comes in spurts probably about once a year. Sometimes there’s a couple of years where it’s been two or three times,” he says. “It’s usually somebody cleaning their aquarium and poisoning themselves.”

A type of zoanthid soft coral in the *Palythoa* genus, purchased from an aquarium store in Maryland, that contained 500 µg of palytoxin per gram of tissue.

CREDIT: JONATHAN DEEDS

“We just don’t know”

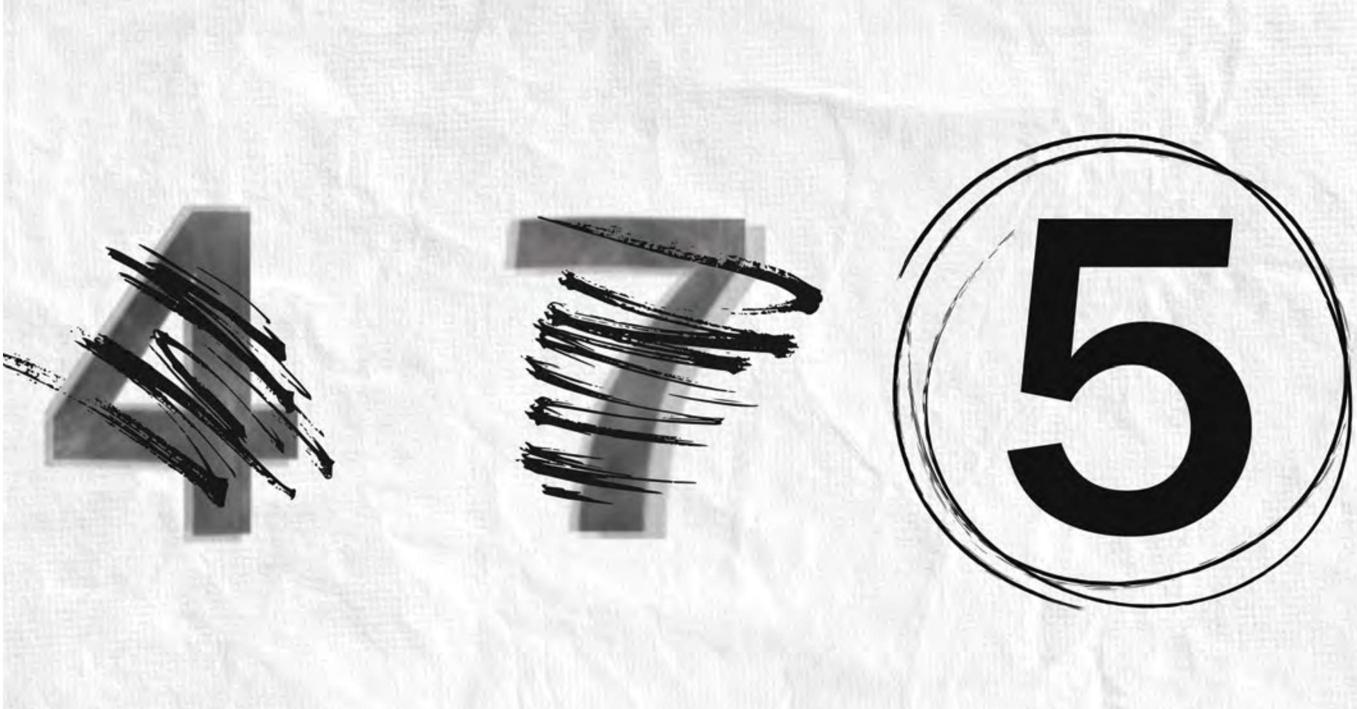
Even though most people exposed to palytoxin inhale the compound, nothing is known about how much aerosolized toxin is required to elicit symptoms. “We can demonstrate exposure from home aquariums, but we can’t show what dose had to get into the human body to cause the effects,” Deeds says. “We just don’t know that yet.”

Part of the difficulty lies in the challenges of quantifying palytoxin and its isomers, especially at the low concentrations that would be found in aerosols. The molecule is large and “very sticky,” according to Tubaro, meaning it gloms on to plastic surfaces, which makes both sampling and analysis difficult. Her group has had success using an antibody- and carbon-nanotube-based electrochemiluminescent biosensor to improve sensitivity over liquid chromatography/mass spectrometry by more than two orders of magnitude (*ACS Nano* 2012, DOI: 10.1021/nn302573c), and the researchers are now developing cheap and rapid assays to use in monitoring seafood and algal blooms.

Deeds also points out that knowledge of how to decontaminate homes after a palytoxin poisoning is woefully thin. “Nobody has done any controlled decontamination studies,” he says. He fields calls from health departments worldwide asking about when it’s safe to allow families back into their homes, he adds. “Wipe everything down with mild bleach is all we know for sure right now.”

As for preventing future exposures, that too is up in the air. Monitoring palytoxin in zoanthids sold for home aquariums doesn’t fall into a clear jurisdiction, Deeds says. FDA regulates only food, and other regulatory agencies monitor traded corals and fish only to ensure that endangered species aren’t involved. No agency is responsible for determining whether a coral or zoanthid species is toxic.

Word of palytoxin’s danger has already spread through online forums and home aquarium hobbyist websites, where users caution against boiling rocks to clean them and recommend wearing gloves and eye protection when handling and cleaning coral and rocks. It’s unclear where to proceed from there, though. “Beyond just putting out information about the risks I’m not sure what the solution is,” Deeds says. ■



CREDIT: WILL LUDWIG/C&EN

INFORMATICS

The drug industry's data integrity problem

A spike in FDA letters citing inadequate data quality at drug plants puts the spotlight on software—and the people who use it

RICK MULLIN, C&EN NEW YORK CITY

As emphasis grows on managing data in pharmaceutical labs and plants—collecting and storing it, sharing it, mining it for pertinence—a basic question often goes unanswered: Is the data any good?

The quality and completeness of data associated with making drugs are, however, huge concerns at agencies such as the U.S. Food & Drug Administration. And drug companies are being forced to pay attention to data in response to a sharp increase in the number of FDA warning letters citing inadequate data integrity.

Quality managers who work on improving the thoroughness and accuracy of data agree that the recent spike in warnings does not reflect a sudden problem with data integrity. It is, they say, the result of industry and regulators coming late to the realization that computer-managed data is in bad shape.

Regulators, in particular, have struggled with the conversion from paper-based to electronic filing, given the difficulty of discovering gaps in experimental data stored electronically. Lab workers, meanwhile, face the question of which data need to be stored in a laboratory information management system (LIMS) and how best to configure all the digital laboratory equipment that feeds data into these systems.

All involved agree that the biggest challenge stems from the human element: the need to adequately train scientists on electronic systems and prevent them from deleting preliminary results that might be of interest to investigators looking for evidence of testing to compliance or flat-out falsifying stored data.

"It's a huge story right now," says Barbara Unger, a former quality and regulatory affairs manager at Eli Lilly & Co. and Amgen who started a data integrity consulting firm in 2014.

Data system remediation projects are under way across the industry—at drug firms and at the contract services firms that manufacture active ingredients and finished drugs for them. Efforts are both time-consuming and costly, Unger says. "And regulatory agencies are aware that it doesn't happen overnight."

FDA, regulators in Europe, and even the World Health Organization stepped up in 2016 with separate guidance documents clarifying requirements under long-standing codes, such as FDA's 21 CFR Part 11 and Part 211, that established the ground rules for electronic data decades ago.

These documents—specifying the need for complete, consistent, and accurate data that indicate safety, identity, strength, quality, and purity of a drug or drug candidate—have also spurred efforts to improve data quality systems and procedures. The scope of the quality of data that regulators require is reflected in an acronym coined by FDA: ALCOA, for attributable, legible, contemporaneously recorded, original or a true copy, and accurate.

Many U.S. drug and drug chemical makers have been lax in initiating data quality programs largely because of a perception that data integrity violations happen overseas, specifically in India. This view was spawned after Ranbaxy Laboratories and a plethora of smaller Indian firms were caught either falsifying or badly transposing lab documentation between 2004 and 2008.

India did lead in FDA data integrity warnings in 2017. But the U.S. was in second, with China close behind.

Indeed, problems in the U.S. made the news at about the same time as the Ranbaxy incident when whistle-blowers alerted FDA about fraudulent data at two drug companies, Leiner Health Products and Able Laboratories, both of which had previously been inspected and received clean bills of health.

Alerted to what to look for, inspectors came back and found sufficient data problems to issue both companies warning letters. Leiner and Able have since gone out of business. And FDA went into training.

"I came at this with the prejudice that it all came out of India," Unger, the consultant, recalls. "But it started in the U.S. and goes back to the 1990s."

The dearth of citations in the U.S. before 2015 and the sharp rise since then resulted from a push by FDA. Spurred by incidents such as those at Ranbaxy, Leiner, and Able, the agency spent several years training its auditors on how to identify problems with computers and work processes that could result in gaps in stored data.

"FDA has taken the lead on this," Unger says. "They started looking far more closely at electronic data capture, approval, review, and archiving mechanisms and at what controls are in place so that analysts can't simply delete data they don't like."

"Based on the increase in warning letters in regard to data integrity, FDA is certainly picking up their inspections, knowledge, and readiness as they go around the world," adds Andrew McNicoll, vice president of quality systems and compliance at Patheon, a provider of manufacturing and other services to the drug industry. Regulators in Canada, the U.K., and elsewhere also have increased their focus on data integrity, he says.

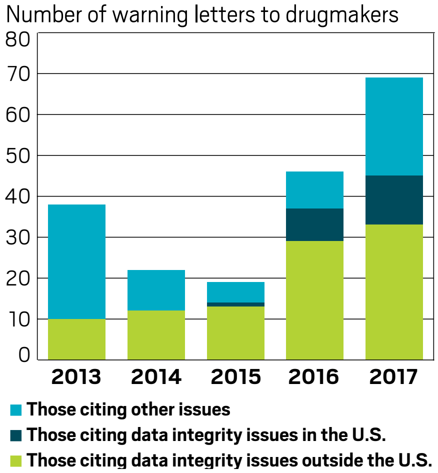
Researchers have obfuscated data on paper since the dawn of research. But redacting data on paper generally leaves a mark. Electronic data that isn't entered into permanent memory, on the other hand, disappears entirely.

Nor are most labs using technology to its fullest potential to manage data integrity, says Monica Cahilly, president of Green Mountain Quality Assurance, a consultancy that has been hired by FDA and other regulators to train inspectors. "This is actually the biggest cause of the uptick in data integrity risk."

Cahilly adds that researchers coming into pharmaceutical labs from graduate school may not realize that eliminating data that doesn't give them the "right answer" compromises an electronic filing. They may also be writing data in paper notebooks and not entering it into an electronic database. The proliferation of stand-alone digital tools, Cahilly says, makes it hard to supervise lab activity and identify researchers in need of training.

Quality alert

FDA's warning letters, especially in the U.S., increasingly cite data integrity issues.



Source: Unger Consulting

Regulators, meanwhile, are on the lookout for data from repeated experiments as an indication of testing to compliance. Lab workers must document why they have made changes that result from necessary repetition. "Truth is an interactive thing," Cahilly says.

Providing compliance-ready data systems has become a competitive front for LIMS vendors and makers of lab instruments such as chromatographs. Most have adapted their systems to support compliance with FDA requirements, Unger says, but success is a matter of effectively implementing these systems in a network with other lab tools.

Heather Longden, marketing manager for informatics and regulatory compliance at Waters Corp., a leading maker of chromatography systems, says the human element, including not only tampering but also system deployment gaffs, poses the greatest threat to data integrity. But she acknowledges that the interconnectivity of chromatography, LIMS, benchtop digital devices, and even financial management software creates a complex data environment and a management challenge.

The integrity of electronic data is further complicated by the enduring preference for paper in laboratories. "We go through laboratories and find that nobody is looking at the electronic data. They are printing it out," Longden says. "They stopped doing that in banking a long time ago."

Longden says Waters's chromatography system, called Empower, has accommodated FDA requirements for data integrity since the agency issued 21 CFR 11 some 20 years ago. The company, she says, spends a lot of time guiding users on implementing the technology. "We are very conscious that just having a tool in your hand is not enough," she says. "You need to know how and when to use it."

LIMS vendors make similar claims. "Our approach is to explain to customers and to auditors how we use our tools," says Trish Meek, director of commercial operations for LIMS at Thermo Fisher Scientific.

Meek notes that problems with data integrity are typically not the result of a technology shortcoming. "If you look at where things fail, it is typically human based," she says. "I think it's really just about understanding the regulations and what needs to be done with system integration and validation with a mind toward ensuring data integrity. People need to be trained on what that is."

Jeff Vannest, senior director of product management at LIMS vendor LabVantage Solutions, says the entry of data into temporary memory is a crux in managing electronic data.

"We spend a lot of our time on behavior, educating the organization."

—**Andrew McNicoll,** vice president of quality systems and compliance, Patheon

Traditional software allows users to delete data entries before saving them, he says. Recent versions of LabVantage's software automatically save data when a user exits a data entry field such as a box in an Excel spreadsheet. The latest version, introduced last year, also queries the user about the reason for changes in data entered.

McNicoll emphasizes the complexity of a problem involving documentation, work practice, and equipment implementation, all of which impact data integrity and all of which are inspected by regulators.

"We spend a lot of our time on behavior—educating the organization," he says. Software developers need to focus on regulators' expectations, he adds, and labs need to keep pace with software upgrades.

Patheon consults with its clients on data management, McNicoll says. "The maturity of programs across the industry varies. Some companies are just embarking; others are further along."

Mark E. Newton, a quality assurance scientist who recently retired from Lilly, is critical of some lab equipment vendors. "Some products don't meet the needs of a regulated laboratory," he says. The biggest problems are at the bench where digital devices on scales, spectroscopy tools, and other equipment do not automatically record data in permanent memory.

"Most of the manipulation of data happens before you get into the big systems such as LIMS," Newton says.

As a result, labs need to design networks that capture required data to stored memory. "We advise configuring systems in which the user cannot see the result of calculations until they save the data they enter," Newton says. This prevents them from omitting differing results from repeated experiments or from flat-out falsifying data.

Drug company quality managers have taken on data integrity collectively through an industry group, the International Society for Pharmaceutical Engineering (ISPE), which recently published its own guidance document for managing data filed electronically with FDA and other agencies.

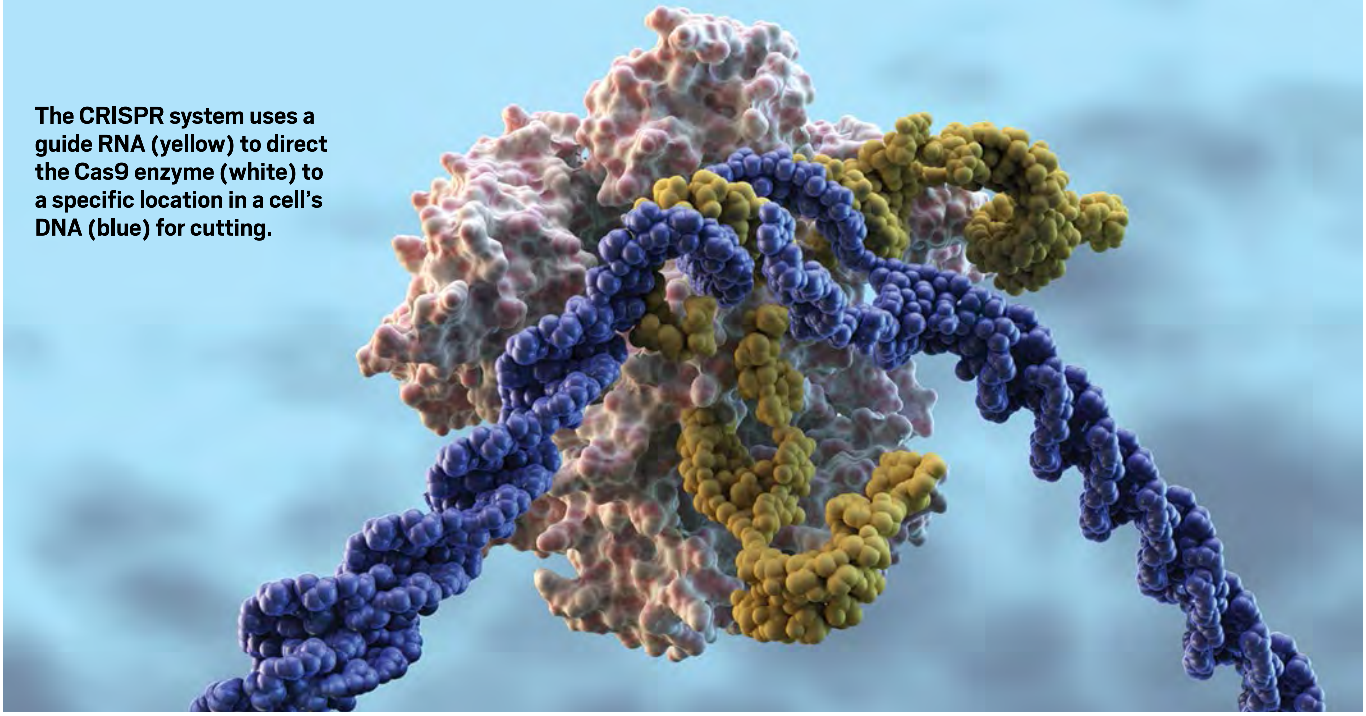
Lorrie Schuessler, computer systems quality assurance manager at GlaxoSmithKline in Collegeville, Pa., is cochair of ISPE's data integrity special interest group. She notes that the current focus on data integrity also results from the geographic dispersal of drug development and manufacturing.

"Studies are no longer done in one place where all the data is generated and analyzed at one point," she says. "It's done all across the globe." This globalization is enabled by computers, she says, but technology can't be relied on to maintain data integrity.

"Technology can only handle so much. There have to be procedures," Schuessler says. "The hope is that systems will get better and technology will support the controls we need, but there will always be human intervention."

Data integrity experts agree that the pharmaceutical industry will be devoting increased resources to systems supporting electronic data and that regulators will keep up the pressure with inspections. "It is an expensive remediation, and it will continue for the foreseeable future," Unger says. "There are some companies who have for the most part done nothing."

Cahilly adds that the cost of maintaining a data system is a crucial consideration. Compliant companies can only get costs down so far. "A site that is falsifying data—or where you go into the lab and instruments are still in their wrappers yet somehow they've got all this 'lab data'—will be able to undercut them on cost all the time." ■



The CRISPR system uses a guide RNA (yellow) to direct the Cas9 enzyme (white) to a specific location in a cell's DNA (blue) for cutting.

BIOTECHNOLOGY

CRISPR comes to the clinic

The first company-sponsored clinical trials of the gene editing system begin this year

RYAN CROSS, C&EN BOSTON

Since its conception in 2012, CRISPR gene editing has spurred headline-making breakthroughs in research labs. In 2018, though, some of CRISPR's biggest firsts are likely to happen in the clinic.

Three biotech firms, each partly founded by one of the three inventors of CRISPR, are gearing up for the first industry-sponsored clinical trials attempting to treat, and potentially cure, genetic diseases. The programs that have recently been garnering the most attention are for two blood diseases: sickle cell and β-thalassemia.

In December, Crispr Therapeutics became the first company to file an application with any regulatory authorities to begin clinical trials for a CRISPR therapy, called CTX001. With permission from European regulators, the trials will begin with β-thalassemia patients this year in Europe, where the disease affects people predominantly of Mediterranean descent.

"It is a momentous occasion for both our company and the field," says Samarth Kulkarni, CEO of Crispr Therapeutics. In the coming months, the firm also plans to ask the U.S. Food & Drug Administration for permission to use CTX001 to treat sickle cell disease, a genetic blood condition more prevalent in the U.S. Vertex Pharmaceuticals will partner with Crispr Therapeutics to develop the drug for both indications.

"I'm hopeful that this is the first in a wave of new treatment options for patients with β-thalassemia and sickle cell disease," says Jacob Corn, a University of California, Berkeley, researcher who has used CRISPR to fix sickle cell mutations in human cells in the lab. Both diseases are ideal for fixing with gene editing, since their precise cause is known: mutations in a gene that makes a subunit of hemoglobin, the protein that carries oxygen throughout the blood.

In sickle cell, the mutation causes normally donut-shaped red blood cells to warp into a crescent shape; the cells get stuck inside blood vessels, depriving tissues of oxygen. β-thalassemia is caused by mutations that prevent the production of fully functional hemoglobin, which for some people can cause severe anemia. Correcting these mutations in a patient's blood stem cells would grant them a perpetual supply of disease-free blood.

CRISPR requires at least two basic components to alter genes: a guide RNA, which carries the code that specifies where to edit a genome, and an enzyme called Cas, which follows the guide RNA to make a cut in a cell's DNA.

Actually changing the DNA sequence, or inserting a new sequence, requires a third component—a DNA template—which has often led to lower rates of successful CRISPR editing. So instead of trying to fix the faulty DNA in sickle cell and β-thalassemia, Crispr Therapeutics is opting for a different approach to boost levels of healthy hemoglobin.

Everyone is born with high levels of a protein called fetal hemoglobin, which is mostly replaced with adult hemoglobin by three months of age—the same time that symptoms of sickle cell and β-thalassemia appear. A gene called *BCL11A* represses

"I'm hopeful that this is the first in a wave of new treatment options for patients with β-thalassemia and sickle cell disease."

—**Jacob Corn,** University of California, Berkeley

CREDIT: CRISPR THERAPEUTICS

fetal hemoglobin production, but a rare genetic mutation in this gene permits fetal hemoglobin production to continue, which effectively counteracts the effects of sickle cell and β-thalassemia mutations.

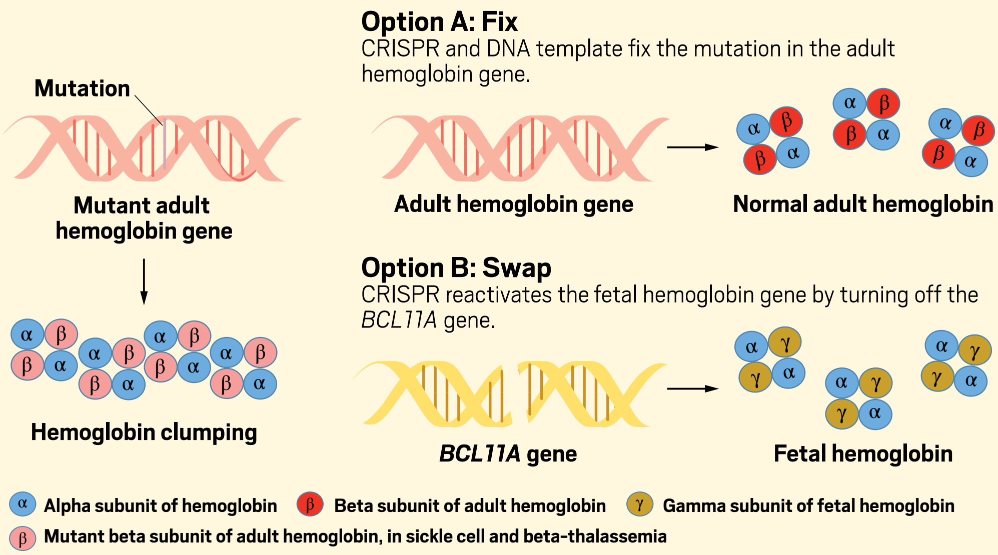
Crispr Therapeutics' lead drug candidate, CTX001, reproduces this mutation's effect. It cuts *BCL11A*, "basically removing the brakes on fetal hemoglobin production," Kulkarni says. The company recently presented results at a hematology meeting showing that its method edited over 90% of blood stem cells removed from patients with β-thalassemia, dramatically increasing fetal hemoglobin in these cells.

Crispr Therapeutics isn't the only company chasing this idea. CRISPR-based Intellia Therapeutics is partnering with Novartis on a similar program. Sangamo Therapeutics and Bioverativ are teaming up to use an older gene-editing technology called zinc finger nucleases to make a break in *BCL11A*. In October, Sangamo received a green light from FDA to commence clinical trials. The company plans to enroll its first subject by mid-2018.

Editas Medicine, another CRISPR company, is working on a potential sickle cell therapy using CRISPR to actually correct underlying mutations in the adult hemoglobin gene. Matthew Porteus, a pediatrician and stem cell biologist at Stanford University, is also developing a clinical trial using this approach.

Repair or replace

Sickle cell disease is caused by a single genetic mutation that creates dysfunctional hemoglobin proteins. CRISPR gene editing can be used to directly repair the mutation in the adult hemoglobin gene. The disease could also be treated by using CRISPR to turn up fetal hemoglobin production, as a replacement for adult hemoglobin.



Editing efficiencies using CRISPR to actually fix a gene used to be very low, just a few percent of cells, Porteus says. "Over the last couple of years, we've twiddled all the knobs," he says, noting that he now sees up to 80% of genes corrected with CRISPR.

The competition to develop sickle cell and β-thalassemia treatments isn't limited to gene-editing. Bluebird Bio, a gene therapy company, has ongoing clinical trials for both conditions using a virus to deliver a healthy copy of the hemoglobin gene into cells. Multiple companies are developing small molecules drugs to help the conditions as well.

"Everyone is working on these diseases because we know exactly what to do," says Stuart Orkin, a hematologist-oncologist at Boston Children's Hospital. "We don't know yet which program will be the best," he says. "But the first one that is shown to be very effective and safe could crowd out the others."

Many people anticipated that the first industry-sponsored CRISPR trial would come from Editas Medicine's program to treat a genetic form of blindness via an injection of CRISPR-filled viruses into the eye. After a delay, the firm now plans to ask FDA for permission to test the therapy in mid-2018.

Crispr, Editas, and Intellia also have earlier-stage programs for diseases of the liver, lungs, muscles, brain, and metabolic system.

But for all the hubbub around the drug company trials, Orkin notes that several Chinese universities began using CRISPR in CAR T-cell immunotherapy trials for cancer in 2016. These therapies involve removing a patient's immune cells, genetically engineering them to target cancer cells, and reinjecting them into the blood.

The University of Pennsylvania also plans to use CRISPR in a CAR T-cell clinical trial, and a large number of preclinical programs in industry could lead to a flood of similar trial announcements in late 2018 or 2019.

Right now, though, CRISPR's spotlight is on genetic blood diseases. Porteus plans to submit an application to FDA for the Stanford clinical trial, which is funded by the California Institute for Regenerative Medicine, in December 2018. Until then, his team will focus on scaling up the CRISPR therapy from a mouse-sized treatment—editing 2 million to 5 million cells at a time—to a human-sized treatment involving 200 million to 500 million cells.

"Is our cupcake recipe going to translate into a wedding cake recipe?" Porteus asks. "It is likely to work, but we have to prove it."

Crispr Therapeutics, meanwhile, has secured a contract manufacturer in Europe that will receive patient blood stem cells, edit them, and ship them back to the clinical trial sites. Patients will then undergo chemotherapy or irradiation in preparation for their edited blood stem cells to be transplanted into the bone marrow, where they will hopefully produce healthier blood cells for life.

A lingering concern in the CRISPR field is the potential for off-target cutting, in which CRISPR accidentally cuts the DNA in the wrong location. Such a cut could result in a new mutation—possibly benign, possibly cancerous. According to Kulkarni, extensive computer prediction, followed by cell and animal testing, led his team to a therapy that has no detectable off-target cutting.

"It is important that they do this very carefully," Orkin says of CRISPR cutting. "Because if there is a mistake or bad effect, it will have repercussions beyond a single patient." It could set the whole field back. ■

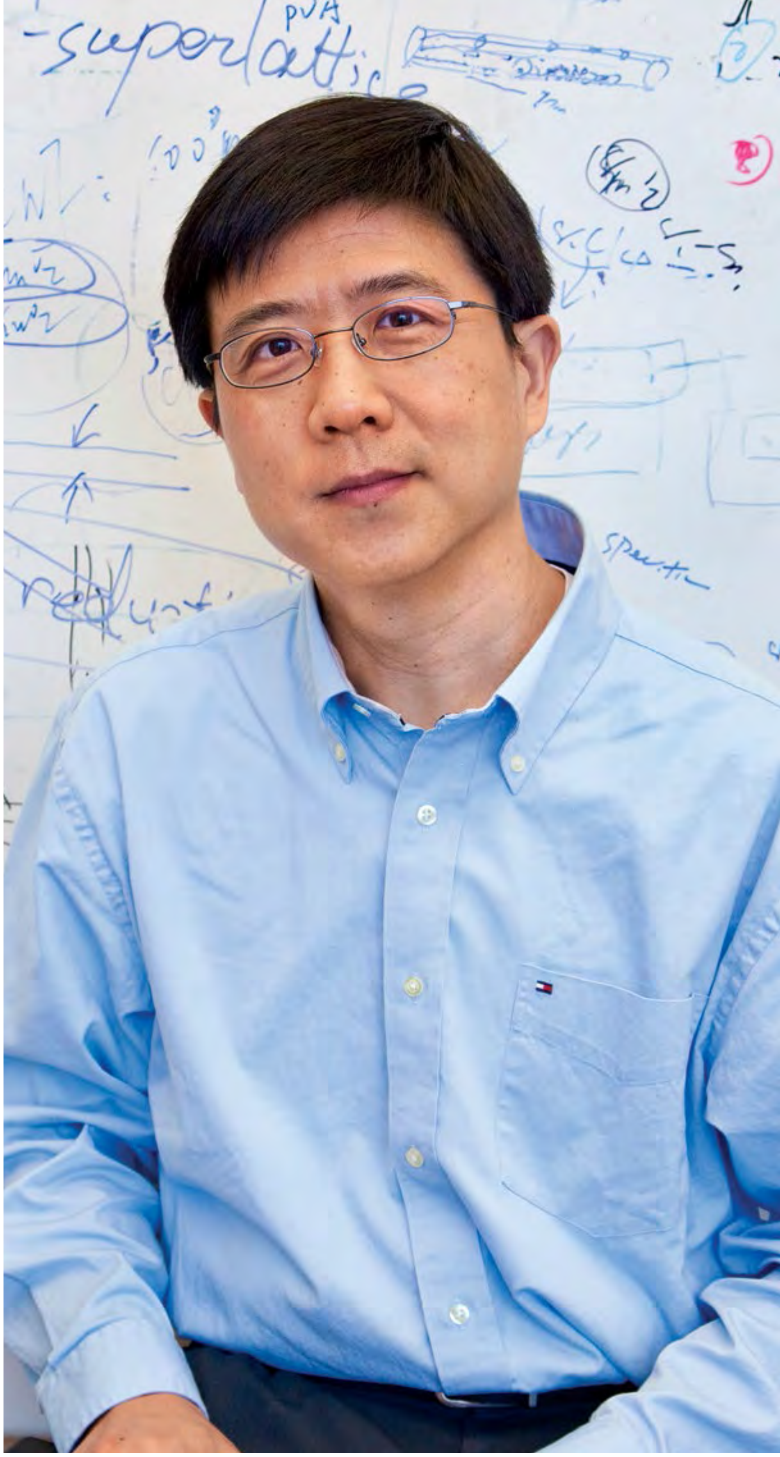
CREDIT: SHUTTERSTOCK/C&EN

ENERGY STORAGE

C&EN talks with Yuegang Zhang, battery troubleshooter

The materials scientist is pushing lightweight lithium-sulfur batteries toward commercialization

KATHERINE BOURZAC, special to C&EN



Yuegang Zhang is determined to make a better battery. The physicist and materials scientist started his career developing new ways to manufacture and use carbon nanotubes. In 2008, while at Lawrence Berkeley National Laboratory, he found himself drawn to perfecting a promising—but challenging—battery technology based on lithium-sulfur chemistry. He tested a variety of carbon nanomaterials to make a sulfur cathode that could pair with a lithium metal anode. In 2012, driven by the desire to commercialize lithium-sulfur batteries for drones and electric vehicles, Zhang returned to his home country of China to start a company. Katherine Bourzac sat down with him to discuss his progress.

Why are lithium-sulfur batteries so promising?

If everything works well, a lithium-sulfur battery can store five times as much energy by mass as current lithium-ion batteries. Because sulfur is lightweight, these batteries have high potential to be used in applications such as drones. And if we increase the lifetime of these batteries to be comparable to lithium-ion batteries, they can also be used in electric vehicles. Let's assume we can keep the size of the battery about the same, but we can double or triple the energy stored. That will extend the mileage of electric vehicles significantly.

Why aren't these batteries in use yet?

For the sulfur cathode, three difficulties prevent its application. One is that sulfur is not conductive; it's insulating. So we have to mix sulfur with conductive carbon. Another thing is that sulfur expands as it takes up lithium ions when the battery discharges. The volume can expand a lot—up to 76%. That requires you to design a cathode that's mechanically stable so it won't pulverize over cycles of charging and discharging. The third challenge is the intrinsic difficulty of the lithium-sulfur chemistry. When lithium ions reach the sulfur cathode, they react to form unwanted compounds like lithium polysulfide. These intermediate reaction products can easily dissolve in most of the organic solvents used in electrolytes, corroding the anode over time so that the battery can store less and less energy.

We handle these challenges with our cathode material design: a careful combination of nitrogen-doped carbon nanostructures that

Vitals

- **Hometown:** Wuhan, China
- **Studies:** B.S., 1986, and M.S., 1989, Tsinghua University; Ph.D., 1996, University of Tokyo
- **Professional highlights:** Researcher, 1996–2000, Nippon Electronics Corp. (NEC); senior researcher, 2002–08, Intel; staff scientist, 2008–12, Lawrence Berkeley National Laboratory; professor, 2012–17, Chinese Academy of Sciences; professor, 2017–present, Tsinghua University
- **Favorite material:** Carbon nanotubes

CREDIT: ROY KALTSCHMIDT/BERKELEY LAB

makes a matrix to hold the sulfur and the polysulfides in place physically and chemically. We build a three-dimensional porous carbon structure by mixing nitrogen-doped graphene and nitrogen-doped carbon nanotubes, cover it with a polymer, and then use low-temperature carbonization to convert this polymer into nitrogen-doped carbon. The polymer acts like solder to hold the nanotubes and the graphene together and improve electrical conductivity. Finally, we load the cathode with sulfur.

Why is now the right time to commercialize this technology?

Before going to Lawrence Berkeley lab, I spent most of my time in industrial laboratories at NEC and Intel, so I know how industry works. I know that to go from the lab to a real product will take 10 years at least. Now it has been about 10 years since we started working on lithium-sulfur. I think it's the time to start working on commercialization of lithium-sulfur; we have solved the scientific problems.

Has moving back to China helped with starting your company?

Wanting to commercialize lithium-sulfur batteries was one of the most important motivations for me to move to China in 2012. I first moved to the Chinese Academy of Sciences. In 2016 I founded my company, Monta Vista Energy Technology, in Suzhou. And this May, I officially joined Tsinghua University in Beijing. Tsinghua has a good atmosphere for commercialization; the university encourages professors to transfer their technologies to market.

Another important factor is that the majority of battery production is now in China. This means there are a lot of battery engineers here, so it is easy to recruit experienced people. We have more chances to exchange information with other battery makers, which helps us transfer our academic R&D into an industrial mode quickly. And we can reach many potential customers in the drone or electric vehicle industry in China. Being close helps us target their needs.

So are lithium-sulfur batteries ready to go on the market?

There are still challenges. Now that we have a good cathode material, we have found a problem on the lithium metal anode side: the pulverization of lithium. When you discharge the battery cell, most of the lithium atoms move to the cathode side. So on the anode side, there's not much lithium left. When you charge the cell, the lithium is supposed to come back to the anode. But this process is not uniform. The ions come back but in some places they don't redeposit on the anode uniformly, so after 30 or 40 cycles the anode is destroyed. We are still working on solutions to this problem.

But we can make a lightweight battery that we can attach to a drone, and it can fly pretty well. Not for a long time, but it can fly.

It sounds like there are problems with these batteries everywhere you turn. Is that exciting for you?

Yes. But now I would say it's getting more interesting. If we're looking at real commercial applications, there are still many problems. But they are engineering problems; they are not scientific problems. I think that they should be solvable, so I'm still very optimistic lithium-sulfur will work.

Katherine Bourzac is a freelance writer. A version of this story first appeared in *ACS Central Science*: cenm.ag/zhang. This interview was edited for length and clarity.

THE FUTURE OF CHEMISTRY: PART NINE

WHAT WILL BE CHEMISTRY'S NEXT BIG THING?

Renowned scientists offer their picks for unsung chemistries that just may change the world.

SPONSORED CONTENT

In 5th-century B.C. Greece, Leucippus of Miletus and his pupil Democritus put forward a new theory stating that all matter was made up of basic units called *atomos*, or atoms. Atoms, they said, were small and indivisible and existed in a constant state of motion within a void. Within this void, they collided, sometimes sticking together and sometimes bouncing off each other. The way they reacted caused changes in matter.

This concept of the atom was largely ignored for millennia. Despite Leucippus and Democritus's extraordinary idea, atomic theory was not confirmed until the work of English chemist John Dalton in the 19th century.

Throughout history, great ideas have been dismissed, ignored, or taken surprising amounts of time to gain traction. Right now, researchers are working on discoveries that will change the world. Will they all get the attention they deserve?

In this final installment of *The Future of Chemistry* series, chemists from around the world name unsung chemistries they believe will be game changers.

Michelle Coote, professor, Research School of Chemistry, Australian National University; associate editor, *Journal of the American Chemical Society*

What? Electric fields as catalysts

Why? The use of electric fields as catalysts is not yet commonplace. The first paper demonstrating the process in a nonredox reaction was published in 2016 in *Nature* (DOI: 10.1038/nature16989). "But I think the potential is enormous and we are just starting to explore it," Coote says. "The timing is also fantastic, as the use of electrochemistry to trigger chemical reactions is also starting to gain traction as a routine tool for organic synthesis."

She believes the use of electric fields as catalysts could have high-tech applications in scanning tunneling microscopes and, on a larger scale, in electrochemical cells. "An exciting prospect is harnessing the fields inside cells to catalyze nonredox reactions taking advantage of high fields in the double layer," she says. "This would be much more scalable."

Exploiting this technique could also be more economical than traditional methods, Coote says. "Electrical fields have a carbon footprint, of course, but don't need to be synthesized or removed from a product later. This is the ultimate in atom economy. Through optimization of field strength and orientation, the regio- and stereoselectivity of a reaction can be improved, making reactions more efficient."

Throughout history, great ideas have been dismissed, ignored, or taken surprising amounts of time to gain traction.

Lili He, assistant professor, department of food science, University of Massachusetts, Amherst

What? Food chemistry

Why? A crucial challenge in future food production will be engineering preservation techniques to reduce food loss during storage, He says. Chemists will develop more effective preservatives, and food chemistry will also transform processing and packaging techniques, she predicts.

For example, active packaging—in which chemical additives interact with contents—will provide additional protection against food spoilage and make shelf life traceable. "This would be greatly appreciated to enhance global food production and security," she says.

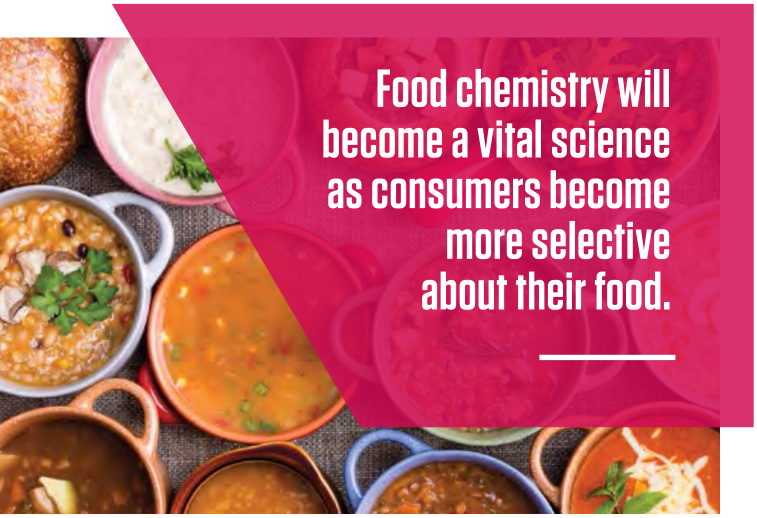
He also argues that food chemistry will become a vital science as consumers become more selective about their food. "We demand natural, organic, non-GMO, low sugar, low salt, and low fat, but the food needs to be delicious and affordable," she notes. As natural additives, such as sweeteners and preservatives, become increasingly desirable, He asserts we'll need good analytics tools for checking purity.

"All these reformulations of our food products require tremendous efforts from our food chemists," she says.

Roald Hoffmann, Frank H. T. Rhodes Professor of Humane Letters emeritus, department of chemistry and chemical biology, Cornell University

What? Synthesis of novel forms of C, CH, and CO

Why? Roald Hoffmann, who co-won the 1981 Nobel Prize in Chemistry for theories on chemical reactions, thinks we need to change the way we think about carbon, graphane (which is completely hydrogenated graphene), and carbon monoxide. "We need good ways to make reasonably pure forms of these [graphane and carbon monoxide] as well as the many calculated metastable allotropes of carbon itself," he says. And, he asserts,



scientists have only scratched the surface of their chemistry. “Reliable calculations show that benzene is not the most stable form of composition CH,” he says, “but a family of graphanes, two-dimensional polymers, is.”

For Hoffmann, though, it’s not the applications of novel forms of carbon, graphane, and carbon monoxide that are crucial, but rather what they’ll contribute to our knowledge of fundamental scientific principles.

Taeghwan Hyeon, SNU Distinguished Professor, department of chemical and biological engineering, Seoul National University; associate editor, *Journal of the American Chemical Society*

What? Crystallization

Why? Crystallization, the process by which liquids and vapors become crystalline solids, is an underappreciated chemistry, Hyeon says. Nucleation, the initial stage when crystal patterns start to form, shows the most promise for future applications.

Apart from abstract thermodynamic models, scientists have a limited understanding of how the atoms and molecules are actually transformed, Hyeon explains. “Although crystallization is the origin of all atomic order and properties of solid state, the microscopic mechanism of atom-by-atom assembly is still elusive and unclear.”

According to Hyeon, crystallization will affect our future understanding of topics as varied as cloud formation, corrosion, drug-particle production, and thin-film fabrication. “Manufacturing of computer chips involves various thin-film fabrication processes, which are basically crystallization processes,” he says. “Consequently, understanding crystallization process, i.e., nucleation and growth, is critical to get high-quality thin films.”

Prashant Kamat, Professor of Science, department of chemistry and biochemistry and Radiation Laboratory, University of Notre Dame; editor-in-chief, *ACS Energy Letters*

What? Chemical bonds and redox states

Why? Kamat believes tailored chemical bonds and redox states will play a pivotal role in future energy storage, helping make energy supplies more reliable and resilient in the face of power-grid threats. Studies have already shown that photoinduced cis-trans isomerization has the potential for energy storage, he explains. “Similarly, oxidized and reduced states of a redox couple have been explored for large-scale energy storage in redox flow batteries.”

Kamat points out that while the amount of energy that can be stored in each molecule is small, collectively, it can be significant. “A more concerted effort is needed to design new molecules that can effectively capture and store light energy, or electrical energy, and deliver it on demand,” he says.

G. Narahari Sastry, group leader, Council of Scientific & Industrial Research, Indian Institute of Chemical Technology

What? Molecular and material composition diagnosis

Why? Sastry predicts that new methods for identifying dangerous and other undesirable molecules in materials will impact areas as varied as security, the environment, food production, and health. Being able to quickly detect molecules used in chemical warfare, explosives, or toxins will greatly improve our quality of life, he explains.

Advanced spectroscopic techniques will be key to identifying the presence of such molecules, he says. Several organizations, including the Organisation for the Prohibition of Chemical Weapons, are already using analytical tools such as nuclear magnetic resonance and mass spectrometry to detect harmful chemicals. Surface acoustic wave detectors, which are devices that separate samples on a membrane and identify agents within them, also have potential. “These efforts, when used wisely and judiciously, will help us to effectively alleviate many bottlenecks in health care, sustainability, and environment sectors,” Sastry says.

His group members are currently looking at how data science and cheminformatics might be used to develop identifiable “fingerprints” for molecules. “While our work is in its infancy, we hope that our computational methods will be of great help in classifying and identifying explosives and chemicals used in warfare.”

THE CHEMOURS COMPANY: **PRECIPITATING THE CONVERSATION**


The Chemours Company's ZERU TEKIE, Global Technical Director, Fluoroproducts (left), and KEVIN LEARY, Global Technology Director, Titanium Technologies (right), look at how collaboration spurs innovation.

Innovation in the chemical industry doesn't happen in a vacuum. It's only through collaboration that the industry can develop cutting-edge applications and products.

We rely on our partnerships with customers to develop and enable market breakthroughs—that's how we uncover and meet their needs. At Chemours, the market, the customer, and our quest for environmental sustainability drive our core research and development, showing us the problems and challenges faced by end users and society.

For example, one thing our customers ask for is new, more efficient ways to generate and store renewable energy. Collaborating with our partners, Chemours has already made progress, reengineering our product Nafion™.

Originally, we developed Nafion™ ion-exchange membrane to help generate energy from fuel cells and to help improve environmental sustainability for the chlor-alkali industry. Now, we've adapted Nafion™ for flow batteries, in which it helps store wind and solar energy, giving us a major boost toward green energy adoption. Advanced flow battery energy storage is also expected to help make power grid management more efficient and cost-effective for utilities.

Our customers also demand improved product performance while reducing the footprint associated with manufacturing the product—a challenge Chemours is willing to meet. Today, we enable our customers to create coatings that last longer and use less paint, thus significantly reducing the amount of energy and materials required to protect structures.

Our industry must also partner with universities to develop a deeper understanding of the science behind our work and to provide new sources of ideas and talent. Such an alliance also helps us in other ways. Few academic institutions today focus on fluoropolymers, for instance. By collaborating with universities, we can help train the next generation of fluoropolymer chemists and engineers, who can help grow our company and advance chemistry itself.

For these reasons and more, Chemours plans to build a new, state-of-the-art research and innovation facility at the University of Delaware's Science, Technology & Advanced Research campus. Scheduled for completion by 2020, the $150 million, 29,000-m^2 facility will employ 330 researchers and help fulfill our quest for innovation.

READ MORE ON HOW CHEMOURS COLLABORATES TO DRIVE INNOVATION AT:
chemours.com/collaborative-innovation

Richard N. Zare, Marguerite Blake Wilbur Professor in Natural Science, department of chemistry, Stanford University

What? Aqueous microdroplets

Why? Tiny water droplets measuring roughly 1 µm, aqueous microdroplets boast special qualities that will bring major advances to chemistry, says Zare (a self-described microdroplet evangelist).

"Droplets can be used in chemical analysis, to understand chemical reactions, and to synthesize chemicals in ways quite different than what takes place in bulk water solutions," explains the 2010 ACS Priestley Medal winner. "We have shown repeatedly that many reactions can be significantly accelerated by carrying them out in microdroplets."

Zare and his team most recently demonstrated this in a paper published in *Angewandte Chemie International Edition* in October 2017 (DOI: 10.1002/anie.201708413). The researchers had previously shown that the addition of water to neat reagents causes an acceleration in chemical reaction rates. Now they've found that in aqueous microdroplets, reactions are further accelerated by a factor of 10^2. "We really do see reactions in microdroplets that are not observed in bulk solution," Zare says.

It even seems water can serve as an environmentally friendly catalyst in some instances, which, he notes, is "not the usual role envisioned for this most common chemical substance."

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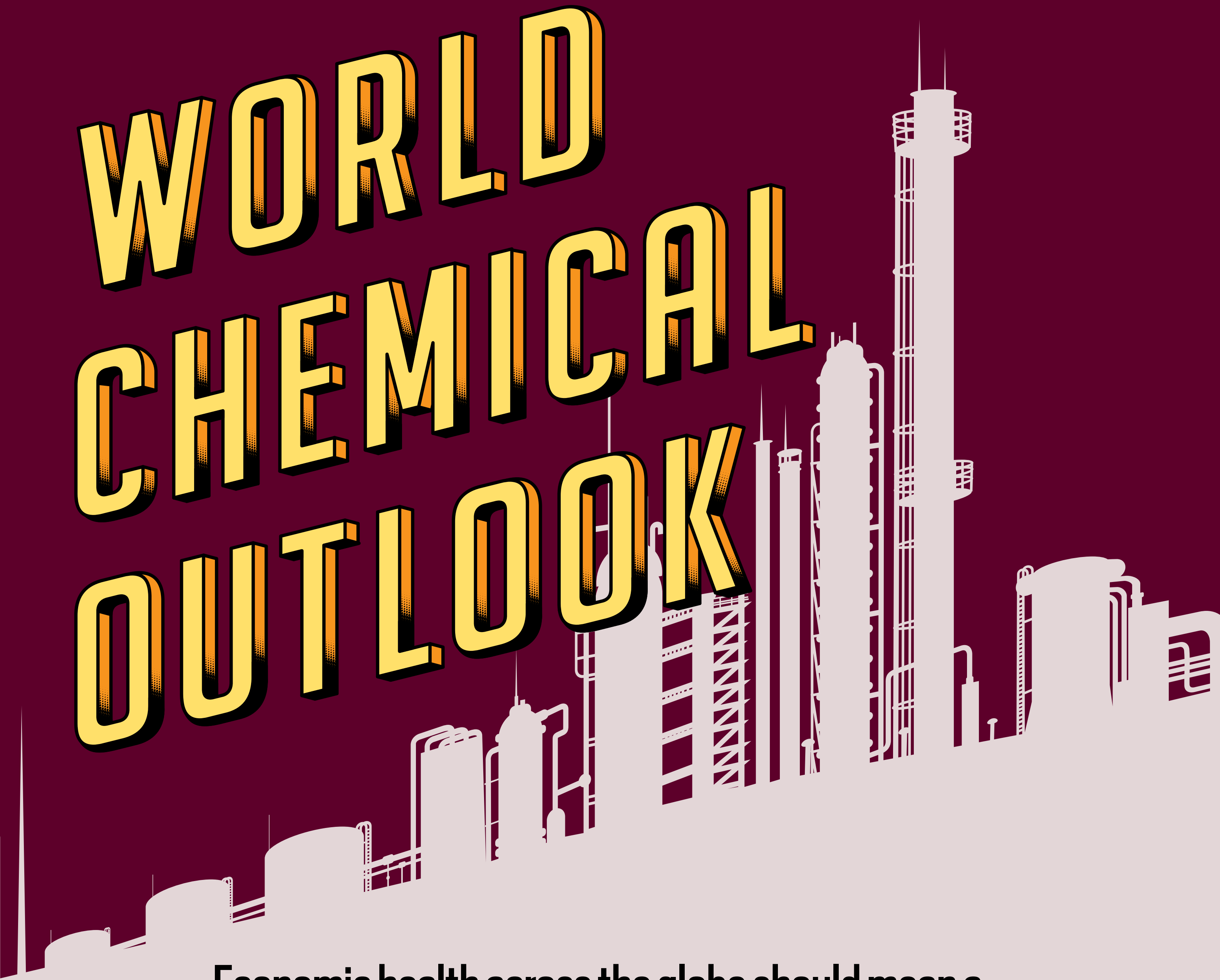
WORLD CHEMICAL OUTLOOK



Economic health across the globe should mean a good 2018 for the world chemical industry

Even when the economic times are good, one region of the globe typically lags. Perhaps Japan is in recession, or Latin America is racked by turmoil, or Europe is struggling with slow growth. But as the calendar flips to 2018, the view is fine pretty much all around. The arrows are pointing up for every economically important country, and the consulting firm PwC predicts that the global economy overall will expand by almost 4%, the fastest rate since 2011. With just a couple exceptions, outlooks for key chemical markets are equally bright. Yes, economies can turn on a dime, but at the moment, 2018 looks to be a very good year for the global chemical enterprise.

CREDIT: WILL LUDWIG/C&EN/SHUTTERSTOCK

ELECTRONIC MATERIALS

Semiconductors are humming, but displays are heading for a fall

The good times will likely keep on rolling for suppliers of semiconductor materials in 2018, at least in the first half. But the display materials market, prone to rapid boom-bust cycles, appears to be heading downward.

"Since demand for DRAM and NAND memory chips remains strong, the first half of 2018 will be good," says Keiji Mihayashi, president of Fujifilm Electronic Materials, which supplies both the semiconductor and display industries. Strong demand for the two types of memory chip is linked to cloud computing, he adds.

Memory chips are a major market for firms like Fujifilm, Mihayashi notes. "High demand for the chips will boost the results of memory manufacturers, and sales of materials will correspondingly be good as well." It's too early to tell what the second half of 2018 will bring, he says.

Lita Shon-Roy, president of the electronic materials consulting firm Techcet, points to other reasons the semiconductor materials market is buoyant. Newly built semiconductor plants in China are boosting demand for materials. And advanced chips are often made using a materials-intensive manufacturing technique called multiple patterning. Meanwhile, supplies of materials remain tight across the semiconductor industry because "producers don't expand capacity just because of one or two good years," Shon-Roy says.

Silicon wafers are in the shortest supply because only a few firms make them. Supplies of high-purity gases and wet chemicals are limited as well. Any unexpected production halt can stress the supply chain, she notes.

The picture isn't so bright for manufacturers of materials used in TVs and other flat-panel displays. The display market is prone to periods of oversupply when large, new plants come on-line, and this is happening now.

"A supply glut is widely expected, which will lead to a decline in panel prices," warns Sang-Ho Kang, display technologies global business director at DowDuPont. "Display materials markets will feel growing price pressure from panel makers."

But newer display technologies will spur both consumer demand and the need for new materials, Kang adds. For instance, the market for organic light-emitting diode displays is small but growing rapidly.

This immersion scanner, made by ASML, is used in multiple patterning, one of several advanced photolithography methods driving demand for semiconductor materials.

And DowDuPont researchers are developing materials for use in foldable displays, which Kang expects to hit the market this year.—JEAN-FRANÇOIS TREMBLAY

RENEWABLES

Paris Agreement sets the global tone

The worldwide fight against climate change took a hit in mid-2017 when the Trump administration pulled the U.S. out of the Paris climate agreement. But the rest of the world—along with 14 states and more than two dozen cities within the U.S.—is moving ahead with policies that put a bull's-eye on carbon emissions.

In December, China kicked off a cap-and-trade carbon market for its energy industry. The market's rules have yet to be announced, but China's need for renewable power will drive a global 20% increase in solar installations this year, the consulting firm IHS Markit predicts.

Meanwhile, the Canadian government is working to impose a carbon tax on provinces that don't meet its standards for reducing emissions.

In the U.S., the new tax legislation preserved key tax credits for the solar and wind industries, which now produce 7% of the nation's electricity. As utilities continue to shutter coal-fired power plants, reliance on renewable sources will rise. The growth of renewables has put a new focus on energy storage, including batteries. The storage market will roughly double in size to nearly 600 MW in 2018, according to GTM Research and the Energy Storage Association.

The New York State Energy Research & Development Authority has invested in 50 energy storage technology projects as part of its commitment to supply 50% of the state's power from renewables by 2030. New York is one of the U.S. states that will uphold the Paris Agreement.

In contrast, the outlook for advanced biofuels has not improved. In the U.S., two of three much-touted cellulosic ethanol facilities—operated separately by DuPont and Abengoa—have been shut down.

After years of planning and construction, Enerkem's plant began producing bioethanol in September.

A few bright spots persist for the biobased chemicals industry in 2018. Projects to produce jet fuels from waste and from purpose-grown crops have attracted corporate support. Firms such as Enerkem and Fulcrum BioEnergy are successfully producing chemicals and fuels from municipal solid waste.

And some industrial biotechnology companies are reporting strong demand. DuPont's Sorona fibers, made with biobased propanediol, are now in everything from jeans to high-end fashion, the company says. Its biobased ingredients are increasingly popular with marketers of cleaning and food products.

"We have been accelerating the pace of our new product introductions over the past few years, and in 2018 you will see new products in basically every market space we serve," says William Feehery, president of DuPont Industrial Biosciences.—MELODY BOMGARDNER

CREDIT: ASML (SCANNER); ENERKEM (PLANT)

PETROCHEMICALS

Market will remain tight despite new capacity

U.S. petrochemical makers are in the midst of commissioning the largest fleet of new ethylene crackers in more than a generation. However, the new supply shouldn't sink profitability anytime soon.

With little capacity coming onstream elsewhere in the world, significant construction delays, and new plants for derivatives such as polyethylene already running, the world will need every metric ton of ethylene the new crackers will crank out. It won't be until the middle of 2018 that they begin to ease a tight market.

The global ethylene market is snug, with effective operating rates—the utilization rate of plants that are running—at 92%, according to Steve Lewandowski, vice president of olefins for IHS Markit. "There is no spare capacity anywhere," he says.

Hurricane Harvey, which made landfall in Texas on Aug. 25, 2017, cut through the heart of the U.S. chemical industry. By Sept. 5, more than half of U.S. ethylene capacity and 36% of ethylene derivative capacity was off-line, according to IHS Markit.

But the region bounced back quickly. Damage to chemical facilities was limited, and all but a few plants were up and running again by the end of the month.

Overall, the industry lost some 750,000 metric tons of ethylene production, nearly a cracker's worth of output for a year. "That doesn't sound like much," Lewandowski says. "But when the whole system is pushing to the maximum operating rate, any disruption is a problem."

Longer-lasting effects of Harvey are construction delays of about six months for two new crackers, each with 1.5 million metric tons of annual capacity, that ExxonMobil and Chevron Phillips Chemical meant to start up by the end of 2017.

These two companies already turned on new polyethylene plants earlier last year. With these and similar additions, Lewandowski says, the U.S. will have much more capacity for derivatives than for ethylene, straining ethylene supplies until the crackers are completed and up to full production around the middle of 2018.

In addition to the ExxonMobil and Chevron Phillips crackers, Indorama is set to restart a long-idled cracker in Lake Charles, La., and Formosa Plastics is due to complete a new cracker in Point Comfort, Texas, Lewandowski says. Shin-Etsu Chemical and Sasol will likely complete their ethylene projects in 2019.

Bob Patel, CEO of polymer maker LyondellBasell Industries, argues that the market for polyethylene won't soften much either. He predicts operating rates for that product may remain above 90%.

Speaking to analysts in October, Patel explained that increases in polyethylene production outstripped demand growth by about 3% in 2017 and will by another 1% in 2018. "If you look across those two years, you end up with perhaps operating rates declining by 3% or 4% coming off very, very high operating rates and what we would consider still to be balanced markets," he said.—ALEX TULLO

Dow Chemical started up this ethylene cracker in Freeport, Texas, last year.

CREDIT: FLUOR

AGRICULTURE

Transformation is coming, despite low crop prices

While the global economy heats up, farmers face yet another year of low commodity prices. After four years of recession for U.S. growers, farm incomes are down about 25% from 2014. Adding insult to injury, corn production remains on track for another record-breaking year.

Cibus plant researchers examine plant clones that have gene-edited, rather than transgenic, traits.

When commodity prices are low, farmers are more sensitive to prices for the inputs they use. Will they make their money back on pricey new biotech seeds and patented pesticides? And with fewer firms competing for their business thanks to an epic wave of corporate consolidation, concerns about affordability will only rise.

Worries over competition have prompted the European Union to delay its deadline for antitrust review of Monsanto and Bayer's proposed merger until March.

In November, the antitrust activist group Open Markets Institute pointed out that Monsanto-Bayer would be the world's largest seller of herbicides and seeds for vegetable and cotton crops. It would be the world's largest owner of intellectual property for herbicide-tolerant seed traits and the largest company researching seeds and traits. Lastly, it would be a huge player in the rise of agricultural data platforms.

But a lot of research and investment is happening outside giant firms like Monsanto, Bayer, and DowDuPont. Start-ups are largely leading innovations in automation and agricultural biotechnology. For example, Cibus used gene editing to develop a nontransgenic canola crop that is tolerant to sulfonylurea herbicides. The website AgFunderNews counts 245 start-ups in plant biotechnology alone.

Highflier Indigo Ag, a four-year-old start-up, raised more than $200 million in a fourth round of funding late last year. Indigo sells seeds coated with specialty microbes that improve row crop yields by helping plants shrug off drought and other stresses. The firm offers a per-bushel premium to farmers willing to adopt the new technology.

Large agriculture firms are also investing in technologies outside their traditional realms of seeds and chemicals. Bayer, for example, recently formed a company with the synthetic biology firm Ginkgo Bioworks to sell microbes that help plant roots fix nitrogen.

Automation may soon begin disrupting markets for traditional crop inputs like herbicides. FarmWise, a new start-up touting internet-connected robots, raised $5.7 million last month to commercialize weed-destroying robots that use computer vision technology to analyze each plant.—MELODY BOMGARDNER

PHARMACEUTICALS

Drug industry strength to buoy fine chemicals makers

Fine chemicals companies finished another strong year, and executives see strength following strength in 2018.

According to the Society of Chemical Manufacturers & Affiliates, a trade group representing fine and specialty chemical firms, sector sales volume increased 4.4% last year. The group expects comparable growth in 2018, thanks to product innovation in markets including pharmaceutical, agricultural, and industrial fine chemicals. For example, the U.S. Food & Drug Administration approved 46 drugs in 2017, more than twice as many as in 2016, and many of them are small molecules being manufactured by the fine chemicals industry.

Much of the growth in drug chemicals stems from customer needs for complex or highly potent molecules. The growth is spurring both investment and consolidation, according to producers. Indeed, the sector's strong performance is attracting diversified companies such as PMC Group, which acquired two pharmaceutical chemical companies late last year.

"I continue to be bullish," says Aslam Malik, CEO of Ampac Fine Chemicals. "More so this year because of tax reform." The lowering of the corporate tax rate will encourage drug companies to invest in the U.S. and put U.S. fine chemicals firms in a stronger position to compete with Europe, he predicts.

Steven M. Klosk, CEO of the pharmaceutical chemical maker Cambrex, is also optimistic. "We continue to expect strong demand for CDMO outsourcing services," he says, referring to contract development and manufacturing organizations. Klosk points to a global pipeline of over 5,000 small-molecule drugs in development.

While the sector appears to have broken from its traditional boom-and-bust cycle, some observers see certain types of bad behavior starting to recur. Consultant James Bruno, president of Chemical & Pharmaceutical Solutions, notes that the move of newcomers into the market is reminiscent of a similar failed rush some 15 years ago.

And the amassing of one-stop shops that combine pharmaceutical chemical and finished dosage manufacturing with other services works against the traditional business model of being small and specialized. "We are very cyclic," Bruno says. "We do the same thing again and again. We screw up and we fix it. And we screw up again."—RICK MULLIN

Pharmaceutical chemical firms such as AMRI, shown here in Rensselaer, N.Y., are benefiting from high drug approval rates.

CREDIT: CIBUS (GREENHOUSE); AMRI (WORKER)

Robust demand should continue in 2018

Persistent growth in the U.S., continued economic expansion in Asia, and a renewal of demand in Europe all bode well for specialty chemical output in 2018, according to the American Chemistry Council. The trade association projects a 3.0% global production rise in 2018 after a 2.5% increase in 2017.

Ever optimistic, ACC had expected output to jump 3.3% in 2017. But despite an overall pickup in the global economy, some industries that depend on specialty chemicals, such as oil and gas drilling, were weak, ACC says. Industry observers say the elements are in place for a better 2018.

Ray Will, a director at the consulting firm IHS Markit, discerns a number of trends likely to increase demand for specialty chemicals. Among them are a shift to electric vehicles and a move away from the use of fluorochemical coolants in home refrigerators.

Hydrocarbons and CO_2 are winning the global battle to fill home refrigerators, says consultant Ray Will.

China, Will says, plans to establish a system of quotas that will require electric vehicles to make up at least 10% of automakers' output beginning in 2019 and increasing annually thereafter. The move is likely to bolster demand for battery materials as well as the electrolyte solutions that shuttle a charge between a battery's anode and cathode.

Chemical makers could be in for a sweet ride if electric vehicles catch on in the U.S., points out credit rating agency Fitch Ratings. While Fitch sets the value of chemicals in a conventional vehicle at $3,000, it estimates the value of chemicals used in electric vehicles at $10,000, mostly related to batteries.

In the world of refrigeration, manufacturers are seeking coolants with low global warming potential. Rather than shift to hydrofluoroolefin refrigerants, many makers of home refrigerators, especially in Europe and Japan, are shifting to hydrocarbon refrigerants, Will says. The hydrofluoroolefins, developed for use in auto air-conditioning, are significantly more expensive, he notes.

The paints and coatings sector should benefit from an uptick in the economy, especially in the U.S., where tax reform will boost capital spending, predicts Phil Phillips, president of Chemark Consulting Group. New machinery and equipment, he says, require a significant amount of paint. Phillips expects paint production to rise about 3.5% in 2018.

Adhesives will grow at a similar rate, Phillips says, singling out a projected increase in demand for urethane adhesives to assemble and seal automobile body components.

Consumer demand for personal care chemicals continues to rise, according to the consulting firm Kline & Co. Trends in the $1.6 billion-per-year specialty ingredients market include growing demand for blue filters said to protect skin from computer screen emissions and cosmetics formulated to protect skin from air pollutants, says Kunal Mahajan, a chemicals project manager with Kline.—MARC REISCH

Manufacturers are seeking coolants with low global warming potential.

CREDIT: SHUTTERSTOCK

CANADA

A petrochemical spending rush is on

When it comes to investing in new chemical capacity, Canada has long dreamed big and delivered modestly. But that changed last month when Canadian firms green-lighted two large projects.

Canadian natural gas pipeline and processing firm Inter Pipeline approved the investment of $2.7 billion to build propane dehydrogenation (PDH) and polypropylene plants near Redwater, Alberta, by 2021.

Some 22,000 barrels per day of propane, half from Inter Pipeline's own processing plant, will enter the facility; 525,000 metric tons per year of polypropylene will leave out the back.

The rationale for the facility is compelling, Inter Pipeline says. Because of a large surplus with no easy outlet to market, propane sells at a substantial discount in Alberta compared with the U.S. Gulf Coast. The company says the facility will be one of North America's most competitive.

A joint venture between Pembina Pipeline and Petrochemical Industries Co. of Kuwait is set to reach a decision later this year on a similar PDH and polypropylene complex in Alberta.

Meanwhile, Canada's largest chemical maker, Nova Chemicals, also approved a long-considered project last month. The company will build a 450,000-metric-ton-per-year polyethylene plant in Sarnia, Ontario, by 2021 and expand its cracker there by 50%.

All the projects are getting support from the government. Alberta is pitching in nearly $400 million in royalty credits for the PDH complexes. Ontario is contributing about $75 million toward Nova's projects.

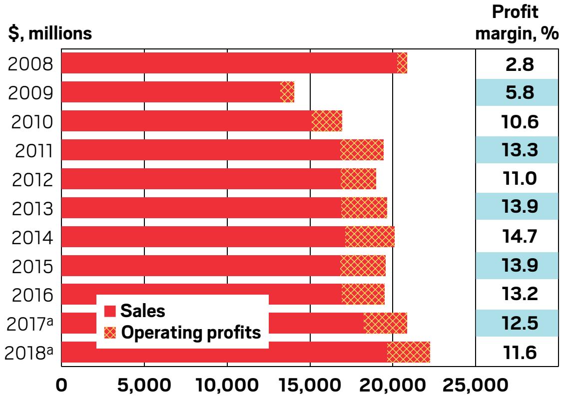
To Bob Masterson, president of the Chemistry Industry Association of Canada (CIAC), such incentives are a must if Canada is to attract investment. U.S. jurisdictions aren't shy about offering packages to prospective investors, he observes.

"It has taken a lot of work to get everybody rowing their oars in the same direction, but we seem to be getting some results," Masterson says, noting that projects worth billions more are under consideration.

The investments are coming at a time of growth for the Canadian chemical industry. In 2017, it saw sales increase by 7% to hit $20.8 billion, according to CIAC. Chemical makers surveyed by the group expect another 7% sales increase this year.—ALEX TULLO

Canadian chemicals

The industry should have another strong year in 2018, though profitability may slip.



a Projected. **Note:** Profit margin is operating profits as a percentage of sales. **Source:** Chemistry Industry Association of Canada

LATIN AMERICA

Finally, growth will kick in

Latin America's economic performance has been sluggish in recent years, with countries such as Brazil even dipping into recession. The past year, however, brought a turnaround for the region, and forecasters expect a return to growth in 2018.

The positives for Latin America, according to economists at the Spanish bank BBVA, include rising commodity prices, currency devaluation leading to increased competitiveness, and a strong world economy. Last year was an "inflection point," BBVA says, "after five years of slowdown and two (2015 and 2016) of contraction."

After two recessionary years, Brazil's economy, the region's largest, is projected to post 0.7% growth for 2017, according to the International Monetary Fund. IMF analysts expect output to increase 1.5% in 2018. However, they caution that the Brazilian economy is still hampered by political uncertainty due to an upcoming presidential election and weak investment.

Chemical sales are showing signs of recovery. Brazilian giant Braskem reported that its polyethylene volumes increased by 4% in the first nine months of 2017 versus the year before. However, the firm's sales of polyvinyl chloride (PVC), which is used by the construction sector for pipes and windows, were down by 3%.

Rina Quijada, a senior director and Latin America analyst for the consulting firm IHS Markit, says Brazilian demand for PVC has fallen 25% since 2015. She sees the market turning the corner in 2018 and demand climbing a modest 2%. Polyethylene demand will increase by 3%, she predicts.

Mexico is on track to grow by 1.9% this year, a slight slowdown from the 2.1% projected for 2017, according to IMF.

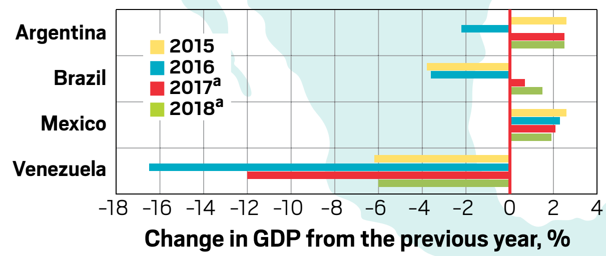
But the chemical industry there has a problem: raw material supply. Ever since Braskem and Grupo Idesa started up a $5 billion ethylene cracker in Nanchital, Mexico, in 2016, their contractual supplier of the raw material ethane, state oil company Pemex, hasn't been able to scare up the ethane needed for its own facilities.

Pemex's ethylene output has plunged 45% since 2015. Output of derivatives such as polyethylene, ethylene oxide, and styrene are also down sharply.

"It has been very difficult for Pemex to produce," Quijada says. She notes that Pemex is evaluating options such as ethane imports from the U.S.—ALEX TULLO

Course reversal

Argentina's and Brazil's economies turned around in 2017, but the recovery will be slow.



a Projected. **GDP** = gross domestic product. **Source:** International Monetary Fund

UNITED STATES

Slow and steady growth ahead

The engines of the U.S. economy are stoked to hum, if not roar, in 2018. Unemployment is low, consumer and business confidence is up, and corporations can look forward to lower tax rates. But recent years' economic growth has not triggered a spike in U.S. chemical output, and it's not clear that will change this year.

In 2017, the U.S. gross domestic product grew by 2.3%, but chemical output rose only 0.8%, much lower than the 3.8% predicted by the American Chemistry Council, the main U.S. chemical trade group. ACC now says 2018 will be the growth year, with output expanding 3.7%.

A recent spate of capacity investment by U.S. industrial companies is good news for the chemical makers that supply them with raw materials. Overall, industrial firms increased capital spending by 8.7% in 2017 and will boost it an additional 2.7% this year, according to the Institute for Supply Management. ACC expects U.S. chemical companies to raise their capital spending 6.9% in 2018.

Another bright spot is home building. The strong jobs market and tight housing inventory caused a key index of builder confidence to jump in December. New construction permits soared by more than 15% compared with the end of 2016, according to Census Bureau data. ACC estimates that each new home requires about $15,000 worth of chemicals.

Auto manufacturing, in contrast, is not expected to add to demand for chemicals overall, though some specialties may see a lift. Sales last year were down from a peak of 17.5 million vehicles in 2016, and they are expected to remain flat.

Other chemical industry customers that ACC expects to grow this year include electronics, appliances, and aircraft parts. The oil and gas sector is expected to improve as oil reaches $55 per barrel. The downside is that chemical firms will see raw material and energy costs increase.

Overall, the global economy will expand by 3.8% in 2018 a bit faster than the expected U.S. rate of 2.6%, according to Deutsche Bank. Rising international demand will benefit U.S. chemical companies, which have a competitive advantage from low-cost shale gas. "With synchronous economic growth around the world, the global appetite for U.S. exports has increased," says ACC economist T. Kevin Swift.

The capacity additions built to take advantage of the shale boom will continue to come on-line, and ACC expects the largest gains to happen this year and next. "In addition, a second wave of investment is on the way," Swift says. "Much of the new production will be exported to customers around the world."—MELODY BOMGARDNER

Big movers

Zacks Investment Research says these U.S. firms will benefit most from industrial demand.

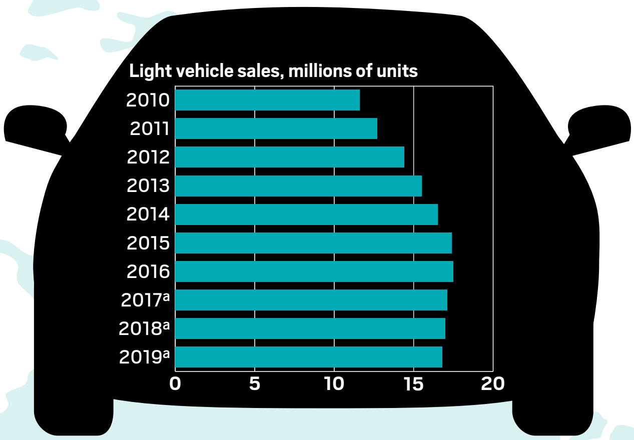
PROJECTED GROWTH RATES COMPARED TO 2017

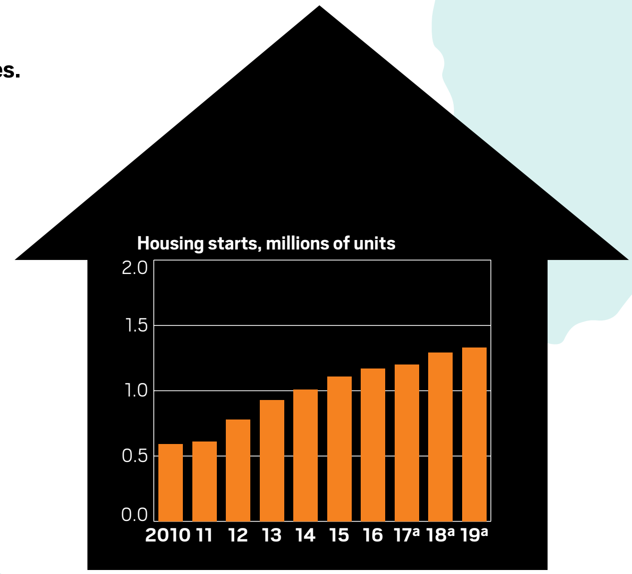
COMPANY	REVENUE	EARNINGS PER SHARE	IN-DEMAND PRODUCT
Kronos Worldwide	41.1%	5.0%	Titanium dioxide
Westlake Chemical	25.7	10.6	Olefins and vinyls
Kraton	30.6	na	Polymers
Albemarle	16.9	14.8	Lithium
Celanese	11.7	9.0	Acetal intermediates, acetate tow

na = not available.

Building boom

While auto sales flatten, demand for housing will spur chemical sales.





a Projected. **Source:** American Chemistry Council

EUROPE

With growth in the cards, confidence returns

Europe's chemical industry has regained its confidence after economic recovery in the region, according to the European Chemical Industry Council (Cefic), a key chemical industry organization. Chemical output is set to increase 2% in 2018, after growing 3% across the European Union in 2017, Cefic says.

"The momentum is growing," says Marco Mensink, Cefic's director general. The growth will help the chemical industry step up investment in R&D and help the region transition to a resource-efficient, low-carbon, and circular economy, Mensink claims.

The cause is robust demand in sectors such as auto manufacturing, construction, metal fabrication, and electronics. Investments in new chemical production capacity are under way, Cefic says. Partly as a result, Europe's chemical industry is now responsible for 1.1% of the EU's gross domestic product and 1.2 million jobs, according to the association.

In Germany, the heartbeat of Europe's chemical industry, the forecast is for chemical sales to rise 3% in 2018 to more than $230 billion. In 2017, Germany's chemical sales increased more than 5%.

"We are confident that the upward trend will last next year," said Kurt Bock, head of German chemical maker BASF, at an end-of-the-year press conference. "But where political aspects are concerned, we need to brace ourselves for persistently turbulent times."

Despite the challenge of Brexit—Britain's planned 2019 exit from the EU—the outlook for the U.K. chemical industry appears to be in line with the rest of Europe.

"We expect to see growth in 2018 … with a possibility it could be just under 2%," says Stephen Elliott, CEO of the Chemical Industries Association, a U.K. trade group. The industry saw 3% growth in 2017.

But Elliott and Steve Bates, CEO of the BioIndustry Association, a biotech group, remain concerned about the potential impact of Brexit. They are calling for the U.K. government to put in place measures that will enable their respective sectors to continue trading with the EU.

Even if such measures are established, U.K. chemical companies will likely take a hit, according to Paul Hodges, chairman of the London-based consulting firm International eChem. European customers of British chemical firms, he says, will be asking whether they can find another supplier or producer outside the U.K.—ALEX SCOTT

In good shape: Europe's chemical industry is poised to grow

- **2%:** Anticipated sales growth in the EU in 2018
- **3%:** Anticipated sales growth in Germany in 2018
- **3.1%:** Growth in EU chemical production in the first half of 2017
- **84.1%:** Plant capacity utilization, which has been growing for more than a year
- **5:** Number of quarters that chemical business confidence has increased in Europe.

Source: Cefic

ASIA

Despite financial risks, region is looking at another banner year

Demand for chemicals is steady in China, Japanese chemical companies are upgrading their profit forecasts, and economic growth is accelerating in India. In sum: The outlook for the Asian chemical industry in 2018 is good.

Predictions of strong economic growth in China, India, and Indonesia translate to "a positive outlook for the Asian chemical industry as a whole," says Steve Jenkins, vice president of chemicals consulting at market research firm PCI Wood Mackenzie.

In Japan, the economy will not be that strong, but chemical companies will be able to grow their margins by focusing on technologically advanced materials, Jenkins says. The continued weakness of the yen will raise profits in yen terms, he adds.

In China, the world's largest market for chemicals, consumer demand is buoying chemical production, Jenkins notes. The widespread use of smartphones to order from online retailers, for instance, is stimulating demand for consumer goods in once-stagnant inland provinces.

Meanwhile, strict enforcement of environmental regulations is changing China's chemical industry, Jenkins notes, in part by leading many firms to upgrade their facilities to stay in business.

Environmental controls are having a wide impact, agrees Peter Huo, vice president for sales and marketing at the Chinese polyurethane chemicals producer Wanhua Chemical.

Even when their operations are compliant, Wanhua and its competitors have had to cut production as a result of China's crackdown. Wanhua, for example, had to temporarily reduce production at some of its plants because "some of the buyers of our products had to stop theirs," Huo explains.

But on the whole, Chinese demand for polyurethane materials and other chemicals was steady in 2017, a trend that Huo expects to continue for at least the first half of 2018. The combination of constant demand and lowered supply due to the crackdown is boosting profit margins, he notes.

The main risks facing Asia are financial. A major slowdown of the U.S. stock market could "derail the current buoyant mood," Jenkins warns. And government officials in China are mentioning more often the need to reduce debt levels in both the private and public sectors, a shift that could dampen the economy as a whole by reducing funds available to invest or expand, Huo says.—JEAN-FRANÇOIS TREMBLAY

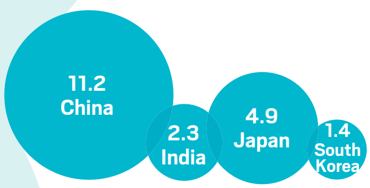
Growth leaders

India and China matched growth in 2017, but India is expected to take the lead again this year.

Change in GDP from the previous year, %

	China	India	Japan	South Korea
2016	6.7	7.1	1.0	2.8
2017[a]	6.8	6.7	1.5	3.1
2018[a]	6.4	7.3	1.1	3.0

Nominal 2016 GDP ($ trillions)



a Projected. **GDP** = gross domestic product. **Sources:** Asian Development Bank, World Bank

Low oil price to accelerate push for diversity

With oil prices widely tipped to stay around $60 per barrel or lower for the next few years, the low-cost-energy advantage enjoyed by the Middle East's chemical sector will continue to evaporate, experts say. As this scenario becomes the new normal, many Middle Eastern chemical companies see 2018 as the year they must shift faster away from basic petrochemicals and toward higher-value specialty products.

"One thing we know for certain: The status quo is not an option," Yousef Al-Benyan, chairman of the Gulf Petrochemicals & Chemicals Association and CEO of the big Saudi firm SABIC, told delegates at the GPCA Annual Forum late last year. "The fundamental change required to deliver a quantum leap in performance is transformation; it is not an incremental improvement."

In addition to the low price of oil, challenges the region faces include lower profit margins, China's rise to self-sufficiency, and the shale-enabled chemical expansion in the U.S., Al-Benyan said.

Using mergers and acquisitions is one way Middle Eastern companies could improve their difficult position, says Mirko Rubeis, a managing director of Boston Consulting Group. He says companies in the Gulf Cooperative Council region—which includes the lion's share of the Middle East's chemical industry—should strive to focus their portfolios in areas such as specialty chemicals while reducing costs through economies of scale.

It's a view echoed by H. E. Khalid A. Al-Falih, Saudi Arabia's minister of energy, industry, and mineral resources and chair of Saudi Aramco. Speaking at the GPCA forum, he called on regional players to think globally and on governments to adopt policies that encourage venture capital investment and greater spending on R&D.

Dow Chemical and Saudi Aramco point to their Sadara Chemical Company joint venture as an example of how to integrate the Middle East's basic chemicals prowess with high-end production of specialty materials.

Last year, Sadara started up a polyurethane raw material plant at its complex in Jubail, Saudi Arabia. It is the last of 26 facilities to be commissioned at the $20 billion site. A raft of downstream facilities—such as a plastics processing plant—are now being built nearby.

Rejecting the downbeat outlook of others producing chemicals in the Middle East, DowDuPont executive chairman Andrew N. Liveris has pledged that he will continue to make specialty chemical investments in the region. For Liveris, at least, the Middle East is still a land of opportunity.—ALEX SCOTT

> "The fundamental change required to deliver a quantum leap in performance is transformation; it is not an incremental improvement."
>
> **—Yousef Al-Benyan, chairman of the Gulf Petrochemicals & Chemicals Association (GPCA)**

Sadara by the numbers

- **6 years:** Time it took to construct Sadara, a joint venture between Dow Chemical and Saudi Aramco
- **3 million metric tons per year:** Amount of chemicals and plastics being produced at the site
- **26:** Number of plants at the site
- **Sept. 17, 2017:** The day Sadara commissioned its final plant, a toluene diisocyanate facility
- **160,000 metric tons:** Amount of steel needed to construct the site
- **2,500 km:** Length of piping at the site

Source: Sadara

Middle East chemicals by the numbers

- **6%:** Share of global production, up from 3% in 2000
- **102:** Number of products being made
- **159 million metric tons:** Production, up 8.5% since 2015
- **$91 billion:** Sales, down 3% since 2015
- **$584 million:** R&D spending, down 20% since 2015
- **49%:** Share of Gulf production attributable to Saudi Arabia

Note: Figures are for 2016 **Source:** GPCA

NATIONAL AWARDS

2018 ACS national award winners

Recipients are honored for contributions of major significance to chemistry

EDITED BY LINDA WANG

The following vignettes highlight the recipients of national awards administered by the American Chemical Society for 2018. Profiles of the Arthur C. Cope Award and Arthur C. Cope Scholar Award recipients will appear in the Jan. 15 issue of C&EN. A profile of Geraldine Richmond, the 2018 Priestley Medalist, will appear in the March 19 issue, along with her award address.

The award recipients will be honored at a ceremony at the spring ACS national meeting in New Orleans, March 18–22.

ACS Award for Computers in Chemical & Pharmaceutical Research: Jürgen Bajorath

Sponsor: ACS Division of Computers in Chemistry

Citation: For the development and application of chemoinformatics and computational chemistry solutions to research problems in medicinal chemistry, chemical biology, and the life sciences.

Current position: professor and chair of life science informatics, University of Bonn

Education: M.S., biochemistry, Free University Berlin; Ph.D., structural biochemistry, Free University Berlin

Bajorath on what gets his creative juices flowing: "I'm inspired by exploring new avenues in research. One of my premises is not to hold onto accomplishments but move on. Trying to develop new ideas going off the beaten path is a driver for me. In addition, working with graduate students and seeing how many of them really get into science is a joy."

What his colleagues say: "Jürgen is a world leader in the development and application of cheminformatics and computational solutions to research problems in medicinal chemistry, chemical biology, and life sciences, and he has done pioneering work in big data analysis and chemistry."—Veerabahu Shanmugasundaram, Pfizer

ACS Award in Surface Chemistry: Stacey F. Bent

Sponsor: Procter & Gamble

Citation: For seminal work on organic functionalization of semiconductor surfaces and for harnessing surface chemistry to gain control over atomic layer deposition processes.

Current position: Jagdeep & Roshni Singh Professor of Engineering, Stanford University

Education: B.S., chemical engineering, University of California, Berkeley; Ph.D., chemistry, Stanford University

Bent on her biggest research challenge: "My biggest research challenge is to understand and control surface chemistry well enough to design materials or processes to achieve whatever properties we desire. A few examples are semiconductors with stable molecular passivation, catalysts with specific selectivity, or optoelectronic devices without interfacial defects."

What her colleagues say: "Her work has provided deep insight into understanding and controlling surface and interfacial chemistry and applying this knowledge to diverse problems in semiconductor processing, nanotechnology, and renewable energy."—Chaitan Khosla, Stanford University

ACS Award for Team Innovation: Vladimir G. Beylin, Brian P. Chekal, Nga M. Do, David W. Fry, Nathan D. Ide, Brian P. Jones, Peter L. Toogood, and Hairong (Angela) Zhou

Sponsor: ACS Corporation Associates

Citation: For scientific innovation leading to the discovery and development of palbociclib (Ibrance), the first CDK4/6 inhibitor for the treatment of metastatic breast cancer.

What their colleagues say: "This team is responsible for the discovery of palbociclib (Ibrance), a first-in-class CDK4/6 inhibitor for the treatment of hormone receptor positive (HR+) human epidermal growth factor negative (HER2–) metastatic breast cancer in combination with letrozole or fulvestrant. This team overcame significant hurdles to discover an agent with suitable pharmacology. Additionally, the demand for rapid advancement from midstage clinical trials to the market required significant process development innovation."—Tony Wood, GlaxoSmithKline

Vladimir G. Beylin

Current position: retired research fellow, Pfizer

Education: M.S., chemical technology/engineering, Leningrad Chemical-Pharmaceutical Institute; Ph.D., organic chemistry, Leningrad Chemical-Pharmaceutical Institute

Beylin on what he's most proud of in his career: "When working in pharmaceutical R&D on many projects and lead compound development, you always hope and dream that one of them will end up being a real remedy for patients in need. When PD-0332991 became Ibrance and started helping thousands of cancer patients, I felt very glad and proud to be a member of the diverse and multidisciplinary team that made this dream a reality."

Brian P. Chekal

Current position: associate research fellow, Pfizer

Education: B.S., chemical engineering, University of Virginia; Ph.D., chemical engineering, Northwestern University

Chekal on what he hopes to accomplish in the next decade: "Over the past 10 years, we have seen significant changes in the way that a laboratory scientist develops an API manufacturing process, with a greater emphasis placed on automated lab reactors with process analytical technology and supported by process modeling tools. I expect that the next decade will see similarly dramatic changes, and I am excited to lead a group of scientists who are leading the use of computational modeling and experimental approaches to develop manufacturing processes with greater process understanding using less time and material."

Nga M. Do

Current position: principal scientist, Pfizer

Education: B.S., chemistry, Purdue University; M.S., chemistry, University of California, Irvine

Do on her biggest research challenge: "The biggest research challenge is the speed of our development work. While intellectually stimulating, the ability to develop efficient processes under the time constraints makes this an ongoing research challenge. The fact that we work on so many different molecules that often require new and different approaches generates new challenges every day."

David W. Fry

Current position: retired scientist, Pfizer

Education: B.S., microbiology, Ohio State University; Ph.D., biochemistry, Ohio State University

Fry on the most important lesson from his scientific career: "The greatest satisfaction from my scientific career has come from my contributions to the field of oncology drug discovery in the area of protein kinases, but even more importantly, the end result of these efforts, which has culminated in new medicines that benefit cancer patients. The most important lesson I learned during my career was that persistence, dedication, and a staunch refusal to accept failure gets you most of the way to achieving your goals."

Nathan D. Ide

Current position: senior principal research scientist, AbbVie

Education: B.S., chemistry, Hope College; Ph.D., chemistry, University of Illinois, Urbana-Champaign

Ide on what he hopes to accomplish in the next decade: "The pharmaceutical industry has brought some truly remarkable treatments to patients over the past decade. Over the next decade, I hope to be part of that continued effort to bring new medicines to patients, working to trim down the list of diseases without effective treatments. I also hope that in the process of delivering effective new medicines, we can help contribute to an improvement in the way that society views the pharmaceutical industry, the field of chemistry, and the broader scientific community."

Brian P. Jones

Current position: senior scientist, Pfizer

Education: B.S., chemistry, Worcester Polytechnic Institute; M.S., chemistry, Worcester Polytechnic Institute

Jones on his biggest research challenge: "My biggest research challenge was developing a crystallization that avoided a particular crystal form of a compound which was prone to fracturing and would therefore filter extremely slowly. The crystallization we developed produced a form of the compound which would not fracture and filtered much more quickly."

Peter L. Toogood

Current position: senior vice president of chemistry, Lycera

Education: B.S., chemistry, Imperial College London; Ph.D., organic chemistry, Imperial College London

Toogood on research dedication: "In addition to teamwork, I think our success with Ibrance derived very directly from a stubborn determination to persist in the search for a single kinase target selective inhibitor."

Hairong (Angela) Zhou

Current position: senior sourcing manager, Genentech

Education: B.S., chemistry, Shandong University; M.S., analytical chemistry, Shandong University; M.S., bioorganic chemistry, University of Wisconsin, Madison

Zhou on what gets her creative juices flowing: "I love working in the pharmaceutical field, where I am part of a team to discover and develop new drugs for treating various diseases. I am inspired by talented and innovative colleagues every day, and the positive energy gets me going. Being able to provide solutions to a challenging situation makes me feel a great deal of accomplishment, not only from running an experiment in the lab for testing a hypothesis but also from coming up with a strategic plan to enable the successful delivery of the goal."

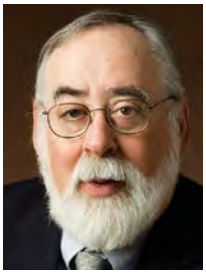
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: George M. Bodner

Sponsor: ACS Exams Institute

Citation: For his contributions to the development of discipline-based educational research on the teaching and learning of chemistry in both introductory and advanced-level courses.

Current position: Arthur Kelly Distinguished Professor of Chemistry, Education & Engineering, Purdue University

Education: B.S., chemistry, University at Buffalo; Ph.D., inorganic and organic chemistry, Indiana University, Bloomington



Bodner on his biggest research challenge: "Getting chemists and science educators to understand each other is a challenge. I've worked to convince chemists that the results of educational research are useful and to convince science educators that the real challenge is extending their work beyond the K–12 level and including both undergraduates and graduate students in an individual discipline, such as chemistry."

What his colleagues say: "Dr. Bodner has focused on overcoming the challenges associated with the teaching and learning of chemistry across the full range of subdisciplines, including analytical, biochemistry, inorganic, organic, and physical chemistry, as well as chemical engineering."—Marcy Towns, Purdue University

F. Albert Cotton Award in Synthetic Inorganic Chemistry: A. S. Borovik

Sponsor: F. Albert Cotton Endowment Fund

Citation: For demonstrating that synthetic inorganic chemistry can harness the power of noncovalent interactions to regulate local environments around metal ions to control their function.

Current position: professor of chemistry, University of California, Irvine

Education: B.S., chemistry, Humboldt State University; Ph.D., chemistry, University of North Carolina, Chapel Hill

Borovik on the people who have had the greatest impact on his career: "I have had several people who strongly impacted my career, including my mentors. However, the most important people are those who have been in my research group. I often come up with a kernel of a project, but it is their hard work, dedication, and creativity that drives the project—often in directions that were unknown at the outset. Without them, nothing happens!"

What his colleagues say: "At all levels—creativity, design, execution, and relevance—professor Borovik's research exemplifies the best in synthetic inorganic chemistry."—Kenneth Raymond, University of California, Berkeley

E. V. Murphree Award in Industrial & Engineering Chemistry: Linda J. Broadbelt

Sponsor: ExxonMobil Research & Engineering

Citation: For distinguished contributions to the field of complex kinetic modeling, particularly the development of automated mechanism generation and mechanistic models applied to industrially important problems.

Current position: Sarah Rebecca Roland Professor of Chemical & Biological Engineering and associate dean for research, McCormick School of Engineering & Applied Science, Northwestern University

Education: B.S., chemical engineering, Ohio State University; Ph.D., chemical engineering, University of Delaware

Broadbelt on what gets her creative juices flowing: "I derive many of my most creative ideas from attending talks given by scientists and engineers from disparate fields. There is nothing more enjoyable than going to a conference and listening to speakers from areas outside my own, as I have found that many guideposts for my research directions have emerged from positioning myself, sometimes uncomfortably, at boundaries and intersections."

What her colleagues say: "Linda Broadbelt is internationally recognized for her contributions in complex kinetics modeling of hydrocarbon chemistry, particularly for the development of automated mechanism generation techniques and methods for specification of rate coefficients. She has expertly developed computational algorithms to automate construction of mechanistic models and continued to improve the capabilities and apply them to topical areas as diverse as metabolic networks, silicon nanoparticle production, atmospheric chemistry, synthesis of antibiotics, and hydrocarbon conversion."—Harold H. Kung, Northwestern University

James Flack Norris Award in Physical Organic Chemistry: Cynthia J. Burrows

Sponsor: ACS Northeastern Section

Citation: For seminal studies to elucidate the mechanistic pathways of oxidation of guanine and its derivatives to further our understanding of DNA damage and repair.

Current position: Thatcher Distinguished Professor and Presidential Endowed Chair of Biological Chemistry, University of Utah

Education: B.A., chemistry, University of Colorado; Ph.D., chemistry, Cornell University

Burrows on the future of her field: "Physical organic chemistry in 2018 is not so much a focused discipline as it is a way of thinking about structure and mechanisms pertaining to carbon-containing molecules. In the 20th century, physical organic chemistry was about reactive intermediates—carbocations, carbenes, radicals. Now it spans materials, devices, catalysis, and biological mechanisms. I'm happy to be a part of this field, grounded in fundamental studies but with ultimately very broad implications."

What her colleagues say: "She is recognized as a world expert in the study of mechanisms of DNA base oxidation. Her work is characterized by keen chemical insight and creative approaches to understanding the broader implications of oxidative DNA damage."—Dale Poulter, University of Utah

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Alison Butler

Sponsor: Alfred R. Bader Fund

Citation: For elucidating the bioinorganic chemistry of the marine environment, including the chemistry of siderophores and vanadium haloperoxidases.

Current position: Distinguished Professor of Chemistry & Biochemistry, University of California, Santa Barbara

Education: B.A., chemistry, Reed College; Ph.D., chemistry, University of California, San Diego

Butler on what gets her creative juices flowing: "A good chemical detective story—like an unusual transition-metal ion composition in a cell, an organism, an ocean (or beyond). I begin imagining what new metalloenzymes are out there waiting to be discovered!"

What her colleagues say: "Alison Butler has a sustained and distinguished set of accomplishments in the fields of bioinorganic and bioorganic chemistry that shows no signs of abating. Her adventurous approach to science has yielded insight into the chemistry of marine organisms and the uptake of iron into microbes. She also has a penchant for prestigious-conference organization, has served in impressive leadership positions in prominent national and international scientific societies, and has devoted much of her considerable energy and enthusiasm to the chemistry community."—Stephen J. Lippard, Massachusetts Institute of Technology

ACS Award in Theoretical Chemistry: Emily A. Carter

Sponsor: ACS Division of Physical Chemistry

Citation: For pioneering development of orbital-free density functional, embedded correlation wave function, and efficient multireference wave function theories, applied to diverse sustainable energy phenomena and materials design.

Current position: dean of the School of Engineering & Applied Science, Gerhard R. Andlinger Professor in Energy & the Environment, and professor of mechanical and aerospace engineering and applied and computational mathematics, Princeton University

Education: B.S., chemistry, University of California, Berkeley; Ph.D., physical chemistry, California Institute of Technology

Carter on what she hopes to accomplish in the next decade: "First, to use my technical expertise to help efficient generation of renewable fuels needed for heavy-duty transportation from photo- or electrocatalysis become a reality. Second, to use my position as an administrative leader to improve the climate in physical sciences and engineering such that an increasing number of talented people of all backgrounds choose to make our disciplines their life's work."

What her colleagues say: "Professor Carter is one of the world's leading developers of new theoretical methods for chemistry and materials. The models she has developed have enabled the accurate theoretical study of a broad array of important grand-challenge problems, such as the discovery and design of molecules and materials for sustainable energy. Her insightful analyses of phenomena that range from surface science to photovoltaics and photocatalysis to metal-oxide semiconductors are legendary."—Mark Gordon, Iowa State University

ACS Award in Pure Chemistry: Mircea Dincă

Sponsor: Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation

Citation: For innovative developments in chemical synthesis enabling permanently porous materials to be endowed with desirable properties such as electrical conductivity.

Current position: associate professor of chemistry, Massachusetts Institute of Technology

Education: B.A., chemistry, Princeton University; Ph.D., chemistry, University of California, Berkeley

Dincă on what he hopes to accomplish in the next decade: "I hope to become a little less intimidated by disorder, in the chemical sense. I find it fascinating that many of the most complex systems, be it biological or human-made, are woefully—and often necessarily—devoid of symmetry or order in the canonical sense. I really want to learn more about how one can make an ally of disorder and asymmetry and ultimately use these concepts to create materials that translate molecular properties to macroscopic function in unexpected ways."

What his colleagues say: "Mircea Dincă is the most creative and insightful young inorganic chemist I have come across in recent years. He is bringing into existence at a blistering pace new knowledge that comes from thinking about materials chemistry at a fundamentally molecular level."—Christopher C. Cummins, Massachusetts Institute of Technology

Award for Volunteer Service to the American Chemical Society: Carol A. Duane

Sponsor: ACS

Citation: For her passion and work in ACS volunteer efforts to empower members with the skills to lead within ACS, their workplace, and their community.

Current position: president, D&D Consultants of Mentor

Education: M.S., chemistry, Ohio State University

Duane on her volunteer role model and why: "My volunteer role models range from chemistry's most eminent scientists to innumerable ACS colleagues and the chemists in my family. With their willingness to give back to the profession and the enterprise, they convinced me that chemists are natural leaders. It is essential that new ACS leaders are prepared to respond to the future with the knowledge and skills that will allow them to lead in the society, their workplaces, and their communities."

What her colleagues say: "Her work is exemplary. She gives freely of her time and talents and treasures truly making a difference in people's lives. I can think of no one who more completely embodies the tenants, purpose, and requirements of this significant recognition."—Tom Lane, retired from Dow Corning and an ACS past president

Earle B. Barnes Award for Leadership in Chemical Research Management: Margaret M. Faul

Sponsor: Dow Chemical Foundation

Citation: For focusing on the career development of scientists to deliver practical solutions to synthesize new chemical entities to treat patients with grievous illnesses.

Current position: executive director of process development, Amgen

Education: B.Sc., chemistry, pharmacology, University College Dublin; M.Sc., organic chemistry, University College

Dublin; Ph.D., synthetic organic chemistry, Harvard University

Faul on what she hopes to accomplish in the next decade: "I hope to continue to advance the commercialization of new drugs to treat grievous illness, especially in the area of oncology. I have lost too many friends and family to cancer. As chemists and engineers, we will be challenged with designing novel, efficient, and scalable processes to bring these medicines from the lab to the factory, and ultimately into the hands of patients. Knowing that my work ultimately serves patients suffering from grievous illness motivates me to come to work every day."

What her colleagues say: "Margaret has had a high-impact career that has led to taking over management responsibilities of increasing magnitude over the last 20 years. She continues to demonstrate excellence in executive leadership and management of highly trained scientific staff."—Jerry Murry, Amgen

Irving Langmuir Award in Chemical Physics: George W. Flynn

Sponsor: ACS and the ACS Division of Physical Chemistry

Citation: For contributions to our fundamental understanding of the structural and chemical behavior of graphene interfaces.

Current position: Eugene Higgins Professor of Chemistry, Columbia University

Education: B.S., chemistry, Yale University; Ph.D., chemistry, Harvard University

Flynn on his scientific role model and why: "Four mentors have had a significant influence in determining the course of my scientific career: my high school chemistry teacher, Mr. Coburn, who made chemistry a remarkably clear discipline and introduced me to independent research; Ali Javan, who taught me to think like a physicist about the interaction of light and matter; and John Baldeschwieler and E. Bright Wilson, who were my Ph.D. mentors and taught me the importance of clear thinking in scientific discussions and about being fearless in attacking new research areas."

What his colleagues say: "In groundbreaking work, he demonstrated that single sheet graphenes are much more reactive than multiple sheet materials. His fundamental work will surely be of great help to investigators who are working on electronic devices based on graphene and doped-graphene materials."—Harry B. Gray, California Institute of Technology

Herbert C. Brown Award for Creative Research in Synthetic Methods: Gregory C. Fu

Sponsor: Purdue Borane Research Fund and the Herbert C. Brown Award Endowment

Citation: For the development of nickel- and copper-catalyzed cross-coupling methods and of nucleophile-catalyzed enantioselective reactions.

Current position: Norman Chandler Professor of Chemistry & Chemical Engineering, California Institute of Technology

Education: B.S., chemistry, Massachusetts Institute of Technology; Ph.D., chemistry, Harvard University

Fu on what he hopes to accomplish in the next decade: "During the next decade, we hope to provide general solutions to coupling a wide range of nucleophiles and alkyl electrophiles, including enantioconvergent processes. We believe that success in this area could be transformative for organic synthesis."

What his colleagues say: "Fu has made several pathfinding contributions to the development of synthetic methods that have impacted the way that chemists think about building organic molecules."—Peter Dervan, California Institute of Technology

Ralph F. Hirschmann Award in Peptide Chemistry: Lila M. Gierasch

Sponsor: Merck Research Laboratories

Citation: For her seminal contributions to peptide structure and function, peptide models for protein folding and function, and roles of peptide and protein aggregation in disease.

Current position: Distinguished Professor of Biochemistry & Molecular Biology and Chemistry, University of Massachusetts, Amherst

Education: A.B., chemistry, Mount Holyoke College; Ph.D., biophysics, Harvard University

Gierasch on what she hopes to accomplish in the next decade: "The environment in a cell is extremely complex and challenging for the process of protein folding, leading to a need for a network of species that protect protein states that are susceptible to aggregation—the protein homeostasis network. We are working with colleagues and collaborators to understand the underlying mechanisms of protein homeostasis from the level of the molecular chaperone machines that act on protein clients to the coordinated action of the network in all of its complexity. We would love to witness and contribute to new discoveries related to these questions, both because of the fascinating basic science involved and because failures in these systems are implicated in a wide array of diseases, including neurodegenerative diseases."

What her colleagues say: "Lila demonstrates the highest levels of scientific creativity in her research. During the past 40 years, she has made seminal contributions to our understanding of peptide structure and function, the mechanisms by which sorting peptides direct intracellular protein trafficking, the roles of molecular chaperones in protein folding, the interplay among secondary structural elements in determining the tertiary structure of proteins, and understanding the role of peptide and protein aggregation in disease."—Joel Schneider, National Cancer Institute

ACS Award in Analytical Chemistry: Michael L. Gross

Sponsor: Battelle Memorial Institute

Citation: For development of mass spectrometry methods that provide insight in physical-organic chemistry, enable environmental protection, offer new approaches in biochemistry and biophysics, and give understanding of human disease.

Current position: professor of chemistry, Washington University in St. Louis and professor of immunology and internal medicine, Washington University School of Medicine

Education: B.A., chemistry, Saint John's University (Collegeville, Minn.); Ph.D., organic chemistry, University of Minnesota, Twin Cities

Gross on his scientific role model and why: "My role model is my postdoc mentor, Fred McLafferty, because he has a passion for science and ambition to contribute something important."

What his colleagues say: "Mike is one of the most recognized leaders in the field of mass spectrometry and analytical chemistry. I have known him for nearly 30 years, and I have been impressed with his productivity, the many students who have come from his lab, his service to the community, and his innovation."—Evan R. Williams, University of California, Berkeley

ACS Award for Affordable Green Chemistry: Frank Gupton and D. Tyler McQuade

Sponsor: Dow Chemical and endowed by Rohm and Haas

Citation: For their outstanding success in developing a sustainable and efficient synthesis of nevirapine through a process intensification that reduced cost and improved access to HIV/AIDS treatment.

What their colleagues say: "The Gupton-McQuade results demonstrate the reinvention of pharmaceutical processes resulting in dramatic reductions in process mass intensity and increasing access to medications through sustainable improvements in process chemistry."—Julie B. Manley, Guiding Green

Frank Gupton

Current position: Floyd D. Gottwald Professor and chair, department of chemical and life science engineering, Virginia Commonwealth University

Education: B.S., chemistry, University of Richmond; M.S., chemistry, Georgia Institute of Technology; Ph.D., chemistry, Virginia Commonwealth University

Gupton on what he hopes to accomplish in the next decade: "We recently established the Medicines for All Institute at Virginia Commonwealth University in collaboration with the Bill & Melinda Gates Foundation. The mission of the institute is to expand global access to lifesaving medications by finding new ways to make them more efficiently. I expect in doing so that we can effect significant improvements in the way drugs are produced in the 21st century."

D. Tyler McQuade

Current position: professor of chemical and life science engineering, Virginia Commonwealth University

Education: B.S., chemistry and biology, University of California, Irvine; Ph.D., chemistry, University of Wisconsin, Madison

McQuade on his work: "It is beyond gratifying on both a personal and professional level to know that Frank and I—with the support of our incredibly talented teams—have not only advanced the field of efficient synthesis in significant ways through our work but have directly improved the lives and health of people worldwide we'll likely never meet."

ACS Award in Applied Polymer Science: Paula T. Hammond

Sponsor: Eastman Chemical

Citation: For her work in polymeric electrostatic thin film assembly and its translational application to the fields of electrochemical energy and controlled drug delivery.

Current position: David H. Koch Chair Professor of Engineering, Massachusetts Institute of Technology

Education: B.S., chemical engineering, MIT; M.S., chemical engineering, Georgia Institute of Technology; Ph.D., chemical engineering, MIT

Hammond on what gets her creative juices flowing: "I get excited when I hear people speak who work in entirely different fields because that is how I get to learn about challenging problems I didn't know existed."

What her colleagues say: "Simply put, Paula is not only an absolutely top innovator in polymer science but is also a most generous human being. Her impact as an iconic, inspirational, and compassionate leader in science and engineering cannot be overstated."—Timothy M. Swager, MIT

George & Christine Sosnovsky Award for Cancer Research: Paul J. Hergenrother

Sponsor: George & Christine Sosnovsky Endowment Fund

Citation: For his many achievements in new compounds, targets, and translational pathways for cancer therapy, including the treatment of canine/feline patients with spontaneous cancer.

Current position: Kenneth L. Rinehart Jr. Endowed Chair in Natural Products Chemistry and professor of chemistry, University of Illinois, Urbana-Champaign

Education: B.S., chemistry, University of Notre Dame; Ph.D., chemistry and biochemistry, University of Texas, Austin

Hergenrother on what gets his creative juices flowing: "It is an amazing time to be in anticancer research, with rapid advances in targeted therapy and immunotherapy. The challenge now is making the leap from short-lived responses and low percentage of responders to durable responses and cures in large numbers of patients. This leap will require a detailed understanding of the vulnerabilities of each patient's cancer, coupled with the identification of drugs that can exploit these defects."

What his colleagues say: "Paul exemplifies all of the best characteristics of an academic scientist dedicated to carrying out translational research that will genuinely impact people's lives. He is willing to take chances in tackling—from start to finish—the most important types of problems, and this approach has reaped dividends; he has taken an anticancer strategy from conception of a novel target, to screening and drug development, and to Phase I clinical trial—a feat that is almost unprecedented in academics."—Scott E. Denmark, University of Illinois, Urbana-Champaign

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Seth B. Herzon

Sponsor: Pfizer Endowment Fund

Citation: For bold and creative contributions to the scalable total synthesis of complex natural products and organic methodology.

Current position: professor of chemistry, Yale University

Education: B.S., chemistry, Temple University; Ph.D., chemistry, Harvard University

Herzon on what gets his creative juices flowing: "Talking chemistry with my students. Nearly every success we've recorded has come directly from a student or from conversations with them."

What his colleagues say: "Seth's research program is simply stunning in terms of demonstrated creativity, capacity to solve truly difficult problems in synthesis, and sheer innovation."—Phil S. Baran, Scripps Research Institute

Frederic Stanley Kipping Award in Silicon Chemistry: Tamejiro Hiyama

Sponsor: Dow Corning

Citation: For the invention of silicon-based cross-coupling reaction and related synthetic reactions.

Current position: professor emeritus, Kyoto University, and RDI Professor, Chuo University

Education: B.Eng., Kyoto University; M.Eng., Kyoto University; D.Eng., Kyoto University

Hiyama on his biggest research challenge: "Because C–Si bonds are quite stable in general, nucleophilic activation is essential for transmetalation from silicon to transition metals. This is the key of the silicon-based palladium-catalyzed cross-coupling reaction and is applied to rhodium-catalyzed conjugate addition of organosilicon reagents to enones and enamides. Naturally, activation of more stable C–H or C–C bonds using transition-metal catalysts is the next challenge for making new C–C bonds."

What his colleagues say: "Although the Nobel Prize in Chemistry for 2010 was given for contributions to palladium-catalyzed cross-coupling reactions, Tamejiro's contributions to expand the approach to silicon-based cross-couplings are similarly remarkable. This was indeed a dream for many organosilicon chemists. Since this discovery in 1988, he has devoted himself to exploring the potential of silicon-based cross-couplings, inventing new reactions that have raised the synthetic value of silicon chemistry in organic syntheses. Needless to say, the reaction is now called Hiyama coupling."—Ei-ichi Negishi, Purdue University

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Jani C. Ingram

Sponsor: Camille & Henry Dreyfus Foundation

Citation: For her outstanding accomplishments in recruiting and mentoring students from underrepresented groups, especially American Indians and Alaskan Natives, into professional careers in chemistry.

Current position: professor of chemistry and biochemistry, Northern Arizona University

Education: B.S., chemistry, New Mexico State University; Ph.D., chemistry, University of Arizona

Ingram on what she hopes to accomplish in the next decade: "I hope to see the number of Native Americans with Ph.D.s in chemistry increase by a factor of 100. There are not many of us now, so I believe that such a large increase is possible with the opportunities that exist as well as the issues that need to be addressed by people within Native American communities."

What her colleagues say: "American Indian and Alaskan Native (AIAN) professionals are the most severely underrepresented U.S. racial or ethnic group in STEM disciplines, and successful degree completion for even a few individuals can impact national totals. Over her time at NAU, Dr. Ingram has directly or indirectly recruited and mentored more than 200 AIAN students in chemistry and related STEM disciplines, at both undergraduate and graduate levels. Her identity as one of a handful of our native faculty in the sciences has been a magnet for minority students, and her insights into academic and cultural barriers have shaped her highly effective approach to mentoring."—Laura Foster Huenneke, Northern Arizona University

ACS Award for Creative Invention: Robert S. Kania

Sponsor: ACS Corporation Associates

Citation: For work leading to the invention of axitinib (Inlyta), a novel VEGFR kinase inhibitor, as a treatment for renal cell carcinoma.

Current position: senior director of oncology drug design chemistry, Pfizer

Education: B.S., chemistry, University of California, Berkeley; Ph.D., chemistry, Harvard University

Kania on what he hopes to accomplish in the next decade: "My goal over the next decade is to contribute to the discovery of a new cohort of small-molecule medicines to treat cancer. Each new breakthrough area in cancer gives me, and the colleagues I work with, opportunities to learn about breaking science and discover small-molecule drugs. Just like the rewarding experience of our drug discovery efforts directed toward finding antiangiogenic drugs and targeted therapies for specific tumor-intrinsic mutations, where we have seen our molecules reach patients, my hope is that our ongoing efforts will lead to the discovery of small-molecule drugs for immuno-oncology and epigenetic targets that will reach patients in the next 10 years."

What his colleagues say: "Rob's invention of axitinib (Inlyta), a rationally designed inhibitor of VEGFR that is effective against a range of solid tumors, is one of the most significant of recent years in cancer chemotherapeutics. Inhibiting VEGFR with a small molecule had long been an unmet challenge. The invention of axitinib will not only benefit countless cancer sufferers but also stimulate further advances in other areas of medicine. Rob has continued to invent and achieve at an extraordinary level and will surely go on to other remarkable feats of discovery."—E. J. Corey, Harvard University

ACS Award for Creative Work in Fluorine Chemistry: Erhard Kemnitz

Sponsor: ACS Division of Fluorine Chemistry

Citation: For his studies on nanoscopic fluorinated materials that provided the foundation for a novel research field, which exhibits a high impact for fundamental and applied research.

Current position: professor of inorganic chemistry, Humboldt University of Berlin

Education: Diplom (master's degree equivalent) and Ph.D., chemistry, Humboldt University of Berlin

Kemnitz on his scientific role model and why: "My professional inspiration is based on Wilhelm von Humboldt's holistic concept of education and the principle of unity of research and teaching. Interactions with my undergraduate and graduate students and collaborators keep me young and creative. Their perspectives impact my research by stimulating questions and reflections on scientific problems. Their input and contributions are invaluable to me to be creative and enthusiastic in what I do as a researcher and teacher."

What his colleagues say: "Professor Kemnitz is one of the world's leading experts in the field of solid-state fluorine chemistry, from fundamental chemistry to industrial applications. A striking achievement was his group's development of the fluorolytic sol-gel route, which has opened new doors into the chemistry of monodisperse nanometal fluorides. Kemnitz and coworkers are the world-leading group in this technique. It is likely to be very useful even beyond academia, and several cooperative projects with industry are still ongoing. In short, professor Kemnitz is an outstanding scientist in the fluorine chemistry community and has made very important contributions to this field."—Sebastian Riedel, Free University of Berlin

James Bryant Conant Award in High School Chemistry Teaching: Brian J. Kennedy

Sponsor: *Journal of Chemical Education* and ChemEd X

Citation: For leadership in promoting student research at the high school level for his students and other students.

Current position: director of the Chemical Analysis & Nanochemistry Research Laboratory, Thomas Jefferson High School for Science & Technology

Education: B.S., chemistry, and B.S., physical science, Radford University; Ph.D., analytical chemistry, University of Wyoming, Laramie; Master of Education, George Mason University

Kennedy on what he hopes to accomplish in the next decade: "I hope to further develop the chemistry research program at my school by creating partnerships with local groups, university researchers, and labs in order to provide students with collaborations and real-world-relevant projects. Toward this end, I would like to be able to develop a high school-level chemical instrumentation textbook so that similar programs can be developed in other schools."

What his colleagues say: "My experiences working in Dr. Kennedy's research lab prepared me incredibly well for college. As a high school student, I experienced all aspects of the research process, from the formation of a research idea to presenting my work at the Virginia State Science and Engineering Fair and tjSTAR school symposium. While always available for guidance when necessary, he allowed me a tremendous amount of independence to develop a procedure, conduct the experiment, and collect data."—Caroline Kerr, University of Virginia

ACS Award in Organometallic Chemistry: Clifford P. Kubiak

Sponsor: Dow Chemical Foundation

Citation: For his groundbreaking and detailed studies of the reduction of carbon dioxide by transition-metal catalysts.

Current position: professor of chemistry, University of California, San Diego

Education: B.S., chemistry, Brown University; Ph.D., chemistry, University of Rochester

Kubiak on his biggest research challenge: "The biggest challenge was setting up my lab as an assistant professor and training the first group of students without any senior students or postdocs in the lab to help. Those first experiments, when they worked, were thrilling. Almost everything since then has seemed easier, even though I think our science is being performed on a higher level. Some of our biggest challenges have been to understand the selectivity of CO_2 reduction catalysts that produce only CO, even when there are enormous quantities of protons available that could be reduced to the thermodynamically more stable product, H_2."

What his colleagues say: "With the tremendous global interest in carbon-based solar fuels, the Kubiak laboratory has become one of the most important centers internationally for studies of the reduction of CO_2. His most recent work defines the best and most advanced understanding of mechanisms of the catalytic reduction of CO_2 to higher energy content carbon-based fuels and fuel precursors."—Guy Bertrand, University of California, San Diego

Francis P. Garvan-John M. Olin Medal: Valerie J. Kuck

Sponsor: Francis P. Garvan-John M. Olin Medal Endowment

Citation: For pioneering research on coatings for optical fibers and copper wire and for transformative achievements leading to a more diverse and inclusive chemical profession.

Current position: retired researcher, Bell Labs

Education: B.S., chemistry, St. Mary of the Woods College; M.S., chemistry, Purdue University

Kuck on what gets her creative juices flowing: "I am driven by the ideal of making things better for the next generation. I am proud to have been the originator of Sci-Mix. It bothered me greatly to see so many young national meeting attendees who were just hanging around the hotel lobbies on Monday night. They had not established their networks, and I reasoned that a large poster session would help them meet other scientists with similar interests. I am also proud of the two presidential symposia, High Tc Super Conductors and Cold Fusion, that I organized in a couple of days just before a national meeting. Those symposia allowed the meeting attendees an opportunity to hear the latest research findings as news of those efforts was just breaking."

What her colleagues say: "In all, Valerie's research led to 25 patents and 26 technical publications published in top peer-reviewed journals. Valerie's service to chemistry and to the American Chemical Society is almost without peer. The theme of her work is creating a more diverse and inclusive chemical profession with a focus on gender, ethnic, and racial diversity, as well as on the needs of bachelor/master's chemists and industrial chemists, who have been underrepresented as recipients of national awards, in holding national offices, and even in ACS programs that serve these constituencies."—Madeleine Jacobs, Council of Scientific Society Presidents

ACS Award in Industrial Chemistry: George P. Lahm

Sponsor: ACS Division of Industrial & Engineering Chemistry

Citation: For his outstanding accomplishments in the discovery of the anthranilamide class of insecticides and the commercialization of Rynaxypyr and Cyazypyr.

Current position: DuPont Fellow, DuPont

Education: B.S., chemistry, State University of New York; Ph.D., organic chemistry, Indiana University

Lahm on what he hopes to accomplish in the next decade: "There is a constant need to renew crop protection products to fight the extraordinary ability of crop pests to develop resistance. The single best way to meet this challenge is to identify molecules that act by new biological mechanisms. My continuing objective is to find these molecules and bring them forward to create a sustainable pipeline of tools for today and well into the future."

What his colleagues say: "Lahm has a truly rare combination of abilities in organic synthesis, scientific leadership, and business acumen combined with an innate ability to recognize the promise of areas which have not yet been exploited. These traits single him out as a true outlier in field of crop protection as someone who is able to make extraordinary contributions to his discipline."—Thomas Stevenson, DuPont

Alfred Burger Award in Medicinal Chemistry: Dennis C. Liotta

Sponsor: Gilead Sciences

Citation: For inventing antiviral drugs that more than 90% of HIV-infected persons on therapy in the U.S. take or have taken.

Current position: Samuel Candler Dobbs Professor of Chemistry, Emory University

Education: B.A., chemistry, Queens College, City University of New York; Ph.D., chemistry, City University of New York

Liotta on his scientific role model and why: "Although I have many scientific role models, the one that inspired me the most was Gertrude (Trudy) Elion, the 1988 Nobel laureate in Physiology or Medicine. She was, of course, brilliant and creative. But she also had to struggle throughout most of her professional life to get the recognition she so amply deserved. When she had an idea that she believed in, she pursued it relentlessly until she figured out how to make it work. Creativity without persistence probably won't result in anything of lasting value."

What his colleagues say: "As one of the discoverers of the antiviral agent FTC and numerous other antiviral agents, professor Liotta has changed the lives of countless numbers of HIV/AIDS patients. Not only are these drugs extremely effective in controlling the virus, but their incorporation into once-daily treatment combinations has significantly enhanced the quality of life of these individuals."—George R. Painter, Emory University

Ronald Breslow Award for Achievement in Biomimetic Chemistry: David R. Liu

Sponsor: Ronald Breslow Award Endowment

Citation: For the development and application of powerful methods that integrate biomimetic chemistry and biological evolution to solve major problems in chemistry, biology, and medicine.

Current position: professor of chemistry and chemical biology, Harvard University, and Richard Merkin Professor and director of the Merkin Institute of Transformative Technologies in Healthcare, Broad Institute of MIT & Harvard

Education: B.A., chemistry, Harvard University; Ph.D., chemistry, University of California, Berkeley

Liu on what gets his creative juices flowing: "Playing! Being fortunate enough to have a job that is almost always highly enjoyable means that every day feels like playing with molecular or cellular Legos."

What his colleagues say: "David Liu is an outstanding, gifted, and remarkably accomplished scientist whose work defines the very essence of modern biomimetic chemistry."—Alanna Schepartz, Yale University

Gabor A. Somorjai Award for Creative Research in Catalysis: David W. C. MacMillan

Sponsor: Gabor A. & Judith K. Somorjai Endowment Fund

Citation: For his pioneering work in the development of organocatalysis, including fundamentally new methods based on radical intermediates, SOMO catalysis, and photoredox catalysis.

Current position: James S. McDonnell Distinguished University Professor of Chemistry and chair of the department of chemistry, Princeton University

Education: B.Sc., chemistry, University of Glasgow; Ph.D., organic chemistry, University of California, Irvine

MacMillan on what gets his creative juices flowing: "An unusual result, a key insight, or a new understanding of a chemical concept that you have found in the lab. It's like finding a hidden trap door in the back of an attic and when you look down inside—it's full of gold (or even wine). It's a great feeling when it happens, and I only wish it would happen more often."

What his colleagues say: "Organocatalysis has become the single most published-on field of catalysis in the world. Moreover, primarily due to MacMillan's contributions, practical applications on large scale have begun to emerge. Further, a second field that he invented, photoredox catalysis, has the promise to be even more important than organocatalysis. MacMillan's work has been carried out with an exceptional level of scholarship, focusing on what is important and conceptually innovative. His work has been and will continue to be used by others."—Stephen L. Buchwald, Massachusetts Institute of Technology

National Fresenius Award: Thomas J. Maimone

Sponsor: Phi Lambda Upsilon, the National Chemistry Honor Society

Citation: For accomplishments in the field of synthetic organic chemistry, especially in the development of streamlined synthetic routes to complex natural products.

Current position: assistant professor of chemistry, University of California, Berkeley

Education: B.S., chemistry, University of California, Berkeley; Ph.D., chemistry, Scripps Research Institute

Maimone on what gets his creative juices flowing: "Being presented with a new target molecule. It's like meeting a new person. You might at first think you have met someone similar and have preconceived notions about them, but as you converse further you realize their uniqueness. If you find that you really like this new molecule (for either biological or structural reasons), you want to get to know it better—and ideally synthesize and study it."

What his colleagues say: "Total synthesis is a barometer for how the field of chemical synthesis is advancing, and the Maimone lab is leading the way in showing that it is possible to make even the most complex terpenes in a practical and innovative way. For anyone that thinks this field is stale, boring, or mature, please just look at the schemes of any one of his papers."—Phil S. Baran, Scripps Research Institute

Kathryn C. Hach Award for Entrepreneurial Success: Javier García-Martínez

Sponsor: Kathryn C. Hach Award Fund

Citation: For his visionary leadership creating a successful, dynamic company bringing mesostructured zeolites to the refining industry.

Current position: professor of inorganic chemistry, University of Alicante

Education: B.Sc., M.S., and Ph.D., chemistry, University of Alicante

García-Martínez on his biggest research challenge: "I am very interested in the mechanism that allows zeolites to rearrange to incorporate mesoporosity into their structure. We have a lot of data that prove that the zeolite crystals reorganize themselves without dissolving, but the actual mechanism behind this new and puzzling phenomenon is still unclear. I am collaborating with some of the best scientists to solve this problem, but it is a major and exciting challenge that will keep us busy for several years."

What his colleagues say: "I have been impressed by Javier's ability to build an excellent team of business and technical employees and advisers."—Hong-Xin Li, Zeolyst International

ACS Award in Inorganic Chemistry: James M. Mayer

Sponsor: Aldrich Chemical

Citation: For explaining and applying the principles of proton-coupled electron-transfer reactions in catalysis and bioinorganic chemistry.

Current position: Charlotte Fitch Roberts Professor of Chemistry, Yale University

Education: A.B., chemistry, Harvard University; Ph.D., chemistry, California Institute of Technology

Mayer on what he hopes to accomplish in the next decade: "The most important thing that I do is to mentor students and postdocs, to stimulate, challenge, and support them from the large freshman classroom to the one-on-one interactions in my research lab. The growth and success of the students is tremendously rewarding. Scientifically, I would like to expand the reach and influence of the concepts of proton-coupled electron transfer. The newest direction in my group is to explore the impact of these ideas in the chemistry of materials and interfaces."

What his colleagues say: "Jim's research, which focuses on the chemistry and mechanism of atom and group transfer reactions, has been creatively conceived, thoughtfully analyzed, and beautifully executed. His early work aimed to understand the nature and opportunities for metal complexes with multiple bonds to O and N. As is typical of Jim and his scholarship, he did not just discover new reactions, he provided broad conceptual models in his book with Bill Nugent, "Metal-Ligand Multiple Bonds," and in insightful analyses in *Accounts of Chemical Research*. This work still stands as a landmark in the field."—Richard Eisenberg, University of Rochester

ACS Award in Separations Science & Technology: Massimo Morbidelli

Sponsor: Waters Corp.

Citation: For outstanding sustained contributions in fundamental understanding of preparative chromatography and development of innovative processes for the application of continuous countercurrent chromatography in biomanufacturing.

Current position: professor of chemical reaction engineering and separation technology, Swiss Federal Institute of Technology (ETH), Zurich

Education: dottore in ingegneria chimica (equivalent to an M.S.), Politecnico di Milano; Ph.D., chemical engineering, University of Notre Dame

Morbidelli on what gets his creative juices flowing: "In my everyday life, I often end up discussing with my students some set of data that they produced or found in the literature. We always try to understand and explain at a fundamental level each detail behind these, and this inevitably generates a number of exciting questions and new ideas." As good engineers, we then select a few based on their impact on industry and society."

What his colleagues say: "Morbidelli's work has been instrumental in transforming the art of biochromatography into its science and engineering. Because of his contributions, more efficient, more robust, and more rapidly developed processes are possible today in biopharmaceutical manufacturing, improving the ability to bring drugs to the patient faster and with reduced cost."—Giorgio Carta, University of Virginia

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Oliver C. Mullins

Sponsor: George A. Olah Award Endowment

Citation: For fundamental contributions codified in the Yen-Mullins model of asphaltenes and asphaltene thermodynamics, in pioneering downhole fluid analysis, and in leading reservoir fluid geodynamics.

Current position: science advisor, Schlumberger-Doll Research

Education: B.S., biology, Beloit College; M.S. and Ph.D., chemistry, Carnegie Mellon University

Mullins on his scientific role model and why: "My father, William Wilson Mullins, is my scientific role model. He was a famous thermodynamicist and loved probing discussions in science and broadly in all areas of human endeavor. I learned more science at our dinner table than anywhere else. He created an atmosphere of open discussion with contribution by all. I try hard to emulate his leadership."

What his colleagues say: "Oliver C. Mullins's name is synonymous with the science of asphaltenes. His pioneering contributions spanning from the early 1990s have unveiled and quantified the nature of colloidal-like asphaltenes. These efforts have been transformational in petroleum science."—Michael L. Klein, Temple University

ACS Award in Chromatography: Janusz B. Pawliszyn

Sponsor: MilliporeSigma

Citation: For the invention, development, and commercialization of universal, ultraviolet, and fluorescence modes of whole-column imaging detection technology.

Current position: professor of chemistry and Canada Research Chair, University of Waterloo

Education: B.S., engineering, and M.S., bioorganic chemistry, Technical University of Gdansk; Ph.D., analytical chemistry, Southern Illinois University

Pawliszyn on what gets his creative juices flowing: "Designing analytical technologies that facilitate reducing the footprint of human activities on Earth. This means developing ethical, miniaturized tools that eliminate use of toxic solvents and reagents and allow on-site screening—reducing the amount of resources required to make analytical measurements."

What his colleagues say: "Janusz has impacted the field of chromatography incredibly, in particular in methods for quantitative and qualitative analysis of trace compounds. As one outstanding example of his contributions to the field, he invented the solid-phase microextraction technique in the late 1980s. This technique has now grown into a preconcentration method that is used in a large range of chromatographic methods, including environmental, forensic, bioanalytical, as well as clinical studies."—Susan V. Olesik, Ohio State University

ACS Award for Research at an Undergraduate Institution: Joseph J. Pesek

Sponsor: Research Corporation for Science Advancement

Citation: For his research on the synthesis and characterization of chromatographic separation materials and the development of analysis methods and protocols.

Current position: professor of analytical chemistry, San Jose State University

Education: B.S., chemistry, University of Illinois, Urbana-Champaign; Ph.D., analytical chemistry, University of California, Los Angeles

Pesek on his biggest research challenge: "When we first introduced silica hydride as a support material for HPLC, it was met with considerable skepticism. Many people thought it was unstable based on a false comparison to small organosilanes. In fact one reviewer made an amusing comparison to cold fusion. After more than 20 years of use in laboratories around the world, I believe that silica hydride has proved to be more viable than cold fusion."

What his colleagues say: "Joe is internationally recognized for his contributions in the development of novel chromatographic separation materials and the development of analysis methods. The silica hydride technology he and his students developed for making liquid chromatographic bonded stationary phases has such unique properties that LC columns made by his methods are commercially available."—Thomas J. Wenzel, Bates College

Peter Debye Award in Physical Chemistry: Paras N. Prasad

Sponsor: DuPont

Citation: For pioneering contributions in nonlinear optics and multiphoton processes in molecular, polymeric, nanoscale, and biological materials with profound impact in nanophotonics, biophotonics, and metaphotonics.

Current position: executive director, Institute for Lasers, Photonics& Biophotonics, and SUNY Distinguished Professor of Chemistry, Physics, Electrical Engineering & Medicine, University at Buffalo

Education: B.Sc., chemistry, Bihar University; M.Sc., chemistry, Bihar University; Ph.D., chemistry, University of Pennsylvania

Prasad on what gets his creative juices flowing: "Imagining big, thinking outside of the box, and coming up with a scientific idea that is groundbreaking and at the same time promises to be broadly impacting. Growing up in rural India without electricity and running water, I spent plenty of time lying in the dark and became a dreamer with a great deal of imagination."

What his colleagues say: "Paras's groundbreaking research over four decades has broadly impacted the field of photonics, advancing our understanding of light-matter interactions. I am aware of the high standards of creativity and pioneering contributions to physical chemistry that are represented by prior recipients. Paras exceeds these standards and deserves to be included in this elite group [with] his pioneering contributions."—Mark Ratner, Northwestern University

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids: Lawrence R. Pratt

Sponsor: ExxonMobil Research & Engineering

Citation: For outstanding contributions to the theory of hydrophobic interactions, polar and ionic solutions, and the statistical mechanical treatment of solvation-free energies.

Current position: professor and Herman & George R. Brown Chair in Chemical Engineering, Tulane University

Education: B.S., chemistry, Michigan State University; M.S., chemistry, University of Illinois, Urbana-Champaign; Ph.D., chemistry, University of Illinois, Urbana-Champaign

Pratt on his biggest research challenge: "Understanding water and aqueous solutions well enough to make cogent and plausible responses to long-term questions of astrobiologist collaborators: 'Is water necessary for life?' Our discussion of the physical chemistry was published in 2012 as 'Is Water the Universal Solvent for Life?' In that publication we identified seven other solvents as possibilities—including formamide, which might be produced in planetary environments by combination of H_2O and HCN, thus making even it an available possibility."

What his colleagues say: "Without question, Lawrence Pratt has played a key role in the conceptual development of many different areas of liquid-state science. His work shapes the way we think today both quantitatively and qualitatively about many fundamental theoretical issues. His research uses the most sophisticated theoretical concepts but very often applies them to real problems of direct practical and experimental interest, in the tradition of Joel Hildebrand himself."—John Weeks, University of Maryland

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Thomas B. Rauchfuss

Sponsor: Strem Chemicals

Citation: For leadership crucial to maintaining high standards and advancing inorganic chemistry and for sustained and creative contributions to synthetic inorganic chemistry.

Current position: Larry Faulkner Research Professor of Chemistry, University of Illinois, Urbana-Champaign

Education: B.S., chemistry, University of Puget Sound; Ph.D., chemistry, Washington State University

Rauchfuss on what gets his creative juices flowing: "For me, a great source of inspiration comes from the international nature of the research enterprise. It is striking how much research priorities vary from country to country. These diverse cultures not only affect my scholarship but improve my enjoyment of research."

What his colleagues say: "As a current friendly (but serious) competitor of professor Rauchfuss in the field of biomimetics of hydrogenase enzyme active sites, I have the greatest admiration of his research. He has been at the forefront of several developing areas of research. He is a chemist's chemist and an excellent scientist who simply loves his work. His group has published extensively on very challenging synthetic methods and new chemistries. I'm also impressed with his devotion to teaching undergraduates."—Marcetta Darensbourg, Texas A&M University

ACS Award in the Chemistry of Materials: Elsa Reichmanis

Sponsor: DuPont

Citation: For pioneering research in design and development of polymer/organic materials and processes for advanced electronics and photonics and service to chemistry society.

Current position: Brook Byers Professor of Sustainability, professor of chemical and biomolecular engineering, and Pete Silas Chair in Chemical Engineering, Georgia Institute of Technology

Education: B.S., chemistry, Syracuse University; Ph.D., organic chemistry, Syracuse University

Reichmanis on her scientific role model and why: "I can't say that I have a single scientific role model. Rather, I have several. They are the managers and colleagues at Bell Labs who created opportunities for me to be successful. They led the way through being excellent scientists and leaders, with a commitment to serving the community and making a difference. It's my responsibility to 'pay it forward."

What her colleagues say: "Elsa Reichmanis is a leader in materials chemistry who was the first to recognize how material structure and associated chemical interactions during processing must be considered together when designing new chemistries for advanced technology applications."—Omkaram Nalamasu, Applied Materials

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry: Carol V. Robinson

Sponsor: Waters Corp.

Citation: For developing fundamental processes that allow membrane and soluble protein complexes to retain biologically significant states during mass spectrometry, prompting new fields of research.

Current position: Doctor Lee's Professor of Chemistry, University of Oxford

Education: M.S., chemistry, University of Wales; Ph.D., chemistry, University of Cambridge

Robinson on what gets her creative juices flowing: "The excitement of seeing a new mass spectrum for a protein complex that I never thought we would be able to get into the gas phase. I then like to brainstorm ideas and use my creative juices to try to design further experiments and to try to gain some new mechanistic insight and find out something novel about this protein complex."

What her colleagues say: "Carol has an incredible instinct for important and new breakthroughs in her chosen field of science and just as importantly the ability to do something about them."—Michael T. Bowers, University of California, Santa Barbara

ACS Award for Encouraging Women into Careers in the Chemical Sciences: Rebecca T. Ruck

Sponsor: Camille & Henry Dreyfus Foundation

Citation: For her outstanding accomplishments aimed at enhancing and encouraging women into careers in the chemical sciences.

Current position: director of process research and development, Merck & Co.

Education: A.B., chemistry, Princeton University; Ph.D., chemistry, Harvard University

Ruck on what she hopes to accom-

plish in the next decade: "I aspire to play a significant role in shaping the field of synthetic organic chemistry, both scientifically and culturally. I intend to leverage my position at Merck Process to help continue to push back the frontiers of science—designing new reactions to synthesize complex drug molecules—and serve as a leader in fostering a chemistry community in which innovation is fueled by diversity and my commitment to women in chemistry transforms known challenges into opportunities."

What her colleagues say: "Rebecca has demonstrated a strong and unwavering interest in the development and promotion of women in chemistry. As such she has sponsored, initiated, and participated in many activities aimed at stimulating interest in the field and promoting professional development of those who have chosen chemistry as an educational and/or career path."—Michael H. Kress, Merck Research Laboratories

Josef Michl ACS Award in Photochemistry: Jack Saltiel

Sponsor: Josef Michl Award Endowment

Citation: For groundbreaking studies of photochemical reaction mechanisms, particularly cis-trans photoisomerization.

Current position: professor of chemistry and biochemistry, Florida State University

Education: B.A., chemistry, Rice University; Ph.D., chemistry, California Institute of Technology

Saltiel on his scientific mentor and why: "I owe my deepest gratitude to my teachers: to Mr. Finfrock at San Jacinto High School, whose love of chemistry was contagious and whose teaching made college chemistry seem easy; to Ted Lewis at Rice University, who guided my first steps in research in physical organic chemistry; and to George Hammond at Caltech, who created that Camelot of modern organic photochemistry and made research such fun."

What his colleagues say: "Saltiel is one of the most original, innovative, and active photochemists today and is expected to dominate the field for a number of years to come."—V. Ramamurthy, University of Miami

E. Bright Wilson Award in Spectroscopy: Richard J. Saykally

Sponsor: E. Bright Wilson Endowment

Citation: For the development of powerful new laser spectroscopy technology and its application for pioneering studies of molecular ions, water, and aqueous solutions and their surfaces.

Current position: Class of 1932 Endowed Professor of Chemistry, University of California, Berkeley, and faculty senior scientist in the Chemical Sciences Division, Lawrence Berkeley National Laboratory

Education: B.S., chemistry, University of Wisconsin, Eau Claire; Ph.D., physical chemistry, University of Wisconsin, Madison

Saykally on what gets his creative juices flowing: "Discussing wild and crazy ideas with smart, creative students."

What his colleagues say: "Rich developed powerful new laser spectroscopy technology and its application for pioneering studies of molecular ions, water, and aqueous solutions and their surfaces. Even more important than all the techniques Rich developed is the science he did with them."—Ben McCall and Martin Gruebele, University of Illinois, Urbana-Champaign

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Dwight S. Seferos

Sponsor: Gray Award Endowment

Citation: For the development and implementation of tellurophene and selenophene polymers and photoactive compounds.

Current position: associate professor, University of Toronto

Education: B.S., chemistry, Western Washington University; Ph.D., chemistry, University of California, Santa Barbara

Seferos on his scientific role model and why: "Professor Gary Lampman at Western Washington University got me started down this path. From him I learned that an equal dose of diligence and curiosity leads to success."

What his colleagues say: "Tellurium chemistry instantly distinguishes Seferos's work from that of others who work in these fields. In undertaking the synthesis of these challenging and previously unknown compounds, Seferos has contributed significant new knowledge in chemistry. This new knowledge is important for solar fuels, electronics, and catalysis, all of which are important for meeting long-term challenges in energy."—Douglas W. Stephan, University of Toronto

James T. Grady-James H. Stack Award for Interpreting Chemistry for the Public: Bassam Z. Shakhashiri

Sponsor: ACS

Citation: For celebrating the joy of chemistry with kids of all ages and sparking appreciation of science in an extraordinary number of public engagements and media.

Current position: professor of chemistry, University of Wisconsin, Madison

Education: A.B., chemistry, Boston University; M.Sc., chemistry, University of Maryland; Ph.D., chemistry, University of Maryland

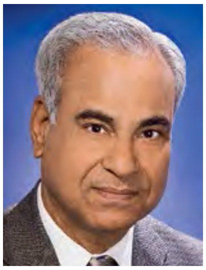
Shakhashiri on what gets his creative juices flowing: "The grand challenges that face society and scientists—the denial of basic human rights, especially the right to benefit from scientific and technological advances, climate change, limited resources, population growth, malnutrition, spreading disease, deadly violence, and war—motivate me to better connect scientists to society and to advocate for our role as scientist-citizens. All in keeping with the ACS mission of advancing the broader chemistry enterprise and its practitioners for the benefit of Earth and its people."

What his colleagues say: "Through an extraordinary number of appearances in person and in the media, Dr. Shakhashiri has shared his love of chemistry with an audience of hundreds of thousands of viewers. Through these outreach activities, he boosts science literacy so the public can make better-informed decisions based on an appreciation of the benefits science brings to their lives."—Glenn Ruskin, American Chemical Society

Glenn T. Seaborg Award for Nuclear Chemistry: Suresh C. Srivastava

Sponsor: ACS Division of Nuclear Chemistry & Technology

Citation: For his outstanding accomplishments in the production and development of many radioisotopes and radiopharmaceuticals that have and continue to provide medical benefit to patients worldwide.



Current position: senior medical scientist emeritus and research adviser in the Collider-Accelerator Department and Medical Isotope Research & Production Program, Brookhaven National Laboratory

Education: B.S., chemistry and biology, Agra University; M.S., organic chemistry, Agra University; Ph.D., nuclear and biological chemistry, University of Allahabad

Srivastava on what he is most proud of: "In the late '70s, I developed the very difficult chemistry behind the medical Tc 'kits' (shake and bake), which continue to be used widely for diagnostic medical imaging. This achievement has saved millions of lives and is still going strong. The most common radioisotope used in diagnosis is technetium-99m, with 40–50 million procedures per year, accounting for about 80% of all nuclear medicine procedures worldwide. There are over 20 million nuclear medicine procedures per year in the U.S."

What his colleagues say: "Srivastava's contributions to radiochemistry and nuclear medicine, and to radiochemistry education, are outstanding. For three decades he has headed the Medical Isotope Research & Production Program at Brookhaven National Laboratory, where he has been instrumental in the introduction and/or development of many important radionuclides and radiolabeling methodologies."—Leonard Mausner, Brookhaven National Laboratory (retired)

ACS Award for Creative Work in Synthetic Organic Chemistry: Brian M. Stoltz

Sponsor: MilliporeSigma

Citation: For the development of efficient methods, particularly cascade reactions, that allow for the efficient synthesis of complex organic molecules.

Current position: professor of chemistry, California Institute of Technology

Education: B.S., chemistry, Indiana University of Pennsylvania; B.A., German, Indiana University of Pennsylvania; M.S., organic chemistry, Yale University; Ph.D., organic chemistry, Yale University

Stoltz on what gets his creative juices flowing: "Creativity is the beauty that underscores the science. I've been incredibly lucky to have had a number of critically important mentors throughout the course of my scientific development. Additionally, I have benefited from exceedingly talented and quite brilliant students and colleagues in my 17 years at Caltech. It is the collective of these individuals that inspires and pushes me to a higher level."

What his colleagues say: "He is well recognized as one of the young leaders in organic synthesis and is one of the few who not only develop both new catalytic methodology but also demonstrate the methods in complex total synthesis."—Robert H. Grubbs, California Institute of Technology

ACS Award for Creative Advances in Environmental Science & Technology: Barbara J. Turpin

Sponsor: ACS Division of Environmental Chemistry, *Environmental Science & Technology*, and *Environmental Science & Technology Letters*

Citation: For revealing the importance of aqueous-phase chemistry in the formation of atmospheric secondary organic aerosol.

Current position: professor and chair of environmental sciences and engineering, Gillings School of Global Public Health, University of North Carolina, Chapel Hill

Education: B.S., engineering and applied science, California Institute of Technology; Ph.D., environmental science and engineering, Oregon Health & Science University

Turpin on what gets her creative juices flowing: "My students will tell you that I can get overly excited during group meetings—brainstorming, daydreaming, and hypothesizing—feeding off the energy that they bring to the room. I love fieldwork, especially in beautiful places. When I go to the field for six weeks, I am able to focus on one thing without interruption. We work in teams helping each other. The camaraderie, beauty, and singleness of mission lead to reflection and creative ideas."

What her colleagues say: "Barbara's creative scientific and technological advances impact even further than air pollution, climate, and human health by contributing to our understanding of how humans are changing the natural cycles of nutrients and thus ecosystems' functioning."—Maria Kanakidou, University of Crete

George C. Pimentel Award in Chemical Education: Pratibha Varma-Nelson

Sponsor: Cengage Learning and the ACS Division of Chemical Education

Citation: For work on face-to-face and cyber versions of Peer Led Team Learning that has facilitated understanding of small-group chemistry learning in the two environments.

Current position: professor of chemistry and founding executive director, STEM Education Innovation & Research Institute, Indiana University-Purdue University Indianapolis

Education: B.Sc., chemistry, University of Pune; Ph.D., organic chemistry, University of Illinois, Chicago

Varma-Nelson on her biggest research challenge: "There were two challenges. First, I started my career at a small institution not known for attracting much external funding, so it was difficult for me to get support for my work. We didn't even have local administrative expertise for how to pursue or manage grants.

Second, although it has been sometimes amusing, it's been challenging to deal with stereotypes about female Indian immigrants being in positions of authority in otherwise traditional settings."

What her colleagues say: "None of her publications, presentations, or awards can begin to describe the personal impact that Dr. Varma-Nelson has had on the field of chemical education, including undergraduates, graduate students, peers, and professional colleagues. No one can interact with Dr. Varma-Nelson without leaving charged with her enthusiasm, passion, and talent for changing how we teach chemistry."—Diane M. Bunce, Catholic University of America

ACS Award in Colloid Chemistry: Håkan Wennerström

Sponsor: Colgate-Palmolive

Citation: For his outstanding contributions to our understanding and applications of the fundamental molecular interactions and forces in complex colloidal, soft-matter, and self-assembling systems.

Current position: professor emeritus in physical chemistry, Lund University

Education: M.S., chemical engineering, Lund University; Ph.D., physical chemistry, Lund University

Wennerström on his biggest research challenge: "Since my days as a graduate student, I have constantly struggled to understand quantum mechanics. I have used the theory to interpret spectroscopic observations and interactions of relevance in colloid science. The work on NMR relaxation highlighted the problem of time reversal symmetry. The interpretation problem is still an enigma, but I constantly make progress in my subjective understanding of the quantum theory."

What his colleagues say: "He is one of our most influential colloidal chemists. Through his long career, he has had a tremendous impact on the field with work that spans from fundamental theory to applications. With his well-known textbook he has also contributed significantly to education."—Ulf Olsson, Lund University

Ernest Guenther Award in the Chemistry of Natural Products: David R. Williams

Sponsor: Givaudan

Citation: For his insightful and creative strategies for the synthesis of biologically active natural products.

Current position: Harry G. Day Professor of Chemistry, Indiana University, Bloomington

Education: B.S., chemistry, St. Lawrence University; Ph.D., organic chemistry, Massachusetts Institute of Technology

Williams on his scientific role model and why: "Remarkable experiences with the late George Büchi and with professors E. J. Corey and the late R. B. Woodward: These iconic leaders fostered the foundation for my career as a researcher and mentor. I have considered Paul Wender and David Evans as outstanding role models of professionalism, scholarship, and creativity. I am also a grateful beneficiary of the unbridled enthusiasm of Al Meyers, Harry Wasserman, and Paul Grieco as they generously took interest in the research of a newly minted assistant professor."

What his colleagues say: "Dr. Williams has a long-standing record of achievement in the synthesis of natural products and in the development of new strategies and methodologies for synthesis, many that are of use in medicinal research and thus of benefit to society. Williams has been a leading figure in natural product chemistry, and his striking and prolific accomplishments are among the finest in the field. His body of work represents the truest traditions of excellence in natural product chemistry."—Paul A. Wender, Stanford University

ACS Award in Polymer Chemistry: C. Grant Willson

Sponsor: ExxonMobil Chemical

Citation: For fundamental advances in synthetic polymer chemistry.

Current position: Rashid Engineering Regents Chair of the departments of chemistry and chemical engineering, University of Texas, Austin

Education: B.S., chemistry, University of California, Berkeley; M.S., organic chemistry, California State University, San Diego; Ph.D., organic chemistry, UC Berkeley

Willson on what gets his creative juices flowing: "Solving problems that matter to others and discussing these problems with terrific graduate students that I have had the honor to work with."

What his colleagues say: "Professor Willson is truly one of the top polymer chemistry innovators of our time and has made many important and impactful discoveries that emphasize the importance of synthetic polymer chemistry. Moreover, his numerous advances have resulted in technological developments with wide-ranging implications. There is no doubt that professor Willson is highly deserving of this award."—Marc Hillmyer, University of Minnesota, Twin Cities

Ahmed Zewail Award in Ultrafast Science & Technology: Xiaoyang Zhu

Sponsor: Ahmed Zewail Endowment Fund established by Newport Corp.

Citation: For his creative study and deep understanding of ultrafast dynamics in nano, molecular, and hybrid materials and interfaces.

Current position: professor of chemistry and Howard Family Chair in NanoScience, Columbia University

Education: B.S., chemistry, Fudan University; Ph.D., physical chemistry, University of Texas, Austin

Zhu on what he hopes to accomplish in the next decade: "What I hope to accomplish will most likely be very different than what I will accomplish. Every research project has turned out to be different than what I outlined in my research proposals and has been full of big surprises. While I focus on fundamental problems of technological or societal importance, such as solar energy conversion, my research path has so far been a random walk guided by my love of solving puzzles."

What his colleagues say: "Xiaoyang has done pioneering work applying ultrafast spectroscopy techniques to energy materials applications. He is among the most creative, ambitious, and successful researchers in ultrafast science at present, both in terms of the novel experimental techniques employed, and in his role in uncovering new understanding of energy and nanomaterials and interfaces, with potentially significant societal as well as scientific impact. He is also a great mentor for the students and postdocs working in his group."—Henry Kapteyn, University of Colorado, Boulder, and KMLabs

Nobel Laureate Signature Award for Graduate Education in Chemistry: Aleksandr V. Zhukhovitskiy (student) and Jeremiah A. Johnson (preceptor)

Sponsor: Avantor Performance Materials

Citation: For pioneering contributions to persistent carbene surface chemistry and the development of materials that bridge polymer networks and supramolecular cage chemistry.

What their colleagues say: "Alex's outstanding, highly productive Ph.D. research in the Johnson lab has contributed profoundly to surface chemistry and polymer network chemistry. In both fields, Alex's innovative work addressed highly challenging questions and opened new areas for investigation by the chemistry community. For example, his surface chemistry work showcased the power of carbenes as functional handles for surface elaboration. Alex also developed polymer metal-organic cage gels, which merged previously disconnected fields of metal-organic cage chemistry and metallogels."—Krzysztof Matyjaszewski, Carnegie Mellon University

Aleksandr V. Zhukhovitskiy

Current position: LSRF Merck Postdoctoral Fellow, University of California, Berkeley

Education: B.A., chemistry, Northwestern University; M.S., chemistry, Northwestern University; Ph.D., chemistry, Massachusetts Institute of Technology

Zhukhovitskiy on his scientific role model and why: "I have numerous scientific role models, including my scientific mentors—beginning with my father, who is also a chemist. Beyond my mentors and my chemistry idols (for example, Hermann Staudinger), I admire such scientists as Richard Feynman and Noam Chomsky for their outspokenness in the face of convention, constitutional curiosity coupled with a genuine knack for and love of teaching, and perhaps most importantly, a profound preoccupation with ethics."

Jeremiah A. Johnson

Current position: associate professor of chemistry, Massachusetts Institute of Technology

Education: B.S., biomedical engineering and chemistry, Washington University in St. Louis; Ph.D., chemistry, Columbia University

Johnson on what gets his creative juices flowing: "Being around brilliant colleagues, including students like Alex, postdocs, faculty, etc. Sometimes, my most creative chemistry-related thoughts occur when I'm playing my guitar, singing in the shower, or dreaming."

COMMENT

Working group looks at immigration's impact on chemistry

TIFFANY HOERTER, CHAIR, ACS COMMITTEE ON ECONOMIC & PROFESSIONAL AFFAIRS
SUSAN BUTTS, CHAIR, ACS WORKING GROUP ON IMMIGRATION & WORK VISAS

In 2016, the ACS Committee on Economic & Professional Affairs (CEPA) chartered a cross-committee working group on immigration and work visas in the U.S. to determine if the American Chemical Society should develop a policy position focused on these topics. Susan Butts, the chair of this working group, provides an update on its progress below. The remainder of this comment is an independent update written by Susan, and the views she expresses are entirely that of the working group.

Hoerter

Butts

Immigration. It is a topic we often hear about in the news, but the focus is usually on terrorism or immigrants who enter a country illegally. How does immigration affect the chemistry community in the U.S.? Has it contributed to the quality of scientific research and the vitality of the economy, or has it created unfair competition for students and workers?

The CEPA-chartered working group on immigration and work visas, which includes representatives from six ACS governance committees having interests related to this policy area, has been gathering information about workforce-related immigration and how ACS members feel about it.

According to the Migration Policy Institute, the percentage of people residing in the U.S. who were not born in the U.S. has remained in the range of 5 to 15% over the past 165 years, dropping to its lowest point in 1970 and climbing to 13.5% by 2015.

Foreign nationals in the U.S. fall in a variety of categories: permanent residents, temporary residents (for example, people with special work visas), or residents living in the U.S. without proper documentation.

Every year, the U.S. grants permanent resident status to approximately 1 million people. These include refugees and asylees, family members of immigrants, immediate relatives of U.S. citizens, and up to 140,000 people with special skills who are admitted under the employment-based preference category. This latter category includes scientists and engineers who are sponsored by their employers.

U.S. universities have attracted many foreign students because of the high quality of undergraduate and graduate education these institutions offer. Data from the 2016 National Science Foundation Survey of Earned Doctorates show that over the past two decades, approximately 40% of chemistry doctorates and 52% of chemical engineering doctorates from U.S. universities have been granted to foreign nationals. However, 2013 data from the NSF longitudinal study of these graduates from U.S. universities, the Survey of Doctorate Recipients, estimates that approximately 95% of chemists and chemical engineers who received Ph.D.s from U.S. universities and are employed in the U.S. are either U.S. citizens or legal permanent residents.

Within some science, technology, engineering, and mathematics disciplines, particularly those related to computer science and other fields in the information technology sector, people are concerned that many jobs in the U.S. are being filled by contracting firms that bring in foreign workers on temporary (typically H-1B) visas. On the basis of data available from the U.S. Department of Labor, it appears that relatively few jobs in the occupation categories of chemist, biochemist, and chemical engineer are being filled by H-1B visa workers.

In addition to concern over foreign students and workers who are in the U.S. legally, people are becoming increasingly concerned about the fate of young people who were brought illegally to the U.S. when they were children. Many are pursuing college education, military service, or employment under the protection of the Deferred Action for Childhood Arrivals (DACA) program (C&EN, April 17, 2017, page 36). Recent action by President Donald J. Trump will end the DACA protections and leave these young people vulnerable to deportation unless the government takes subsequent steps.

The ACS working group polled the members of its constituent ACS governance committees at the recent ACS national meeting in Washington, D.C. When asked, "Do you think that immigration of chemists and related scientists and engineers is good for the U.S. chemistry enterprise?" a majority replied, "Yes." This, however, was a very small sample, and the working group would like to hear from more of our 156,000-plus ACS members.

The working group has created a brief survey about immigration and its impact on the chemistry enterprise to which any ACS member can respond. It includes a few specific questions and a field for comments. To find the survey, go to www.acs.org/policyinput and click on the link under Workforce Related Immigration Policy. Alternatively, members can share their thoughts or questions about workforce-related immigration via an email to policy@acs.org.

Views expressed are those of the author and not necessarily those of C&EN or ACS.

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The Max-Planck-Society strives for gender equity and welcomes applications from all backgrounds. We actively encourage applications from persons with disabilities. Prof. Dr. David G. Heckel, Managing Director, Max Planck Institute for Chemical Ecology, Hans-Knoell-Str. 8, 07745 Jena, Germany, **research@ice.mpg.de, www.ice.mpg.de**

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Newscripts

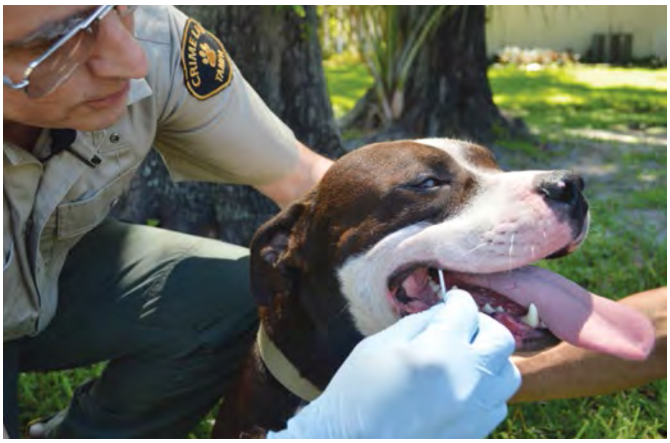
Curating quirky science since 1943

Don't pooh-pooh the solution

Dog poop is something most people avoid. Some even shun the word "poop," preferring "dog mess" instead. But Mark Guarino uses the word in about "every other sentence," he tells Newscripts. That's because the 53-year-old entrepreneur from Tampa, Fla., is building an empire based on thousands of carefully packaged pieces of pooch poo mailed to him from across the country.

A few years ago, Guarino was searching for something new to do after nearly 20 years at his website-hosting and software company. After a couple of false starts at starting a new company, a friend asked Guarino, "Why don't you go pick up dog poop?"

That crappy proposition led Guarino to launch his own pooper-scooper business, Mr. Dog Poop, in January 2015. He soon heard about another company, Knoxville, Tenn.-based BioPet Laboratories, that was offering a dog poop DNA testing service called PooPrints to convict stealthy poopers and help property managers fine the negligent owners.



Profiled pooch: Mark Guarino collects saliva from a dog to add its DNA to his company's database.

"That's stupid, way over the top, and totally unnecessary," Guarino thought at the time.

He quickly changed his mind.

"We packed up the poop-scooping business to become a high-end dog poop DNA company," Guarino says. The rebranded firm now charges property managers $34.95 to submit saliva samples from each resident's dog to build up a DNA database. When a mystery stool from a participating property is mailed to Mr. Dog Poop's lab and matched to a canine culprit in the database, the property is charged $49.95—and the dog's owner is subsequently fined that much, or more.

Starting the genotyping company was harder than Guarino expected. "I had no idea what I was doing," he says. For instance, Guarino bought an old DNA sequencer for a bargain, only to later hear from a geneticist he hired that they would need a newer model. And since sequencing the full genome of every dog would be expensive, Guarino and his team also had to devise a short list of 23 genetic markers that could be amplified from the dog poop while still accurately linking a poo to a pooch.

Canine culprit: When DNA from an anonymous poop matches a dog's DNA from Guarino's database, the owner is fined.

Another unexpected challenge was simply getting stools and saliva from the same dog to see if the DNA matching program was accurate. "No one wanted to work with me," he says. Guarino even tried chasing dogs down in his neighborhood to collect their poop and saliva, to no avail. "A lot of people laughed at us." It was trial by feces.

Eventually Guarino posted an advertisement on Craigslist, offering to pay $40 for a saliva swab and poop sample from the same dog. "We did it around Christmastime, and people lined up," he says. "I think in one day I spent $500 on poop."

Starting the business ended up being more expensive than expected, but Guarino says it's starting to look like it will pay off.

The company's website, replete with cartoons of pooping pooches and detectives investigating the crime scenes, was an instant hit. "People were calling from all over the country," Guarino says. He estimates his lab has processed more than 20,000 dog poop samples from 500 locations in the continental U.S. "We have samples being shipped in on a daily basis," he says. "The local post office is inundated with dog poop."

Mr. Dog Poop has a waiting list of 600 locations. The firm is now the biggest competitor of BioPet, which works with over 2,600 properties.

Both BioPet and Mr. Dog Poop claim their programs have led to cleaner residences. "It holds dog owners accountable," says Jay Retinger, President of BioPet. He notices that more dogs are allowed at some apartments after they join the program.

When a dog's poop is identified, most owners learn their lesson. "We've only caught the same dog twice 25 times," Guarino says.

Ryan Cross wrote this week's column. Please send comments and suggestions to newscripts@acs.org.

CREDIT: MR. DOG POOP (BOTH)