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# Quote of the week

# "Train beats truck; ship beats train."

--Capt. Bill Diehl (ret.), president, Greater Houston Port Bureau Page 18



Illustration by David Mack/ Science Source



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# Editorial No place like home

ast week, the American Chemical Society hosted in Washington, D.C., the 254th ACS National Meeting. Although a large portion of the society's staff is based at CAS in Columbus, Ohio, you could say that D.C. is our home turf because our headquarters are located here. And there is no place like home to celebrate chemistry.

This D.C. meeting came after the record-breaking San Francisco spring event, where nearly 19,000 attendees gathered to talk chemistry, so we started the fall meeting on a high.

And the high continued for the C&EN team. Last week, we were proud to host the second edition of C&EN's Talented 12 symposium. It was the third time that we featured young scientists in the chemical sciences in this way in the magazine but only the second time that we also held a live event.

Our keynote speaker, Caltech's Harry Gray, kicked the morning off, and he was eloquent, entertaining, and insightful. He spoke about his early days and reflected on key events in his life during that time, sharing his view on the thrills of starting an independent career in chemistry and providing guidance on the challenges.

One of the things Gray told the Talented 12 is that "your students think you are better than you really are." He cautioned that "it's okay to make mistakes" and insisted that early-career researchers must make sure "your students understand you can be wrong." He also advised to "hang out with other chemists"-which is not difficult during ACS national meetings-and treasure the moments spent with students and postdocs, especially early in your career, because many will become lifelong friends. He also made a tongue-in-cheek comment about it being okay to collaborate with physicists too, as occasionally they may have ideas worth exploring.

Gray was followed by the Talented 12, who gave TED-style talks highlighting their lines of research. They represented academia, industry, and government and discussed all manner of science, including bioelectronics, immunotheranostics, synthetic opioids, superresolution microscopy, and a field whose name I think was first coined by one of the Talented 12: metalloendocrinology.

These sessions were recorded, so you will be able to get a flavor of what happened when we publish them on C&EN's newly revamped YouTube channel. We'll give you a heads up via social media and our newsletters when they are ready to be viewed in a few weeks. If you can't wait, you can read more about the Talented 12 at talented12.cenmag.org.

We are already accepting suggestions for 2018, and the nomination form is up and running at cenm.ag/t12nom. If you think you have what it takes to become a member of the Talented 12 or know someone who does, please nominate. In 2017, we received over 150 nominations, of which 50% were put forward by our panel of experts and 50% came from the nomination form.

In terms of other ACS national meeting news and events, you can find highlights in the pages that follow or read our coverage in full at acsmeetings.cenmag.org. You can also watch our archived broadcasts from key events from the meeting through C&EN's Facebook channel. These broadcasts include a lively panel discussion with the Talented 12, a 360° video of attendees watching the eclipse while our reporters answered questions about why you shouldn't stare at the sun, a tour of Sci-Mix and what it's all about, an interview with the three professors we profiled in our "A year in the life of a new professor" feature, a conversation with ACS President-Elect Peter Dorhout about chemical safety, and more.

See you next spring in New Orleans.

Editor-in-chief @BibianaCampos

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

# Reactions

# Letters to the editor

## **Open access**

The editorial in the June 19 issue (C&EN, page 2) speaks about the used [open access (OA)] types (i.e., the well-known gold and green) but also mentions two rather new OA types (i.e., diamond and black/guerrilla). Initially I thought that the editor was referring to the so-called predator OA journals with poor refereeing (if at all), uncertain storage security, and very high handling charges when she mentioned black OA. Answering her question at the end of the editorial, I want to address another category.

Perhaps it should be mentioned explicitly that we know and often use one other, easily available category of OA, namely the FOC (free of charge) open access.

As any recent scientific article in any scientific journal is available (often only) through internet access and because any scientist wishing to access a recently published article needs to use the internet to go to the indicated site for a (free) download, there is also the possibility of using the legal and free method to obtain a PDF. Since a number of years, all publishers-at least in natural sciences-provide [for] all publications

# How to reach us

#### **Chemical & Engineering News** Letters to the Editor

- ▶ Our e-mail address is edit.cen@acs.org.
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- Comments can be left at cen.acs.org.
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▶ Letters should generally be 400 words or fewer and should include the writer's full name, address, and home telephone; letters and online comments may be edited for purposes of clarity and space. Because of the heavy volume of mail received at C&EN, writers are limited to one letter in a six-month period.

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Leiden. the Netherlands



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## Re: Lawsuits progress against Sci-Hub

Readers commented on Sci-Hub and ACS's lawsuit online.

## cenm.ag/scihub

Elsevier brought a lawsuit against SciHub. That's OK. We all know that Elsevier is a greedy corporation. We all know that SciHub is outside the jurisdiction of any US court.

But ACS? In what way does this action serve scientific progress? ACS is supposed to be [a] non-profit organization. This is really a disgrace. **Gabor Lente** 

Instead of wasting our money on lawyers, work on a solution that gives true reasonable access to scientific papers to the many research libraries ... and scientists (university or public, academic researchers or "citizen scientists"[)] that cannot afford the exorbitant prices of research articles. You don't like Sci-Hub, then offer a better solution!

#### Pedro M. Pereyra

ACS certainly has a not-so-good history of futile lawsuits to protect its publishing empire. The costs of publication by ACS are not at all transparent. The authors get nothing; reviewers get the same. Authors are sometimes required to sign indemnity clauses that are hardly reasonable. ACS should level with us about the itemized true costs of publication. That said, we do need trustworthy publishers. However much we may object to ACS pricing and policies, they run legitimate journals. If their copyrights are rendered worthless, they will not be able to continue to do so. Open access can't seem to provide the same assurance of quality.

## Roger Barth

The results of research that is funded by the public, which means tax payers money, must be publicly available and should not be hidden behind a pay wall. Period. I can't applaud sci-hub enough for what they do for science. Even in a first world country like Belgium sci-hub is the only way to access publications that are essential for my research.

#### Mathias Glassner

This is why so many faked data can get

through. Without open and free access to scientific data, only a few eyes get to see it and decide to review it. Science needs to be open and shared freely. It is for societies best interest. **Christina Matlick via Facebook** 

## Join the conversation.



# Corrections

▶ Aug. 7, page 28: In the cover story, "Supporting mental health," the date given for Jason Altom's death was incorrect. He died in 1998, not 1988.

► Aug. 14/21, page 46: In the "By the numbers" section of the Talented 12 cover story, we stated that Harry B. Gray was one of the six most common academic ancestors for this year's class of rising stars. He is a common ancestor, but he is not in the top six.











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# Concentrates

Chemistry news from the week

## ACS NEWS

# Washington, D.C., hosts ACS national meeting

Members take in the eclipse; society narrowly rejects financial support for international chapters

Coinciding with the historic solar eclipse, the 254th ACS National Meeting & Exposition is one that attendees will likely never forget. On Monday afternoon, around the

peak of the eclipse, attendees poured out of the Washington, D.C., convention center. Standing shoulder-to-shoulder and smiling ear-to-ear, they donned eclipse glasses and gazed at the sky with anticipation and awe.

Although attendance at the D.C. meeting, which took place Aug. 20–24, did not eclipse the record-breaking attendance in San Francisco in April, attendance was nevertheless strong, with nearly 13,000 attendees.

Programming by 29 technical divisions and five committees highlighted the meet-

#ACSDC by the numbers

- Attendance: 12,944
- Papers presented: ~9,370
- Exhibiting companies: 282

▶ Job seekers at the ACS

- Career Fair: 364 Employers at the ACS
- Career Fair: 36
- Positions at the ACS Career Fair: 90

ing's theme, "Chemistry's Impact on the Global Economy." Roughly 9,370 papers and 2,720 posters were presented at the meeting. The plenary session featured a talk by Joseph DeSimone of Carbon Inc. and the University of North Carolina, Chapel Hill, on lowering the cost of three-dimensional printing.

Prashant Jain of the University of Illinois, Urbana-Champaign, presented



# Highlights

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Jain (left) and Aizenberg.

The Kavli Foundation Emerging Leader in Chemistry Lecture on the topic of turning photons into chemical bonds. And Joanna Aizenberg of Harvard University gave The Fred Kavli Innovations in Chemistry Lecture on using liquid-filled nanostructured materials to make antifouling surfaces.

In society news, the ACS Board of Directors, among other actions at its executive session, approved the advance member registration fee for national meetings held in 2018. The board also approved program funding requests for the ACS Online Course in Laboratory Safety and New Faculty Workshop Series.

At the ACS Council meeting, the Committee on Budget & Finance reported that ACS's projected 2017 revenues will reach \$553 million, which is \$26.2 million higher than they were in 2016. Net contributions from operations will reach \$25.3 million, and total expenses will reach \$527.6 million.

The council voted by a sliver of a margin to reject a petition to permit ACS's International Chemical Sciences Chapters to receive financial support from the society and to be entitled to representation on the council. The council also rejected a petition to establish a probationary Division of Space Chemistry.—LINDA WANG

## SYNTHESIS

# Flow process streamlines assembly of essential antibiotic

Continuous synthesis produces ciprofloxacin salt in nine minutes

Flow chemistry—in which reagents course through a series of reactors to form new compounds—allows chemists to build molecules in a fast and efficient assembly-line-like way. But with each additional step, the reaction becomes more challenging: Solubility issues with intermediate compounds arise, and unwanted by-products can clog the reactor tubing.

Researchers have now overcome some of these limitations to engineer a flow process for making ciprofloxacin, an essential antibiotic. The overall reaction consists of six telescoped steps followed by a filtration and crystallization step to give the ciprofloxacin hydrochloride salt in 60% yield. Telescoped steps are those in which the flow isn't paused for offline purifications. According to the team, this is the longest linear sequence of telescoped flow steps so far achieved (*Angew. Chem. Int. Ed.* 2017, DOI: 10.1002/anie.201703812).

The flow sequence takes nine minutes. Batch chemistry, a more traditional process that produces molecules in discrete amounts, rarely generates product molecules within minutes, according to Timothy Jamison, whose group developed the new ciprofloxacin process in collaboration with Klavs Jensen's lab at Massachusetts Institute of Technology. A current batch process for making ciprofloxacin in comparable yield takes more than 100 hours.

Hongkun Lin, a postdoctoral researcher in the Jensen lab, disclosed the synthesis last week during a Division of Organic Chemistry poster session at the ACS national meeting in Washington, D.C.

The method "illustrates how to overcome many of flow chemistry's problems," This antibioticproducing reaction contains the longest linear sequence of telescoped flow steps, researchers say.

#### Ciprofloxacin hydrochloride

said Christopher Smith, an organic chemist now at the University of Reading who formerly conducted work in the Jensen lab as a postdoc. For instance, the team addressed the low solubility of multiple intermediate reaction steps by screening various solvent systems and engineering the system to heat up to 180 °C then rapidly cool back to room temperature.

Filtration, crystallization

steps

Six steps in nine minutes via continuous flow

The team also sidelined an amine by-product in one step that would have interfered with a subsequent step by introducing acyl chloride. The compound reacted with the excess by-product to keep it from impeding the process, a very "clever" move, said Eindhoven University of Technology's Timothy Noël, who is an associate editor of the *Journal of Flow Chemistry*.—TIEN NGUYEN

## **MICROFLUIDICS**

# Watching proteins diffuse through lymph nodes

Microfluidic device provides easy way to monitor migration

Proteins called cytokines that are secreted by cells within the lymph nodes are often used as drugs to manipulate immune responses. But something so basic as how these proteins travel through lymph node tissue is poorly understood.

At last week's ACS national meeting in Washington, D.C., in a Division of Analytical Chemistry symposium, Ashley E. Ross of the University of Cincinnati described a microfluidic platform for studying the diffusion of cytokines through mouse lymph node tissue. She did the work while still a postdoc with Rebecca R. Pompano at the University of Virginia. The device is a simplified version of one they published earlier this year (*Analyst* 2017, DOI: 10.1039/ c6ano2042a).

Ross studied the diffusion of fluores-

cently labeled cytokines in parts of the lymph node and measured how it differed in normal and inflamed tissue. These measurements

enabled Ross to calculate diffusion coefficients for various cytokines through the tissue. By combining the measured values with the diffusion coefficients of the cytokines in solution, she was able to determine the so-called tortuosity of the tissue, which was slightly less than that of brain tissue. "That explains the extent of hindrance that proteins experience in the tissue," she said.

Grégoire Altan-Bonnet, head of the immunodynamics group at the U.S. National Institutes of Health, has studied cytokine diffusion in mice (*Immunity* 2017, DOI: 10.1016/j.immuni.2017.03.011). "You really



A microfluidic device allows spatially resolved delivery of fluorescently labeled cytokines to lymph node tissue. Shown here is an image of IFN- $\gamma$  (red) on mouse lymph node tissue with labeled B cells (green).

are much better off with a microfluidic device than with mice," especially for studying multiple cytokines at a time, Altan-Bonnet told C&EN. "We can inject stuff into blood, but in terms of spatial, temporal, and quantity control, it will never compare to what we can do in a microfluidic device."

"The next thing we want to do is to study actual drugs in lymph node tissue," Ross said. Understanding how therapies transport through diseased versus healthy tissue, she added, may aid the development of more effective immunotherapies.—CELIA ARNAUD

# **ACS** Meeting News

## NATURAL PRODUCTS

# Licorice compounds can inhibit drug-metabolizing enzymes

Botanical supplements used to treat menopausal symptoms can interact with many biological targets

Women seeking relief from menopausal symptoms sometimes reach for botanical dietary supplements. Extracts from licorice, hops, and red clover contain phytoestrogens that help mitigate hot flashes, for example.

These extracts also contain a "mush" of other compounds that act on a multitude of biological targets with possible unintended

OН CH<sub>2</sub>O Licochalcone A

consequences, according to Judy Bolton, head of the medicinal chemistry and pharmacognosy department at the University of Illinois, Chicago (UIC).

Bolton organized a session last week at the ACS national meeting in Washington, D.C., to discuss research elucidating the biological effects of botanical supplements. In one talk, researchers reported that licorice extracts can interfere with drug-metabolizing enzymes.

This suite of cytochrome P450 (CYP) enzymes in the liver degrades potentially toxic molecules, including by-products of normal metabolism. The enzymes also are responsible for two-thirds of the breakdown of pharmaceuticals in the body.

Drugs or other molecules people ingest can alter the activity of certain CYP enzymes and disrupt drug metabolism. Inhibiting an enzyme that chews up a

certain drug can lead to buildup of that medication, potentially to toxic levels. Enhancing enzyme activity, on the other hand, will accelerate clearance of the drug

from the body, rendering the medication less effective.

Studying these kinds of drug-drug interactions is required by the U.S. Food & Drug Administration in pharmaceutical development, but no such requirements exist for botanical supplement development. Richard B. van Breemen, a colleague of Bolton's at UIC and director of the NIH-funded Center for Botanical Dietary Supplements Research, works to fill in that knowledge gap. His team at the center identifies potentially harmful botanical-drug interactions.

During a Division of Chemical Toxicology session at the ACS meeting, van Breemen discussed a recent study of extracts



from three licorice plant species. His team looked for possible interactions between CYP enzymes and the extracts themselves, as well as 14 compounds isolated from the extracts. The team found that many of the extracts and compounds inhibited various CYP enzymes and that one licorice species in particular, Glycyrrhiza inflata, was extremely potent because of a compound called licochalcone A (Eur. J. Pharm. Sci. 2017, DOI: 10.1016/j.ejps.2017.07.034). Licochalcone A irreversibly inhibits the CYP3A4 enzyme, a critical component of the CYP family.

Van Breemen's team has three Phase II clinical studies approved, two of which are already under way, to study how licorice, hops, and red clover extracts interfere with drug metabolism in menopausal women.

Mary F. Paine, an associate professor of pharmaceutical sciences at Washington State University, said interaction studies such as this one are "very valuable." The ultimate goal, according to Paine, is to share definitive knowledge with consumers and health care providers about potential adverse botanical-drug interactions.—EMMA HIOLSKI

# CHEMICAL BONDING Triplet diradical cyclobutadiene spotted

Carbon and silicon share many chemical properties, yet their low-coordinate compounds behave quite differently: For example, although C=C bonds are ubiquitous, Si=C and Si=Si bonds are rare, and the latter can be isolated only when sterically protected by large substituents.

Those bonding differences stem from parameters including differences in electronegativity and the size of bonding orbitals, according to Yitzhak Apeloig of Technion-Israel Institute of Technology. During a lecture last week at the ACS national meeting in Washington, D.C., Apeloig described how he and his colleagues used that knowledge to observe an elusive diradical. Apeloig spoke in a symposium on theoretical modeling of

chemical bonding hosted by the Division of Physical Chemistry to honor Nobel Laureate Roald Hoffmann of Cornell University.  $(CH_3)_3Si$ 

Apeloig explained how double-bonded carbon and silicon anions and radicals have different structures and properties, and that silicon

radicals are thermodynamically more stable than carbon radicals. By understanding that stability, Apeloig, working with Technion's Boris Tumanskii, the University of Tsukuba's Akira Sekiguchi, and others, used a combination of electron paramagnetic resonance spectroscopy (EPR) and computational work in 2015 to observe the first triplet diradical-a radical in which the two

unpaired electron spins are aligned in parallel—in a Si=Si compound.

Si(CH<sub>3</sub>)<sub>3</sub>

 $Si(CH_3)_3$ 

▲ ▲

 $(CH_2)_2Si$ 

That work enabled the same team to now report the first spectroscopic observation of a triplet diradical electronic state of a heated cyclobutadiene (shown), albeit one stabilized by trimethylsilyl

groups (Angew. Chem. Int. Ed. 2017, DOI: 10.1002/anie.201705228). Cyclobutadiene is a classic model compound used to study antiaromaticity, but the triplet diradical of cyclobutadiene had not been observed because of its low stability. Studying the elusive species could aid organic synthesis and help design new electronic materials, Sekiguchi told C&EN.—STEVE RITTER

# Science Concentrates: ACS Meeting News

## CATALYSIS

# Copper dimers reduce NO<sub>x</sub>

# Unusual catalytic mechanism plays key role in diesel exhaust cleanup

High schoolers aren't the only ones who pair up and break up frequently. Catalytic species in the systems that clean up engine exhaust do it too, according to a study presented last week at the ACS national meeting in Washington, D.C.

The work, presented in the Division of Catalysis Science & Technology, uncovered an unusual mechanism in the selective catalytic reduction (SCR) process, which reduces smog-causing nitrogen oxides  $(NO_x)$  in diesel engine exhaust to nitrogen and water via reaction with ammonia.



Single copper ions in a zeolite catalyst (white geometric shapes) bind two ammonia molecules, migrate through the zeolite, and form oxygen-bridged dimer complexes, which catalyze exhaust cleanup. Cu is orange; N is blue; H is white; O is red.

SCR systems, which rely on chabazite zeolite treated to incorporate copper in its lattice, come standard on many diesel vehicles, yet details of how they work remain a subject of debate.

Rajamani Gounder of Purdue University, William F. Schneider of the University of Notre Dame, and coworkers found that in the presence of ammonia, copper ions form  $Cu(NH_3)_2$  complexes. The NH<sub>3</sub> moieties make the species mobile, allowing them to migrate through openings that interconnect hollow cages in the porous zeolite framework. As the copper species move about, they briefly and reversibly form dimers that are bridged by a pair of oxygen atoms. The dimers facilitate an O<sub>2</sub>-mediated Cu(I) to Cu(II) redox step that's central to reducing NO<sub>x</sub> to nitrogen and water (*Science* 2017, DOI: 10.1126/science.aan5630).

Fine-tuning the distribution of copper ions in the zeolite could lead to lower  $NO_x$  emissions at cooler operating temperatures than is possible with current SCR systems.

"Exquisite" is how Robert J. Davis described the team's techniques for exploring this SCR system. Davis, a catalysis specialist at the University of Virginia, remarked that this exciting finding regarding the mobility of copper ions and the dynamic formation of paired copper species may also be relevant to the high selectivity of Cu-treated zeolites used for oxidizing methane to methanol.—MITCH JACOBY



INFECTIOUS DISEASE

# Antimicrobial agents in dragons' blood

Peptides from Komodo dragons could inspire new ways to fight infections

Some reptiles sport tough immune systems that help them fend off infections after suffering gnarly wounds. For example, Komodo dragons can avoid infections after bites from other Komodo dragons even though the reptiles' mouths can harbor up to 50 strains of pathogenic bacteria.

At the ACS national meeting in Washington, D.C., last week, researchers reported a method to discover antimicrobial peptides in the blood of these resilient reptiles. The peptides could inspire novel antibacterial therapies, even against multi-drug-resistant pathogens, the researchers said.

This bioprospecting approach in reptiles "is a unique take on natural products isolation chemistry," said Coran Watanabe of Texas A&M University, who was not involved in the work.

All vertebrate animals, not just reptiles, rely on antimicrobial peptides as part of their immune response. These short, positively charged peptides can poke holes in the membranes of pathogenic bacteria, disrupt bacterial gene expression, and turn on other parts of animals' immune systems to launch an attack on invaders.

In the Division of Biological Chemistry, a team led by Barney M. Bishop and Monique L. van Hoek of George Mason University presented a method to prospect for antimicrobial peptides in the blood of American alligators and Komodo dragons.

The method relies on custom hydrogel microparticles made from cross-linked poly(*N*-isopropylacrylamide). The particles contain negatively charged "bait" groups, such as acrylic acid or 2-acrylamido-2-methylpropanesulfonic acid, to attract positively charged molecules. The polymer cross-linking helps the particles preferentially capture small peptides and exclude larger proteins.

The scientists incubate these particles in  $100-\mu$ L samples of plasma and then recover the collected peptides using solvents. They analyze the peptides' sequences using mass spectrometry.

Using this technique, Bishop and van Hoek's team has discovered dozens of novel antimicrobial peptides from alligators and Komodo dragons. The scientists used the sequence of one of the dragon peptides to design a synthetic peptide called DRGN-1 that accelerated healing of wounds in mice that were infected with *Pseudomonas aeruginosa* and *Staphylococcus aureus* (*npj Biofilms* & *Microbiomes* 2017, DOI: 10.1038/s41522-017-0017-2). The team is now investigating ways to incorporate DRGN-1 into possible wound dressings.—MICHAEL TORRICE

# Nature's waterslide reinvented

Skinny nanotubes move water faster than record-holding protein aquaporin

The membrane protein known as aquaporin, which shuttles water in and out of cells, has long held the record as the most efficient water-trafficking system. Now, scientists have discovered one that's six times as fast: a membrane full of skinny carbon nanotubes. The finding could lead to desalination membranes that resist biofouling and operate more efficiently.

The nanotubes in the new system are just 0.8 nm in diameter, so water molecules must slide through them single file—a process that speeds the molecules' transport (*Science* 2017, DOI: 10.1126/ science.aan2438). Aquaporin also makes water travel single file, but amino acids on the inside of its channel hydrogen bond to the water molecules and slow their transit compared with those sliding along the molecularly smooth nanotubes' interior.

"There is always interesting physics to observe by just looking at how things are done in nature," says Aleksandr Noy, the Lawrence Livermore National Laboratory scientist who led the research. "Then you can go back to the lab and use that information to design new systems and materials." Noy says that aquaporin was his inspiration to create the skinny-nanotube system and that it "was always the molecule to beat."

"What is most exciting," says Zuzanna Siwy, an expert in nanopore physics at the University of California, Irvine, is that Noy and coworkers "have identified a man-made system that is even more efficient than the biological system of aquaporin."

Karl Johnson, a chemical engineering professor at the University of Pittsburgh who studies carbon nanotubes for desalination, says that "while this work is of tremendous scientific interest, I do not see how it provides a pathway for constructing membranes that can actually be



This computer-generated image shows a skinny nanotube embedded in a lipid membrane.

used for large-scale water desalination and other applications."

Siwy is more optimistic. There are obviously challenges, she says, such as making desalination membranes of sufficient area and with enough nanotube pores, but she points out that carbon nanotubes are amenable to different types of processing, unlike delicate aquaporin, and should therefore be strong contenders for desalination membrane components.—BETHANY HALFORD



A comic collaboration between C&EN and ChemScrapes cartoonist Brendan Burkett



## **Orbital parking lot**

# More online

To see more of Burkett's work, go to chemscrapes.net. To see more Sketch Chemistry, visit **cenm.** ag/sketch.

# Science Concentrates: ACS Meeting News

## **SYNTHESIS**

# One-two punch converts benzenes to cyclohexenes

Aromatic compounds are largely untapped as precursors for synthesizing cyclohexadienes and cyclohexenes, typically because of the harsh conditions needed to overcome the stability of the delocalized ring. But Katy B. Wilson has developed a tungsten-mediated reaction system that makes this dearomatization seem easy. Working in W. Dean Harman's research group at the University of Virginia, Wilson has found that including a trifluoromethyl group on the benzene ligand of a tungsten complex, [trispyrazolylborate]W(NO)[P(CH<sub>3</sub>)<sub>3</sub>]  $(\eta^2$ -benzene), enhances the metal-arene interaction and exerts control over the sequential protonation and attack of two nucleophilic reagents on the aromatic ligand.



#### R = trispyrazolylborate

The result, as Wilson described at the ACS national meeting, is a new tandem addition reaction for preparing highly functionalized trifluoromethylated cyclohexenes with regio- and stereocontrol, such as the example shown (J. Am. Chem. Soc. 2017, DOI: 10.1021/jacs.7b05118). Harman's group has a history of using this type of metal complex to induce unexpected reactivity in aryl molecules, including dearomatization of aromatic and heteroaromatic rings and enabling pyridines to undergo Diels-Alder reactions. Dearomatizations are often a key step in building the core structures of natural products and other bioactive compounds. Wilson said the team isn't out to synthesize natural products but is looking for reactions useful in midstage functionalizations during the optimization of drug leads.-STEVE RITTER

## **GREENHOUSE GASES**

# Nitric oxide gets a new role

Fertilizer runoff from farmlands can create algae blooms that cause hypoxic dead zones

## WATER

# Water quality revealed in a droplet

Consumers want to know what is in the water coming out of their taps. But there is a huge variety of water-quality tests on the market, which can be daunting for the average person. At the ACS national meeting, Rebecca H. Lahr, a civil and environmental engineer at Michigan State University, presented a simple, low-cost, "open source" water test. Her method is based on the unique residue patterns formed by water droplets as they dry. This phenomenon,

called the coffee-ring effect, occurs as the water evaporates, moving particles within the droplet to its outer edge and leaving behind residue that resembles a stain created by spilled coffee. Users simply place a drop of water on a piece of polished aluminum sheeting. After the water evaporates, they snap a photo of the remaining residue using a jeweler's magnifying glass and a cell phone camera. Lahr's



Residues left from evaporated water droplets show different patterns and could help people identify what is in a water sample. The droplets were from "hard" water (left) and water treated with softener (right).

team is creating a library of residue patterns for various tap water components. Users could then compare the patterns they see to those in the library to identify what is in their water. Because this method is so straightforward, Lahr hopes teachers will use it in classrooms to inspire curiosity about chemistry and tap water. A quick, cost-effective test for baseline water quality could also be useful for other scientists and utility managers, she said.-EMMA HIOLSKI

in rivers, lakes, and oceans. But the runoff can also lead to the release of nitrous oxide (N<sub>2</sub>O), a greenhouse gas that can also destroy the

ozone layer. In soils and during wastewater treatment, microbial enzymes convert fertilizer ammonia (NH<sub>2</sub>) into other nitrogen compounds through a process called nitrification. Nitric oxide (NO) is a key intermediate in the nitrification pathway rather than a by-product, as previously thought, reported Cornell University researchers at the ACS national meeting. Postdoc Jonathan D. Caranto and his adviser, Kyle Lancaster, studied nitrification in Nitrosomonas europaea, which is the dominant ammonia-oxidizing bacteria species in wastewater treatment plants. One enzyme converts NH<sub>3</sub> to hydroxylamine (NH<sub>2</sub>OH).



Previously, researchers thought that a second enzyme, hydroxylamine oxidoreductase (HAO), then oxidized NH<sub>2</sub>OH to NO<sub>2</sub><sup>-</sup>. Under anaerobic conditions, NO<sub>2</sub><sup>-</sup> gets reduced to  $N_2O$ , yielding some NO from incomplete catalysis. Instead, Caranto and Lancaster found that HAO converts NH<sub>2</sub>OH to NO (Proc. Natl. Acad. Sci. USA 2017, DOI: 10.1073/pnas.1704504114). A third enzyme would then take NO to  $NO_2^{-}$ . Depending on conditions, some NO could escape and undergo side reactions to form  $N_2O$ . Meanwhile, the race is on to identify the enzyme that oxidizes NO to NO2-.--JYLLIAN KEMSLEY

### DRUG DISCOVERY

# Steering clear of opioids' downsides

Current opioids cause pain relief typically by binding to the µ-opioid receptor on nerve cell surfaces. But these opioids famously cause addiction, so scientists have been eveing another member of the opioid receptor family, the  $\kappa$ -opioid receptor, as a target for treating pain. Activating this receptor doesn't induce euphoria, which drives opioid abuse, but when compounds bind to it, they can trigger an unknown biochemical pathway that leads to sedation and dysphoria, or strong feelings of unease. Late last year, Laura Bohn of Scripps Research Institute Florida and collaborators used cell assays to identify compounds called biased agonists that bind to the  $\kappa$ -opioid receptor and activate a G protein signaling pathway but avoid a  $\beta$ -arrestin pathway, which the scientists think leads to sedation and dysphoria (ACS Med. Chem. Lett. 2017, DOI: 10.1021/ acsmedchemlett.7b00224). One of these



biased agonists, called triazole 1.1, reduced pain and itch in mice without decreasing the animals' locomotion or lowering their dopamine levels—a sign of In these cutaway views of the  $\kappa$ -(left) and  $\mu$ -opioid receptors (right), inhibitors nestle into the binding pockets of the receptors.

dysphoria. Although the results are encouraging, accurately linking a particular pathway with corresponding physiological responses is still a major challenge for the field, Bohn said at the ACS national meeting. To address this issue, her team studied biased agonists for the better-known µ-opioid receptor and developed a predictive model that correlates data from cell-based assays with physical outcomes in mice. The researchers screened u-targeting compounds and observed a direct correlation between those that triggered the  $\beta$ -arrestin pathway in cells and those that caused respiratory depression-another common opioid side effect—in mice.—TIEN NGUYEN

## PUBLISHING

# Debate over chemistry preprint servers

Thomas Faust

#### Replying to @davidImobley @steven\_albanese

Really important symposium, ACS recognise that community input is critical for ChemRxiv success. Also, honest discussion is key for progress

Follow

10:17 AM - 22 Aug 2017 from Washington, DC

For years, many chemists have been calling for a preprint server for their community. Physicists already have arXiv, and biologists have bioRxiv. In just the past few weeks, organizations launched two chemistry preprint servers—ChemRxiv (a joint effort by ACS, the Royal Society of Chemistry, the German Chemical Society, and others) and Elsevier's Chemistry Research Network, or ChemRN. Now that the servers are here, questions linger about how they operate, how peer-reviewed journals will interact with them, and how they'll change the way chemists work. At the ACS national meeting last week, journal editors and chemists gathered to discuss these issues. C&EN was on the ground, live-tweeting the session. To see all the back-and-forth dialogue, visit **cenm.ag/preprint**.—LAUREN WOLF

## CATALYSIS

# Reaction plays favorites in polyols

Chemists would like to be able to modify compounds containing multiple hydroxyl groups, such as the antiparasitic drug ivermectin, to generate useful new molecules. One way to do this would be to selectively oxidize individual hydroxyls to ketones, which are synthetically versatile groups in that they can be readily converted to nitrogen-based groups. As described at the ACS national meeting last week, John F. Hartwig and Christopher K. Hill of the University of California, Berkeley, have now designed a catalyst capable of such a feat (Nat. Chem. 2017, DOI: 10.1038/nchem.2835). Dehydrogenating selected hydroxyls to ketones in multihydroxylated compounds known

a ketone and then further elaborated

with nitrogen-based groups.

as polyols has been difficult. A common strategy is to add protecting groups to the hydroxyls you don't want to react and then deprotect them later. But this is laborious, requiring multiple reactions instead of just one. The Berkeley team developed a catalyst that oxidizes polyol secondary alcohol groups-hydroxyls on carbon atoms that are bonded to two other carbon centers—much more readily than primary alcohol groups—hydroxyls on carbons connected to only a single carbon center. The catalyst has strongly electron-donating phosphine ligands that make its ruthenium center electron rich, enhancing its selectivity. The researchers demonstrated the catalyst's power by using it to selectively oxidize a single hydroxyl group in over a dozen polyol natural products and using subsequent catalytic reactions to convert the resulting ketones into nitrogen-modified products.—STU BORMAN



# Business Concentrates

## CONSUMER PRODUCTS

# New effort to develop meatless meat

UC Berkeley, Givaudan partner to make meat alternatives tastier

A new lab at the University of California, Berkeley, aims to develop plant-based meat alternatives appealing enough to make meat lovers abandon their favorite steak. The university says it will make its innovations available for free to encourage more entrepreneurs to enter the market.



Students at the University of California, Berkeley, taste their plant-based fish alternative. The lab will be part of Berkeley's Sutardja Center for Entrepreneurship & Technology. Ikhlaq Sidhu, the center's founder, says

meat alternatives are a big opportunity for start-ups.

Animal-free meat is also attracting investors. Last week, Bay-area-based Memphis Meats raised \$17 million from investors including Cargill and Bill Gates. The company makes a variety of meats from animal cells raised in a bioreactor.

Berkeley jumped on the plant-based meat trend earlier this year, when it launched what it calls the world's first course focused on the topic. Now 40 students will have the opportunity to solve both technical and business dilemmas facing the nascent industry. The team includes chemical engineering, liberal arts, science, and business students.

To improve the taste, texture, and smell of current offerings, the lab will work with the Swiss flavors and fragrances maker Givaudan. The company hopes the students can create an easy-to-manufacture product with intracellular fats and water that mimics the umami flavor of meat.

"We must collaborate to truly move forward," says Flavio Garofalo, Givaudan's business manager for protein.

Market research firm Mintel says buyers of meat alternatives want products made with natural ingredients—a potential challenge for lab-based businesses.

One leading contender, Impossible Foods, adds soy leghemoglobin to its plant-based hamburger. It produces the bloodlike protein from genetically modified yeast.

Earlier this month, Impossible Foods said it is responding to a request by the U.S. Food & Drug Administration for more information to support the company's determination that soy leghemoglobin is generally recognized as safe, or GRAS.—MELODY BOMGARDNER

## BY THE NUMBERS

**400** 

Sources: Start-Up Nation Central, AgFunder

## The number of Israeli

start-ups developing agricultural technologies. The companies are spread across 12 categories, including water management, biotechnology, crop protection, and robotics. Last year the tiny nation claimed 2% of global agtech venture investments, or \$52 million.

## GLOBAL HEALTH

# Novartis advances new malaria drug

Novartis and the nonprofit Medicines for Malaria Venture (MMV) have launched patient testing of an antimalarial compound they claim has the potential to treat drug-resistant strains of the malaria parasite. The compound, KAF156, will be tested for efficacy in combination with a new formulation of the existing antimalarial lumefantrine.

The first test is being performed at a center in Mali. The partners plan to follow it with tests at 16 other centers in nine countries in Africa and Asia this year.

KAF156 belongs to a class of antimalarial compounds called imidazolopiperazines. The compound has proved fast acting in Phase IIa clinical trials in clearing both *Plasmodium faliciparum* and *P. vivax* parasites, Novartis says.



#### KAF156

The push for new antimalarial drugs is in response to recent reports of parasite strains resistant to standard regimens for battling malaria, such as combinations of artemisinin with mefloquine or piperaquine. Moreover, these drugs must be taken once or twice daily over three days, often leading to incomplete courses of treatment. The long-term goal of MMV is the development of single-dose combination therapies.

KAF156 was discovered and developed in a partnership between two Novartis research arms and the Swiss Tropical & Public Health Institute with support from MMV, the Wellcome Trust, and Singapore Economic Development Board.—RICK MULLIN

# Big ag merger probed

# Regulators fret over power of a combined Bayer and Monsanto

The European Commission is opening an in-depth investigation into Bayer's planned \$66 billion purchase of rival Monsanto. Regulators are concerned about the market heft the two firms would have if they combine businesses in agricultural chemicals, seeds, and crop traits.

Together, Bayer and Monsanto would be the world's largest supplier of crop protection chemicals. Their nearly \$25 billion in annual sales would be ahead of Dow Chemical and DuPont, which are set to complete their merger at the end of this month.

European commissioner for competition Margrethe Vestager worries that the combined Bayer and Monsanto may be too large. "We need to ensure effective competition so that farmers can have access to innovative products, better quality, and also purchase products at competitive prices," she says. Bayer and Monsanto submitted a proposal last month for addressing the EC's preliminary issues reso with the merger, but their remedies were apparently insufficient. Bayer says it will work constructively with the EC, which has set a deadline of Jan. 8, 2018, to complete its review.

As part of its further investigation, the EC will delve into the two companies' herbicide units. Monsanto makes glyphosate, used with its Roundup Ready seeds, while Bayer offers glufosinate, used with its special LibertyLink seed. The EC points out that glufosinate is one of the few available alternatives to glyphosate. It also notes that the two companies are among the few researching new active ingredients to combat weed resistance to herbicides.

These concerns do not come out of the blue. In May, Bayer received conditional



A Bayer scientist inspects cotton fibers at a research facility in Lubbock, Texas.

approval for the merger from South African authorities provided it divest Liberty-Link-related assets.

The EC is also concerned about the overlap the companies would have in seeds. For example, it points out that Monsanto is the European market leader in rapeseed and Bayer is the largest supplier globally.

The EC is looking at the merger in the context of a wave of consolidation in agricultural chemicals. In March, the EC cleared the Dow-DuPont deal provided that DuPont sell a portion of its crop protection business. In April, the EC approved ChemChina's purchase of Syngenta on the condition that it divest a number of generic pesticides.—ALEX TULLO

## **EMPLOYMENT**

# Nonprofit scientists head to industry

Novartis, other drugmakers see discovery talent in academia

Several top researchers are leaving academic and government posts for jobs in the pharmaceutical industry. The moves are a sign that the once sharp line between the for-profit and nonprofit scientific realms is becoming increasingly blurred.

The Swiss drug giant Novartis is a pioneer in recruiting scientists from academia. When it set up the Novartis Institutes for BioMedical Research (NIBR) in Cambridge, Mass., in 2003 the company hired Mark C. Fishman, a Harvard Medical School professor, as its president.

In 2015 Jay Bradner, also of Harvard Medical School, took over the top job when Fishman retired. Last year, two more Harvard researchers—Peter Hammerman and Jeff Engelman—joined Novartis in its oncology unit.

Now, Shaun Coughlin, director of the University of California, San Francisco's Cardiovascular Research Institute, has agreed to move East to become NIBR's global head of cardiovascular and metabolism. He is scheduled to start work Nov. 1.

AstraZeneca, meanwhile, is recruiting two senior scientists from outside the corporate realm. Jean-Charles Soria will leave South-Paris University to become head of oncology innovative medicines.



UCSF's Cardiovascular Research Institute, shown here, lost a top researcher to Novartis.

And Geoffrey Kim has left the U.S. Food & Drug Administration, where he directed the oncology products division, to become AstraZeneca's head of oncology strategic combinations.

Separately, Thomas Wynn has left the U.S. National Institutes of Health, where he was a senior investigator, to head early discovery in Pfizer's inflammation and immunology unit.

Big pharma firms are looking harder at academia for research talent, says Ron Malachuk, a principal at the executive search firm Korn Ferry. "Developing intellectual property and increasing innovation is critical for drug companies," he says, "and academicians possess the critical thinking skills to lead such initiatives."

For their part, academic and government scientists are more open to the "for profit" world these days, Malachuk says. Reasons include increased competition for tenured academic positions and professors' growing comfort with the corporate world through roles as technical advisers or consultants.—MICHAEL MCCOY

# Business Concentrates

## **3-D PRINTING**

# BASF goes deeper into 3-D printing

BASF has acquired Innofil<sub>3</sub>D, a Dutch producer of filaments used in three-dimensional printing. BASF already sells



plastic pellets used to make such filaments, which are

Equipment on which Innofil3D creates its 3-D printing filaments.

extruded to manufacture objects in the layer-by-layer 3-D printing process. "With this acquisition, BASF is moving one step

further along the value chain," says Volker Hammes, managing director for BASF New Business.—MICHAEL MCCOY

### **BUSINESS**

# SK Capital re-ups investment in Archroma

The investment firm SK Capital says it has reinvested an undisclosed sum in Archroma, a supplier of chemicals to textile, paper, coatings, and other markets. SK acquired Archroma in 2013 from the Swiss specialty chemical maker Clariant. According to published reports, SK tried putting Archroma up for sale in January. SK now says its new investment will give Archroma the financial flexibility to build its competitiveness and market position.—MICHAEL MCCOY

## LATIN AMERICA

## Dow may exit Argentina shale

Dow Chemical is reevaluating its Argentine shale partnership with the state oil company YPF, Argentine energy minister Juan José Aranguren told Bloomberg News in an interview. Dow wouldn't confirm to C&EN whether it is considering a sale. "Dow,

# Ingevity will buy a pine chemicals business

The pine-based chemicals maker Ingevity has agreed to acquire the pine chemicals business of the paper company Georgia-Pacific for \$315 million. The business will add about \$105 million in annual sales to Ingevity's sales, which were \$908 million last year. The business produces pine-based tall oil fatty acids, tall oil rosin, and tall oil rosin esters used in adhesives, paints, mining, and other applications. It manufactures most of its products at a plant in Crossett, Ark., that employs 70 people. The sale continues the exit of paper manufacturers from the pine chemicals business. Ingevity itself was formed last year when the paper company MeadWestvaco spun off its chemical business. And Kraton's pine chemicals business was once part of International Paper. The addition of the Georgia-Pacific business will result in about \$11 million in annual savings because of manufacturing optimization and lower logistics costs, Ingevity says.—MICHAEL MCCOY

which was an early investor and supporter of both YPF and the government's strategy, remains fully committed to our strategic relationship with YPF and constantly evaluates new strategic opportunities in every region," the company says. Dow has been developing shale gas wells in Argentina's Neuquén province since 2013. The company consumes natural gas at an ethane extraction joint venture and a downstream petrochemical complex in Bahía Blanca, Argentina.—ALEX TULLO

## CONSUMER PRODUCTS

# Modern Meadow moves to New Jersey

Modern Meadow, a start-up making lab-derived animal materials, including leather, will move its headquarters from Brooklyn, N.Y., to Nutley, N.J. The 7,300-m<sup>2</sup> site, on a former Roche campus, will also house lab space and a pilot manufacturing facility. Modern Meadow engineers cells to grow collagen, which self-assembles into fibrils that in turn are converted into leather. New

This piece of Modern Meadow leather was made in the lab. Jersey pitched in tax credits worth up to \$32 million. Modern Meadow says it will grow its



Brooklyn-based design and research studio.—MELODY BOMGARDNER

## SPECIALTY CHEMICALS

# Albemarle to add 200 jobs in North Carolina

Albemarle plans to bring 200 jobs to North Carolina. In Kings Mountain, the specialty chemical maker will add 170 jobs and invest \$10.5 million over the next five years in a manufacturing and services facility. The project was facilitated by a Job Development Investment Grant from the state and supported by the state Department of Commerce and the Economic Development Partnership of N.C. Albemarle will also add 30 jobs at its headquarters in Charlotte.—RICK MULLIN

## FOOD INGREDIENTS

# Frutarom adds European flavor firms

The Israeli flavors and fragrances firm Frutarom is continuing its international shopping spree with its fifth and sixth acquisitions this year. It bought England-based Flavours & Essences, a developer of flavors and natural colors, for \$19.5 million. F&E had sales of \$17.4 million in the prior 12 months. Frutarom also purchased the Swiss firm Mühlehof Gewürze, which specializes in savory flavors for convenience foods, for \$7.0 million. Mühlehof's sales for the prior 12 months were \$3.4 million. Both of the acquired firms focus on local markets and tastes; Frutarom says the moves will increase its market share in Europe.—MELODY BOMGARDNER

### AGRICULTURE

# Monsanto gains a CRISPR platform

Monsanto has signed a deal to use the CRISPR/Cas9 gene-editing platform of Seoul, South Korea-based ToolGen to develop products for agriculture. Gene-editing tools can add, delete, or change genes in plants much more quickly than traditional plant breeding and biotechnology methods can, Monsanto says. Monsanto is working to catch up with DuPont Pioneer, the first agricultural company to access CRISPR tools. Early this year Monsanto signed a nonexclusive deal for CRISPR/Cpf1 technology from the Broad Institute of MIT & Harvard.—MELODY BOMGARDNER

## NUCLEIC ACIDS

# AstraZeneca, Ethris sign mRNA agreement

AstraZeneca will pay Ethris roughly \$30 million as part of a five-year collaboration to develop RNA therapies for respiratory diseases. Under the pact, Ethris will develop messenger RNA therapies based on its technology, which allows a nonimmunogenic transcript to be delivered into cells. The companies will work on treatments for asthma, chronic obstructive pulmonary disease, and idiopathic pulmonary fibrosis. Since 2013 AstraZeneca has been working with Moderna Therapeutics to develop mRNA-based drugs for cardiovascular, metabolic, and renal diseases.—LISA JARVIS

## INFORMATICS

# GSK amps up Al with Insilico pact

Aiming to bolster its abilities in the hot area of artificial intelligence research, GlaxoSmithKline will collaborate with Insilico Medicine. Under the deal, which follows a pilot pact, GSK will use technology from Baltimore-based Insilico to look for novel biological targets and pathways. Meanwhile, GSK has lost its head of drug discovery and preclinical development, Ian Churcher, to BenevolentBio, a subsidiary of another AI firm, BenevolentAI.—LISA JARVIS

## BIOLOGICS

# Samsung, Takeda team for new biologics

Samsung Bioepis and Takeda Pharmaceutical are joining to develop new biologic therapies for areas of unmet medical need. The partners' first program is TAK-671, a



Samsung Bioepis focuses on innovating expedited drug development processes.

treatment for pancreatitis. Samsung Bioepis launched in 2012 as a manufacturer of the generic biologic drugs known as biosimilars. "Takeda's extensive knowledge and expertise in drug development makes the company an ideal partner for us as we open a new chapter at Samsung Bioepis," says CEO Christopher Hansung Ko.—RICK MULLIN

## INFECTIOUS DISEASE

## J&J deepens TB drug commitment

Johnson & Johnson has teamed with India's Institute of Microbial Technology (IM-TECH) to develop new treatments for tuberculosis. The goal is safer, more effective, all-oral treatments for multi-drug-resistant TB, as well as TB drugs with novel mechanisms for all people with TB. Scientists from J&J and IMTECH will work together to tackle TB, which in 2015 killed nearly 500,000 people in India. In late 2012, J&J received approval for Sirturo, the first new TB treatment in 40 years.—LISA JARVIS

# **Business Roundup**

► Lubrizol's life sciences business will invest \$10 million to expand its silicone contract manufacturing site in Franklin, Wis. The 6,600-m<sup>2</sup> expansion will grow the facility's product development and production capacity and add clean rooms for making implants and drug-eluting devices.

**Eastman Chemical** is hiking capacity for glycol-modified polyethylene terephthalate (PETG) at its plant in Kuantan, Malaysia, by 20%. PETG is a durable polyester copolymer used in retail fix-tures and signage.

▶ **Sun Chemical** has acquired Joules Angstrom U.V. Printing Inks, a maker of ultraviolet inks based in Pataskala, Ohio. Sun says the purchase expands its offerings to packaging and other markets.

► **Syngenta** has sold certain herbicides and fungicides marketed in Mexico to American Vanguard. Mexican regulators required the sale before they would allow ChemChina to acquire Syngenta.

▶ **DSM** will provide its bioerodible polymer technology to Aerie Pharmaceuticals for use in delivering compounds to the eye. Aerie plans to apply the polymer to the developmental small molecule AR-13154.

▶ **StanChem** has been acquired by Artemis Capital, a private equity firm, for an undisclosed sum. Based in East Berlin, Conn., StanChem makes emulsion polymers, adhesives, and coatings. ► Eli Lilly & Co. and Topas Therapeutics will jointly study antigen-specific tolerance induction. The partners will initially focus on antigens that can induce inflammation and autoimmune disease. Topas was spun off from Evotec in early 2016 with \$15 million in financing.

▶ CRISPR Therapeutics has formed a two-year research pact with Massachusetts General Hospital Cancer Center to develop T cell therapies for cancer. The partners will use CRISPR/Cas9 gene editing to improve drugs currently in development.

### SAFETY

# **CSB reaches out to ACS**

Safety board seeks to collaborate with the society

Two top officials with the U.S. Chemical Safety & Hazard Investigation Board (CSB), a federal agency that investigates chemical-related accidents, said they are exploring the potential for collaboration with ACS.

In separate presentations at the ACS national meeting on Aug. 21, CSB Chairperson Vanessa Allen Sutherland and Kristen Kulinowski, a CSB board member and longtime ACS member, applauded the society's recent efforts to elevate the importance of safety among chemists. Particularly, they pointed to policies that call for authors to address and emphasize safety concerns associated with work reported in ACS journals and the inclusion this year of safety as a core value in the society's strategic plan. ACS publishes C&EN. In introducing Sutherland during a talk in the presidential events, ACS President Allison A. Campbell stressed CSB's importance as an independent investigator of chemical-related accidents.

"They do not shame or blame. They are not there to punish but to get the facts," Campbell said. The board investigates the cause of accidents and makes recommendations to regulatory agencies, facilities, and others to improve safety, she continued.

Sutherland said that in the two years since she took over CSB leadership, much of her emphasis has been on building relationships with industry, academia, and others over safety, work she wants to expand with ACS.

With a staff of 40 and an \$11 million



This image is from ACS's 2015 video on a safer version of the rainbow flame demonstration.

annual budget, Sutherland described an agency stretched thin. President Trump has proposed defunding CSB, though it's up to Congress to decide whether and how much to fund it.

The paths of ACS and CSB have crossed before, Kulinowski said, primarily on investigations of accidents at academic labs or in classroom demonstrations gone bad. Beyond lab work, Kulinowski did not have specific initiatives in mind, but she said safety opportunities on which the two organizations could align were plentiful.—JEFF JOHNSON, special to C&EN

### POLLUTION

# Treated sludge harbors antibiotic-resistance genes

## Findings raise public health concerns

To kill microorganisms that can potentially cause disease, the world's most advanced sewage treatment plants essentially pressure-cook wastewater. But new research indicates that this process may not get rid of genes that impart antibiotic resistance to microbes.

Because treated sludge is regularly spread on lands used to grow crops for human consumption, this finding could have public health implications, said Sarah Fischer, an environmental chemist at the University of Maryland, College Park, during a Division of Environmental Chemistry session at the ACS national meeting in Washington, D.C.

The U.S. Environmental Protection Agency estimates that more than 7 million metric tons of biosolids—the residue from wastewater treatment, also called sludge—is applied to U.S. lands each year as fertilizer. Increasingly, organic farmers are debating the possible use of biosolids, pointed out Mustafa Selim of East Carolina University's Brody School of Medicine, who co-organized the symposium. The U.S. Department of Agriculture now bans the use of biosolids on crops certified as organic.

Fischer is part of a team that is studying antibiotic resistance at an advanced wastewater treatment plant in the U.S. There, thermal hydrolysis units heat wastewater to 180 °C under pressure to reduce fecal coliform.

After the autoclave-like treatment, the residue undergoes anaerobic digestion, in which microbes break down organic material for 22 days before the remaining biosolids are hauled out of the facility.

Fischer and colleagues checked materials moving along the treatment process for the presence of seven known genes that provide resistance to antibiotics. They found that thermal hydrolysis greatly reduced the presence of active, pathogenic bacteria and of the resistance genes. But after the anaerobic digestion step, the levels of the genes increased.



Construction of thermal hydrolysis units at a wastewater treatment plant. The research team has two hypotheses on why this is happening, Fischer continued. One is that the

thermal treatment process doesn't destroy genetic material, leaving DNA that surviving organisms can take up directly from their environment, which many bacteria can do. The other hypothesis focuses on sludge that is added to wastewater in anaerobic digesters. This material contains bacteria that could carry the resistance genes, thus reintroducing the genetic material to the heat-treated wastewater, she said.

The researchers are next exploring whether the antibiotic-resistance genes in the treated sludge persist in agricultural fields, Fischer told C&EN. "The long-term survival of the genes has been shown to decay in agricultural settings," she adds.—CHERYL HOGUE

## POLLUTION

# At least 50 million in Pakistan at risk from arsenic contamination

The first-ever hazard map of arsenic contamination in Pakistan's groundwater shows 50 million-60 million people are at risk, according to a new study (Science Advances 2017, DOI: 10.1126/sciadv.1700935). Swiss, Chinese, and Pakistani researchers worked together to make the first largescale estimates based on a model that combined local geology and a set of 1,200 new groundwater quality samples, which had found contamination many times the World Health Organization's recommended groundwater limits. This finding shows that more needs to be done to protect Pakistan's people, including those in the major population centers of Lahore and Hyderabad. "This is an alarmingly high number, which demonstrates the urgent need to test all drinking water wells in the Indus Plain," says lead author Joel E. Podgorski, a geophysicist at the Swiss Federal Institute of Aquatic Science & Technology. Some 150 million people worldwide were already estimated to be dealing with arsenic contamination of their groundwater. Even low concentrations of arsenic in water can cause symptoms ranging from skin discoloration to liver, heart, and kidney impairment or cancer.—ANDREA WIDENER

## SYNTHETIC BIOLOGY

# Report provides map for assessing threats from biotechnology

Most biotechnology applications are being pursued for legitimate purposes that could benefit human health, the environment, or the economy, but various reports have reached different conclusions about the potential for people to use such techniques to intentionally cause harm. To better understand how much of a threat biotechnology, especially synthetic biology, poses to human health, the U.S. Department of Defense commissioned the National Academies of Sciences, Engineering & Medicine to investigate potential security vulnerabilities related to manipulating biological functions, systems, or microorganisms. In an interim report released on Aug. 21, the committee provides a framework for examining possible security concerns related



## PHARMACEUTICALS

# Trump signs FDA user fee legislation

President Donald J. Trump on Aug. 18 signed into law legislation (H.R. 2430) that will allow the U.S. Food & Drug Administration to continue collecting fees from industry to help pay for the agency's safety and efficacy reviews of new drugs and medical devices. The legislation renews FDA's authority to collect fees from fiscal 2018 through fiscal 2022. The agency's current authority expires Sept. 30, the end of fiscal 2017. Although President Trump urged lawmakers to allow FDA to collect 100% of its total budget from industry paid fees, he did not get his wish. The new law instead authorizes FDA to collect about \$1.4 billion, or 28% of its budget, in user fees from pharmaceutical companies and medical device manufacturers each year. It also aims to improve postmarket drug safety and gives generic drug manufacturers earlier access to FDA staff in the hope of getting more low-cost drugs to market. The measure passed the House of Representatives on July 12 and the Senate on Aug. 3.—BRITT ERICKSON

to synthetic biology in the near, medium, and long terms. The framework also provides options for mitigating such concerns. The committee is accepting input on the framework until Sept. 5. Once it finalizes the framework, the committee plans to use it to assess the security threats posed by synthetic biology. Those threats and options to address them will be the subject of a future report.—BRITT ERICKSON

## REPRODUCIBILITY

# Industry and academia can improve their partnerships

Cultural differences between academic and industrial researchers are increasingly straining scientific collaborations, but those partnerships are essential to the health of the research enterprise. A commentary in Science suggests ways to improve those relationships (2017, DOI: 10.1126/science. aan4906). The heart of the problem is a fear by industry that academic research is not reproducible, according to the multiauthor commentary, which is the result of an American Association for the Advancement of Science workshop. "Irreproducible research wastes time, money, and resources. Academic researchers, universities, and other institutions, industry, funding agencies, and [journal] editors all have a role to play in raising research standards and creating an environment of trust between communities," said the authors, who laid out suggestions for those players to help improve reproducibility. The commentary also outlines questions industrial and academic partners should ask when they form a partnership. They should decide up front what proprietary data can be shared and in what format, for example. They should also determine what will happen with the academic partner's research and data after the collaboration ends.—ANDREA WIDENER



### PETROCHEMICALS

# **Clearing the Gulf Coast logjam**

As a massive wave of chemical plants comes online, companies chart different courses to the market

### ALEXANDER H. TULLO, C&EN NEW YORK CITY

he heavy lift vessel *Zhen Hua* 13 departed from Shanghai last month carrying three new, 120-meter-tall cranes. The big ship should reach its destination on the Houston Ship Channel by early October.

The new cranes are part of a \$700 million upgrade project at Barbours Cut, one of the ship channel's two container terminals. The improvements will allow its wharves to accommodate the larger vessels soon to arrive through the newly expanded Panama Canal and boost container handling capacity by 60%.

Both the expansions and the bigger ships will provide the capacity the port needs to handle the flood of exports that officials are expecting from the Houston area's new polymer plants.

Cheap, shale-gas-derived feedstocks have induced chemical makers to spend tens of billions of dollars on multiple new plants in the U.S. Around the Gulf Coast, companies will start up 10 ethylene cracker complexes—most complete with plants for derivatives such as polyethylene within the next few years. A few projects, among the largest of the coming wave, are starting up already. Major players Dow Chemical, Chevron Phillips Chemical, and ExxonMobil Chemical are all commissioning polyethylene plants in Texas.

With the buildup at hand, chemical company logistics managers are concerned about whether the region's port, rail, and truck transportation systems will be able to handle the flood of resins that will leave the country through the Gulf Coast. They are working on strategies to use local ports as effectively as they can—and on contingency plans to circumvent the entire region if they need to.

The consulting group Accenture forecasts that U.S. polyethylene capacity will increase by one-third between 2015 and 2018. By 2020, it expects 4.6 million metric tons of new annual polyethylene exports. This is enough to fill 255,000 standard 20-foot (about 6-meter) shipping containers, which in turn would fully load 51 container ships. By itself, polyethylene would represent a more-than-10% increase in traffic through Port Houston, which handled 2.2 million standard containers last year.

"A lot of the resin capacity hasn't turned on yet, but when it does, there are a lot of concerns about congestion," says Paul Bjacek, chemicals and natural resources research lead at Accenture.

Until recently, U.S. chemical executives didn't have to think about the issue, Bjacek notes, because exports weren't essential to their business. For polyethylene, for example, exports made up roughly 10 to 20% of shipments. "Now, whole polymer plants are being built for export," he says.

"The U.S. has not had the kind of construction going" that it now has, Chevron Phillips's chief executive officer, Mark Lashier, told an audience at the IHS Markit World Petrochemical Conference earlier this year. Lashier estimated that 60% of the new polymer capacity will be exported. "How is it all going to get out of the country?" he asked.

Today, most plastic resin leaves Gulf Coast plants in hopper cars. At large domestic customers, such as those that convert the resin into milk bottles, the cars roll right up to the plant gates. For international shipments, the cars go to packaging firms around Houston that repackage the bulk resin into 25-kg sacks, which are loaded into shipping containers and trucked to terminals on the Houston Ship Channel.

"The waterside is absolutely ready," says retired Capt. Bill Diehl, president of the Greater Houston Port Bureau. The big new cranes, he notes, are on their way. The waters around Barbours Cut and Bayport, the ship channel's two container terminals, have been dredged down to a depth of 14 meters. The upgrades will allow the port to bring in the larger ships that have begun to transit the new lane of the Panama Canal, which opened last year.

Before the expansion, the canal could handle container ships carrying 4,500 containers. Now, ships laden with as many as 13,000 can make it through. With its improvements, Houston will handle ships bearing 9,000 containers, Diehl says.

The bigger ships will spur the port of Houston's growth, Diehl argues. The boost in size of the ships will decrease the cost of shipping each box, improving the competitiveness of Houston and East Coast ports against ports on the West Coast.

Additionally, Diehl says, Houston is strategically suited to take advantage of the larger ships. Many U.S. ports suffer from a container imbalance because they import more than they export. In Los Angeles, which is an arrival point for Chinese imports, boxes go back to China empty, driving up the cost of shipping because half of the shipping and handling is wasted on unused boxes.

Houston, in contrast, is a large export port because of all the local industry. A

# The chemical export boom by the numbers

► **4.6 million metric tons:** The amount of additional annual polyethylene exports from the U.S. expected by 2020.

 255,000: The number of 20-foot (about 6-meter) shipping containers that the polyethylene will fill.
 51: The number of container ships it

will take to transport those containers.

2.2 million: The number of containers Port Houston handled in 2016.

11%: The increase in Port Houston container traffic over the past three years.

Sources: Accenture, Port Houston

good balance between imports and exports helps containers go in and out fully loaded and keeps shipping costs relatively low. Diehl sees a virtuous cycle. As plastics exports ramp up, shipping companies will increasingly use the port because they know they will be able to fill the boxes for the return trip from Houston.

But even if Port Houston manages the growth, chemical companies may have plenty of transportation problems to worry about. Earlier this year, the consulting firm PricewaterhouseCoopers (PwC) conducted a study, sponsored by the American Chemistry Council trade group, of how railroads, trucks, and ports will handle the coming wave of production.

PwC forecasts that U.S. chemical shipments will increase roughly 36 mil-

lion metric tons over the next three years. Producers will require additions of 270,000 railcars, 723,000 trucks, and 808,000 shipping containers.

The increased traffic will stress each mode of transportation differently: The rail system's long-standing infrastructure is difficult to expand, trucking faces a limited supply of drivers, and marine shipping capacity has to grow as fast as the chemical exports.

The rail system will be strained particularly around hubs such as Houston; Corpus Christi, Texas; Baton Rouge, La.; and New Orleans. Chemical companies are already experiencing delays of four days on average for their rail deliveries, PwC reports.

"We expect those delays to get much worse based on trying to put additional production through the existing infrastructure," says Mark Lustig, a principal at PwC, noting that delays are on track to double by 2025.

The railroads are investing. Union Pacific, for example, will spend about half a billion dollars on Texas rail infrastructure this year. But making improvements around Houston is a challenge, Lustig points out. "The rail network inside of Houston has been there for quite a while. The city has grown up around it," he says. "It makes it difficult to expand."

On the waterfront, the issue isn't efficiently loading and unloading ships at Houston's docks but rather getting shipments from trucks and trains to the docks. And despite the assurances of port officials, many chemical companies are also anxious about whether Houston will have enough containers and ships to handle the surge.

Company logistics managers are increas-





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ingly considering options such as sending shipments by rail to Los Angeles and other West Coast ports. About one-third of U.S. chemical exports run through ports outside the Gulf of Mexico already, PwC says.

Diehl of the Greater Houston Port Bureau cautions that such routes could be expensive. "Is it better, faster, cheaper for me to come out of Houston and go to Dallas by truck or train, touch the shipment again, and go by truck or train to Los Angeles or the East Coast?" he asks. "Or is it cheaper for me to just get it to the dock?"

"Train beats truck; ship beats train," Diehl says, quoting an adage that describes the relative costs of long-distance shipping.

Overall, PwC expects costs to mount for shippers. For example, by 2025, the chemical industry will need to keep \$22 billion worth of additional inventory because of all the products that will be tied up through delays and longer routes. Operating costs will increase by \$29 billion over the same period, largely because of higher shipping rates. Capital expenditures will total \$23 billion as companies require more railcars and other equipment, PwC predicts.

As production ramps up, each of the major chemical companies is developing its own strategy for navigating shipments through the growing traffic.

Chevron Phillips established new packaging facilities in Fort Worth and Charleston, S.C., to ensure it can move product out of its two new 500,000-metric-ton-per-year polyethylene plants in Old Ocean, Texas. The resins arriving in Fort Worth will be sent to ports on the West Coast. The product processed in Charleston will find ships at Charleston's large container port.

"This doesn't mean we are unhappy with the Houston Ship Channel. They are important for our business today and will be in the future," CEO Lashier told the Houston audience. "But when you're betting \$6 billion, you want to have a lot of options."

Dow is putting a lot of emphasis on communication. Karen Bryant, Dow's director of logistics, says the firm will collaborate with the ports of Houston and New Orleans to clear the way for its products.

"These two ports have made physical upgrades as well as operational upgrades such as increased hours of service, and we believe the increase in volume will be manageable," Bryant says. Dow will also collaborate with steamship lines to coordinate vessel space and containers, she adds.

Bryant expects to see rail congestion

around Houston even though the railroads are adding storage track for parking railcars to ease the squeeze, she says. Dow is also contracting with resin repackagers for storage space.

"Dow does have contingency plans in

"Train beats truck; ship beats train."

-Capt. Bill Diehl (ret.), president, Greater Houston Port Bureau place in the event Houston and New Orleans become congested or experience a shortage of containers," Bryant says. Options include using packaging facilities in the Dallas/Fort Worth area to stage exports to the East and West Coasts.

The firm could also use the port of Freeport, in the shadow of its own massive Freeport complex. The container terminal there handles about 100,000 boxes per year. Dow may also send shipments through Monterrey, Mexico.

With its new polyethylene plants in Mont Belvieu, Texas, ExxonMobil is taking an approach to logistics unique in the U.S. chemical industry. ExxonMobil will dedicate all the new plants' 1.3 million metric tons of annual production capacity to the export market. The company will do its own packaging on-site. Some 200 trucks per day will haul loaded containers about 30 km to Port Houston. The new plants don't even have a rail connection for the domestic market.

"This was built to be an efficient export machine," says April Feick, ExxonMobil Chemical's vice president of global supply chain.

Finding drivers, Feick says, hasn't been a problem because it's easier to hire truckers for short, routine hauls than it is for long ones. The Texas legislature recently passed legislation easing the weight restrictions for trucks on Texas highways within 48 km of a container port. The limit for trucks with six axles increased from 38 to 42 metric tons. The difference will allow ExxonMobil to fully load containers and take 10% of its trucks off the road.

A new polyethylene plant that Exxon-Mobil is planning for Beaumont, Texas, which is farther from Houston, will be connected by rail and have more of a domestic orientation. The company, Feick says, may further optimize its system by dedicating Beaumont to the U.S. and directing more of the polyethylene output at its older Mont Belvieu facility toward the export market.

If it remains adaptable, the chemical industry should succeed in moving all its new product to market, Feick predicts. "The key on this is going to be logistics flexibility," she says, "and really working through every element of the supply chain." ■

# China readies new insurance scheme

Government wants to make it compulsory for manufacturers to buy coverage against environmental damage

### JEAN-FRANÇOIS TREMBLAY, C&EN HONG KONG

hen a chemical producer in China accidentally or intentionally causes serious damage to the environment—be it through a spill, an explosion, or another way—the company is usually ordered to cease operations. Its managers can be fined or even jailed.

But most of the time, no compensation is paid to those affected. Local communities have to bear the cost of contaminated wells from which residents can't drink, toxic soil that farmers can't till, or polluted lakes that fishermen can't fish.

This could soon change. The Chinese government is on track to approve regulations requiring manufacturers in high-risk industries to buy environmental liability insurance. Draft regulations, supported by the Chinese Ministry of Environmental Protection and the China Insurance Regulatory Commission, were unveiled last month to allow industry and the public to comment. The next step will be approval by the State Council, the top organ in the Chinese government.

Some in the Chinese chemical industry support the move. "You need such insurance in the chemical industry," says Shuguan Gan, chairperson of Jingzhou Jianghan Fine Chemical, a producer of

silane coupling agents based in the central China province of Hubei. "The insurance helps the company to survive if it has an accident that affects the community."

Jianghan voluntarily purchased third-party environmental liability coverage several years ago, Gan notes.

In the U.S., chemical producers don't have to get insurance to cover their environmental liability, notes David J. Dybdahl, president of the American Risk Management Resources Network, an insurance broker specializing in environmental

coverage. "Chemical companies may need to purchase environmental liability insurance if it is related to their waste streams, but not their operations as a chemical company," he says.

First proposed in China more than a decade ago, compulsory environmental liability insurance will mark another step in Chinese efforts to control the damage that industry can cause to the environment. The theory is that manufacturers will improve their environmental performance because not doing so would result in higher insurance premiums.

The insurance proposal is one of multiple measures that China has implemented in recent years to make manufacturers more accountable. The increasing scrutiny has led to plant closures and higher prices for certain materials.

Environmental liability insurance has multiple benefits, Dybdahl explains. For example, it helps bankers who are making loan decisions calculate the environmental risks their capital will be



Silane chemicals producer Jingzhou Jianghan chose to buy environmental liability insurance. exposed to. It can also help governments decide what risks certain producers pose. "If something is uninsurable, it is always a good idea from a public policy standpoint not to allow those activities or to modify the activity to make it insurable," he says.

When Jianghan bought its environmental policy, the insurer came to inspect the company's facilities for three days. "The main purpose of the insurance is to provide coverage for communities against damage caused by industry," Gan notes. "It's not to protect the environment." But the audit's goal was to determine whether Jianghan can adequately manage its environmental performance.

"They looked at everything: our equipment, our manufacturing data, our wastewater treatment plant," Gan recalls. "They wanted to make sure that our facilities can satisfy all regulatory requirements." If Jianghan didn't have a wastewater treatment plant, the insurer wouldn't have agreed to sell the firm coverage, he says.

Over the past 10 years, the Ministry of Environmental Protection has run trial insurance programs all over China. The Chinese insurance industry spent the long trial period studying how to set premiums in policies covering environmental liability. When the program is rolled out nationally, several industries, including chemical production and hazardous waste handling, will have to get the coverage. Failure to do so will result in fines and sanctions by regulators.

China's largest petrochemical producers are already required to get environmental liability coverage because of the outsize risk they pose, says the manager of a medium-size manufacturer of intermediate chemicals. He asked for anonymity because of his critical view of the government's plan to require environmental liability insurance.

The government also encourages medium-size producers to buy environmental liability insurance, he says. But requiring such firms to get coverage may not do

# "If you're a marginal producer with poor compliance, you will be shut down."

-Steve Wang, general manager, Join King Fine Chemicals

# **NMR Proton Shifts for Residual Solvent Impurities**

# **Globally Harmonized System of Classification and Labelling** of Chemicals (GHS)

Solvent Acetic Acid	Synonyms Ethanoic acid	Mol Wt 60.05	BP °C	Linear Formula CH <sub>3</sub> COOH	H-Signal Multi CH <sub>3</sub> s	2.13	<b>D</b> <sub>2</sub> <b>O</b> 2.08	CD <sub>3</sub> OD	(CD <sub>3</sub> ) <sub>2</sub> SC	(CD <sub>3</sub> ) <sub>2</sub> CO	D CD <sub>3</sub> CN 1.96	C <sub>6</sub> D <sub>6</sub> 1.55	
Formic Acid	Methanoic Acid	46.02	101	HCOOH	H s	8.02	8.22	8.08	8.18	8.11	8.03	-	
1-Butanol	n-Butanol / 1-Hydroxybutane / n-Butyl alcohol	74.12	117.6	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> OH	CH <sub>3</sub> t CH <sub>2</sub> (3) m	0.94 1.39	0.91 1.35	0.93	0.86	0.90	1.29-1.39	-	
					CH <sub>2</sub> (2) m CH <sub>2</sub> (1) m	1.56 3.65	1.53 3.61	1.51 3.54	1.39 3.38	1.44-1.52 3.49-3.56	1.42-1.49 3.45-3.51		
2-Butanol	sec-Butanol / 2-Butyl alcohol / 2-Hydroxybutane	74.12	99	CH <sub>3</sub> CH(OH)CH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub> (4) t CH <sub>3</sub> (1) d	0.93	0.84	0.91	0.83	0.89	0.88	-	
					CH <sub>2</sub> m CH m	1.48 3.73	1.42 3.71	1.44 3.63	1.32 3.49	1.33-1.47 3.56-3.66	1.33-1.42 3.54-3.62	-	
tert-Butanol	t-Butyl alcohol / 2-Methyl-2-propanol	74.12	83	(CH <sub>3</sub> ) <sub>3</sub> COH	CH3 s	1.28	1.24	1.40	1.11	1.18	1.16	1.05	
Ethanol	Ethyl alcohol	46.06	78	C <sub>2</sub> H <sub>6</sub> O	CH3         t           CH2         q	1.25 3.72	1.17 3.65	1.19 3.60	1.06 3.44	1.12 3.57	1.12 3.54	0.96 3.34	-
Ethylene Glycol 1-Hexanol	Ethane-1,2-diol / 1,2-Dihydroxyethane n-Hexanol / Hexyl alcohol / Caproic alcohol	62.06 102.18	196-198 156-157	HOCH <sub>2</sub> CH <sub>2</sub> OH CH <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub> OH	CH s CH <sub>3</sub> t	3.76 0.86-0.93	3.65 0.88	3.59 0.87-0.94	3.34 0.86	3.28 0.88	3.51 0.89	3.41	
					CH <sub>2</sub> (3-5) m CH <sub>2</sub> (2) m	1.24-1.44 1.52-1.61	1.24-1.39 1.50-1.59	1.26-1.40 1.48-1.57	1.19-1.32	1.24-1.39	1.22-1.38	-	
<ul> <li>iso-Amyl alcohol</li> </ul>	3-Methyl-1-butanol / iso-Pentyl alcohol	88.15	130	(CH3)2CHCH2CH2OH	CH <sub>2</sub> (1) m CH <sub>3</sub> d	3.64	3.69	3.53 0.91	3.35-3.40 0.85	3.37 0.89	3.44-3.50 0.89	-	
		00.15	130	(OH <sub>3</sub> ) <sub>2</sub> OHOH <sub>2</sub> OH <sub>2</sub> OH	<i>CH₂</i> CH q	1.47	1.44	1.42	1.31	1.39	1.37	-	
<u> </u>					CH m CH₂OH m	1.66-1.78 3.68	1.61-1.71 3.64	1.64-1.77 3.58	1.65 3.41	1.72 3.53-3.59	1.67 3.51	-	
iso-Butanol	iso-Butyl alcohol / 2-Methyl-1-propanol	74.12	108	(CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> OH	CH₃ d CH m	0.92	0.88	0.90	0.82	0.87	0.86	-	(.
Methanol	Methyl alcohol	32.04	64.7	CH <sub>3</sub> OH	CH <sub>2</sub> m CH <sub>3</sub> s	3.41 3.49	3.38 3.34	3.30 3.34	3.15 3.16	3.26-3.34 3.31	3.25 3.28	- 3.07	C
Pentanol	n-Amyl alcohol / Pentyl alcohol	88.15	137-139	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> OH	CH <sub>3</sub> t CH <sub>2</sub> (3-4) m	0.91	0.88	0.92	0.86	0.89	0.90	-	E
					CH <sub>2</sub> (2) m	1.58	1.55	1.53	1.41	1.45-1.55	1.43-1.52	-	
1-Propanol	n-Propanol / Propyl alcohol	60.10	97	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> OH	CH <sub>2</sub> (1) t CH <sub>3</sub> t	3.64 0.93	3.60 0.90	3.53 0.92	3.37 0.87	3.37 0.89	2.46 0.88	-	
V					CH <sub>2</sub> (2) m CH <sub>2</sub> (1) t	1.60 3.60	1.55 3.56	1.54 3.49	1.45 3.38	1.44-1.55 3.44-3.51	1.43-1.52 3.40-3.47	-	
2-Propanol	IPA / Isopropanol / iso-Propyl alcohol	60.10	82	(CH <sub>3</sub> ) <sub>2</sub> CHOH	CH <sub>3</sub> d CH m	1.20 4.03	1.18 4.02	1.14 3.92	1.04 3.78	1.10 3.90	1.09 3.67	0.95	• Se
Anisole	Methoxybenzene / Methyl phenyl ether	108.14	154	C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub>	CH <sub>3</sub> s	3.76	3.85	3.77	3.76	3.78	3.77	-	• (
					CH (a/p) m CH (m) m	6.93 7.29	7.06 7.41	6.90 7.25	6.93 7.29	6.88-6.95 7.24-7.31	6.89-6.98 7.27-7.34	-	
Benzene Pyridine		78.11 79.10	80.09 115-116	C <sub>6</sub> H <sub>6</sub> C <sub>5</sub> H <sub>5</sub> N	s CH (2) m	7.37 8.62	7.44 8.52	7.33 8.53	7.37 8.58	7.36 8.58	7.37 8.57	7.15 8.53	
1					CH (3) m CH (4) m	7.29 7.68	7.45 7.87	7.44 7.85	7.39 7.79	7.35 7.76	7.33	6.66 6.98	
Toluene	Methylbenzene	92.14	111	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	CH <sub>3</sub> s	2.36	-	2.32	2.30	2.32	2.33	2.11	
					CH (o/p) m CH (m) m	7.17 7.25	-	7.16 7.16	7.18 7.25	7.10-7.20 7.10-7.20	7.10-7.30 7.10-7.30		
p-Xylene	1,4-Dimethylbenzene / p-Xylol	106.17	138	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	CH₃ s CH s	2.30 7.06	2.30 7.18	2.26 7.02	2.24 7.05	2.26	2.27	-	
Chloroform 1,2-Dichloroethane	Trichloromethane / Formyl trichloride EDC / Ethylene dichloride / Glycol dichloride	119.38	61 81-85	CHCl <sub>3</sub> CICH <sub>2</sub> CH <sub>2</sub> CI	CH s CH <sub>2</sub> s	7.26	-	7.88 3.78	8.32 3.90	8.02 3.87	7.58	6.15 2.90	
Dichloromethane	DCM / Methylene dichloride	84.93	39-40	CH <sub>2</sub> Cl <sub>2</sub>	CH <sub>2</sub> s	5.30	-	5.48	5.76	5.63	5.44	4.27	
Acetonitrile Dimethylformamide	AcCN / Methyl cyanide / Cyanomethane DMF / Formyldimethylamine	41.04 73.09	81-82 153	CH <sub>3</sub> CN HCON(CH <sub>3</sub> ) <sub>2</sub>	CH <sub>3</sub> s CH s	2.10 8.02	2.06 7.91	2.03 7.98	2.07 7.95	2.05 7.96	1.96 7.92	1.55 7.63	
•					CH₃ s CH₃ s	2.96 2.88	3.00 2.86	2.99 2.85	2.89 2.73	2.94 2.78	2.89 2.77	2.36 1.86	
Dimethyl sulfoxide n-Butyl acetate	DMSO / Methyl sulfoxide / (Methylsulfinyl)methane 1-Butyl acetate	78.13	189 126-127	(CH <sub>3</sub> ) <sub>2</sub> SO CH <sub>3</sub> CO <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>	CH <sub>3</sub> s CH <sub>3</sub> CH <sub>2</sub> t	2.62	2.71 0.91	2.65	2.54	2.52	2.50	1.68	
In Dutyr accitate	1 Butyr acetate	110.10	120 121	0113002(0112)30113	CH <sub>2</sub> m	1.38	1.37	1.39	1.32	1.32-1.43	1.31-1.42	-	
					<u>CH₂</u> m CH₃CO s	1.61 2.04	1.63 2.09	1.61 2.01	1.54	1.54-1.62 1.97	1.54-1.63 1.97	-	
Ethyl acetate	EtOAc / Ethyl ethanoate / Acetoxyethane	88.11	75-78	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	CH <sub>2</sub> CO t CH <sub>3</sub> CH <sub>2</sub> t	4.07	4.11	4.06	3.99 1.18	4.02	4.02	- 0.92	-
					CH <sub>3</sub> CO s CH <sub>2</sub> q	2.05 4.12	2.07 4.14	2.01 4.09	1.99 4.03	1.97	1.97 4.06	1.65 3.89	
Ethyl formate	Ethyl methanoate / Formic acid ethyl ester	74.08	54	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	CH₃ t	1.29	1.29	1.27	1.24	4.05	-		
•					CH <sub>2</sub> q CH s	4.22 8.04	4.28 8.16	4.20 8.06	4.17 8.23	-	-	-	Com
iso-Propyl acetate	iPrOAc / 1-Methyl ethyl acetate / 2-Propyl acetate	102.13	88.8	CH <sub>3</sub> CO <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	(CH <sub>3</sub> ) <sub>2</sub> CH d CH <sub>3</sub> CO s	1.23 2.02	1.25 2.07	1.22 1.99	1.17 1.96	1.19	1.19 1.94	-	
Methyl acetate	Methyl ethanoate / Methyl acetic ester	74.08	57.4	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	CH m CH <sub>3</sub> CO s	4.99 2.05	4.98 2.09	4.95 2.02	4.86 1.92	4.91 1.98	4.91 1.99	-	
					OCH <sub>3</sub> s	3.67	3.68	3.64	3.61	3.59	3.60	-	
n-Propyl acetate	Acetic acid propyl ester / Propyl ethanoate	102.13	102	CH <sub>3</sub> CO <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> t CH <sub>2</sub> CH <sub>3</sub> m	0.94	0.92	0.94	0.88	0.92	0.92	-	• G
					CH <sub>3</sub> CO s CH <sub>2</sub> CO t	2.05 4.02	2.09 4.06	2.02 4.01	2.00 3.95	1.98 3.97	1.98 3.97	-	
tert-Butyl methyl ether	MTBE / 2-Methyl-2-methoxy propane	88.15	54-56	(CH <sub>3</sub> ) <sub>3</sub> COCH <sub>3</sub>	CCH <sub>3</sub> s OCH <sub>3</sub> s	1.19 3.22	1.22 3.24	1.15 3.20	1.11 3.08	1.19 3.13	1.14 3.13	1.07 3.04	
Diethyl ether	Ether / Ethoxyethane	74.12	34.6	(CH <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> O	CH₃ t	1.20	1.17	1.17	1.09	1.11	1.12	1.11	
- 1,2-Dimethoxyethane	DME / Dimethylglycol	90.12	84-86	CH3OCH2CH2OCH3	CH <sub>2</sub> q CH <sub>3</sub> s	3.48 3.40	3.56 3.37	3.49 3.35	3.38 3.24	3.41 3.28	3.42 3.28	3.26 3.24	
1,4-Dioxane	Diethylene ether / Diethylene dioxide	88.11	101	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	CH <sub>2</sub> s CH <sub>2</sub> s	3.55 3.71	3.60 3.75	3.52 3.66	3.43 3.57	3.46 3.59	3.45 3.60	3.33 3.35	
Tetrahydrofuran	THF / Oxolane / Diethylene oxide	72.11	66	C4H8O	CH <sub>2</sub> m CH <sub>2</sub> O m	1.85 3.76	1.88 3.74	1.87 3.71	1.76 3.60	1.79 3.63	1.80 3.64	1.40 3.57	
Cyclohexane	Linstone / Dissonder the second	84.16	81	C <sub>6</sub> H <sub>12</sub>	CH <sub>2</sub> s	1.43	-	1.45	1.40	1.43	1.44	1.40	
<i>n</i> -Heptane	Heptane / Dipropyl methane	100.21	98	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>	CH3         t           CH2         m	0.89	-	0.90	0.86	0.88	0.89	-	
n-Hexane		86.18	69	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub>	CH <sub>3</sub> t CH <sub>2</sub> m	0.88	-	0.90	0.86	0.88	0.89	0.89	
Methylcyclohexane	MCH	98.19	101	CH <sub>3</sub> CH(CH <sub>2</sub> ) <sub>5</sub>	CH <sub>2</sub> CH (ax) m CH <sub>3</sub> d	0.82-0.93	-	0.82-0.94	0.80-0.90	0.87-0.93	0.88-0.94	-	
					CH <sub>2</sub> (4) (ax) m	1.06-1.17	-	1.09-1.20	1.04-1.14	1.07-1.17	1.08-1.18	-	
		_			CH <sub>2</sub> (3) (ax) m CH m	1.17-1.28 1.33	-	1.26 1.31-1.39	1.14-1.25 1.32	1.24	1.25		
n-Pentane		72.15	36	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>	CH <sub>3</sub> t CH <sub>2</sub> m	0.88	-	0.90	0.86	0.88	0.89	0.87 1.23	
Acetone 2-Hexanone	2-Propanone / Dimethylketone MBK / Methyl butyl ketone / Propyl acetone	58.08 100.16	56 127	CH <sub>3</sub> COCH <sub>3</sub> CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> COCH <sub>3</sub>	CH <sub>3</sub> s CH <sub>3</sub> t	2.17	2.22 0.88	2.15	2.09	2.09	2.08	1.55	
2-Hexanone	MBR / Methyr butyr ketone / Propyr acetone	100.16	127	UH3(UH2)3UUUH3	CH <sub>2</sub> m	1.32	1.30	1.32	1.24	-	-	-	(
					CH <sub>2</sub> m CH <sub>2</sub> CO t	1.56 2.42	1.53 2.56	1.53 2.47	1.43 2.41	-	-	-	(
<ul> <li>Isobutyl methyl ketone</li> </ul>	MIBK / 4-Methylpentan-2-one / Isopropylacetone	100.16	117.4	(CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> COCH <sub>3</sub>	CH <sub>3</sub> CO s (CH <sub>3</sub> ) <sub>2</sub> CH d	2.13 0.92	2.21 0.90	2.12 0.85	2.07 0.85	- 0.88	- 0.88	-	
- isosayi metryi ketolle				0.13/20110112000113	CH m	2.13	2.08	2.00	2.00	2.02-2.11	2.02-2.08	-	Harn
					CH₃CO s CH₂ d	2.12 2.30	2.21 2.43	2.05 2.28	2.05 2.28	2.06 2.31	2.05 2.29	-	
	MEK / Ethyl methyl ketone / 2-Butanone	72.11	80	C <sub>2</sub> H <sub>5</sub> COCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> t CH <sub>3</sub> CO s	1.06 2.14	1.26 2.19	1.01 2.12	0.91 2.07	0.96 2.07	0.96 2.06	0.85	<ul> <li>Irritation (s</li> </ul>
Methyl ethyl ketone					CH₂CH₃ q	2.46	3.18	2.50	2.43	2.45	2.43	1.81	• Ac
	TEA / Diethylamingethane	101.19	90	(CoHe) N	CH <sub>2</sub> t		0.99	1.05	0.93	0.96			
Triethylamine	TEA / Diethylaminoethane	101.19	90	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	CH <sub>3</sub> t           CH <sub>2</sub> q	1.03 2.53	0.99 2.57	2.58	0.93 2.43 7.07	0.96 2.45	2.45	2.40	
	TEA / Diethylaminoethane Methanamide / Formic amide Long chain, linear aliphatic hydrocarbons	101.19 45.04	90 210	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N HCONH <sub>2</sub>									<ul> <li>Specific target (drowsiness or c</li> <li>Hazard</li> </ul>



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 May cause fire or explosion Strong oxidizer May intensify fire



• Acute toxicity (fatal or toxic)



· Hazardous to the aquatic environment (acute or long term)



much to improve the environment, he adds. Whether they have insurance or not, he says, smaller companies that damage the environment will likely try to cover it up.

"If a company reports to its insurer that it had a mishap, the government will learn about it," he says. Fear of official sanctions, including the possible arrest of managers, will discourage firms from disclosing spills to their insurers, he contends.

The proposed insurance coverage is part of the government's effort to improve industrial company compliance with environmental regulations, according to Steve Wang, general manager of Join King Fine Chemicals, a producer of chemicals used in the pharmaceutical and agrochemical industries. For instance, he says, government inspectors have over the past two years been visiting manufacturing facilities more frequently, and their scrutiny is becoming increasingly thorough. In Wang's view, more-frequent inspections are a stronger tool for enforcing compliance than compulsory insurance ever could be.

In Hangzhou, China, a chemical trader who buys chemicals from a variety of suppliers and also asked for anonymity tells C&EN that stricter environmental rules have raised the price of several intermediates used in the pharmaceutical industry. The insurance, he argues, will not work as intended in China. "If you look at Chinese state-owned banks, many of them have a lot of bad loans on their balance sheets," he says. "This is not because the banks cannot select good borrowers; it's because the government orders them to make those loans."

In the case of environmental liability insurance, he expects the government will order insurers to cover certain companies that might otherwise be uninsurable. "In fact, having insurance coverage could encourage those manufacturers to worry even less about their environmental performance," he speculates.

While similarly skeptical chain about liability insurance, Jiangh Join King's Wang says the increasing pressure on companies to im-

prove their compliance has been good for his business. In recent years, he says, Join King's profitability has improved because of reduced competition as other firms are pressured out of business.

"If you're a marginal producer with poor compliance, you will be shut down," he says. "Investing in environmental abatement raises a company's business sustainability."

At Jianghan, Gan says even a temporary closure of facilities for environmental reasons can dramatically alter the competitive landscape. "Even if one of our competitors has to shut down for only three months af-

> ter a government inspection, that's enough for some of their customers to permanently switch to us," he says.

Although opinions vary on whether compulsory environmental liability insurance will help China's environment, the country on the whole appears to be making progress in reducing the damage caused by industry. And if the insurance can be made to work as intended, notes Dybdahl, the U.S.

insurance executive, it will play an important role in encouraging companies to limit their environmental risk.

"Safer firms pay less for insurance than risky firms, and they can use these lower insurance costs to finance their investments in safety and other loss control measures," he says. ■

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## "The main purpose of the insurance is to provide coverage for communities."

# -Shuguan Gan, chairperson, Jingzhou

Jianghan Fine Chemical



# 2-D MATERIALS C&EN talks with Tomás Palacios, 2-D materials visionary

MIT professor wants to integrate electronics everywhere and anywhere

## KATHERINE BOURZAC, special to C&EN

n recent years, the family of two-dimensional materials has expanded from simple graphene to include almost 1,000 materials that exist—or are predicted to exist—in an atomically thin form. These 2-D materials are flexible and transparent, and their unusual properties make researchers eager to apply them in electronic devices. Electrical engineer Tomás Palacios of Massachusetts Institute of Technology believes ultrathin materials will allow engineers to completely reimagine what electronics look like and where they can go, enabling electronics to be placed almost anywhere and everywhere. He described his vision to Katherine Bourzac.

# Can you tell me about your concept for ubiquitous electronics?

What my group is trying to do is find applications for these truly amazing 2-D materials. We strongly believe that we should be able to change the form of electronics, allowing us to bring electronics to completely different objects than what we have been used to so far. One way to bring us closer to the vision of ubiquitous electronics is to make electronic systems so large that we can wrap entire buildings with them. We are now starting to print electronics in the same way that we can print newspapers, so we can think of covering everything with smart materials. A different approach to ubiquitous electron-

# Vitals

- Hometown: Jaén, Spain
   Studies: B.S. and M.Sc., 2001, Polytechnic University of Madrid; M.Sc., 2004, and Ph.D., 2006, University of California, Santa Barbara
- Childhood hobby: Building inventions, including attempted perpetual motion machines
- Current hobbies: Playing the piano, hiking, reading, and spending time with family
   Favorite material: "I try to be
- opportunistic in the sense that I will use any material that serves the purpose I need. That's one of the advantages of 2–D materials. You can mix and match in any way you want."
- ► Early inspiration for syncells: "When I was very little, six or seven years old, I watched a science fiction movie, "Fantastic Voyage," where they were able to shrink a submarine to bring it inside the arteries of a patient. I have been asking myself, How can we bring that vision closer to reality?"

ics is to make these microsystems so tiny that we can have them everywhere and not even realize they are there. It's about embedding functionality and intelligence in just about every object that we have.

# How might you embed functionality into a building or another large object?

We modified a 3-D printer to be able to print structural materials, such as polymers, and electronic materials based on graphene and other 2-D materials. For example, we worked with NASA to print the body of a small unmanned aerial vehicle and embed it with sensors to be able to monitor its structural properties and mechanical strain.

#### What about going small?

With conventional electronics, it's very difficult to find anything smaller than maybe 1 mm<sup>3</sup>. But nature is able to build extremely complex microsystems with a volume that is orders of magnitude smaller than that. Every single one of our cells is an amazing microsystem that I would argue is a lot more complex and interesting than many of the electronic microsystems we've made so far. So a couple years ago we started a large effort to try to demonstrate what we call synthetic cells, or syncells, based on 2-D materials. They are the only materials we know of that are inherently flexible, transparent, and multifunctional, just like biological cells.

#### How do you make them?

The idea is to fabricate simple building blocks made of 2-D materials on a silicon wafer. One building block could be a light-emitting diode transmitter or a solar cell energy harvester. Another could be a chemical sensor of some sort. Then you detach these building blocks from the wafer and have them in solution. To increase the density of our structures, we are working with Peng Yin and his group at Harvard University. They are developing ways to use DNA to fold the 2-D materials and lock them in place.

The final goal of our research is to be able to develop artificial organelles with specific functionality that you could combine in arbitrary ways to make different types of syncells. For one syncell you take a few chemical sensors, and you combine those with memory and an LED communication building block. Then you wrap everything with a graphene membrane to hold it together. The goal is to demonstrate microsystems smaller than anything anyone has fabricated before with conventional silicon.

Once you have these tiny syncells floating in solution, you can start thinking about how to make the syncells interact with each other. How might you combine syncells that have slightly different properties to build more complex microsystems? Or, how might you embed them in materials such as asphalt, plastic, or paint to bring them to every object around us?

#### Your ideas about electronics are very imaginative. Where do you get your ideas?

I'm at a university, so I am paid to come up with ideas that, although they may seem crazy today, may become a reality in a few years. My time horizon is very different from the time horizon of companies that are expected to make money in the next quarter.



Katherine Bourzac is a freelance writer. A version of this story first appeared in ACS Central

*Science*: cenm.ag/palacios. This interview was edited for length and clarity.



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# BURGEONING

# **BRINGS NEW OPPORTUNITIES**

MALORYE A. BRANCA, C&EN BRANDLAB CONTRIBUTING WRITER

t was an incurable tumor on her baby daughter's optic nerve that led Tracy Ryan to cannabis.

Ryan and her husband were told that chemotherapy might slow the tumor's growth but that was the most they could hope for, and the effect might be short-lived. After recovering from their shock, the Ryans did some research that led them to cannabis oil. Although there is not any clinical data suggesting cannabis oil has any efficacy in cancer, her parents gave it to Sophie during chemotherapy in hopes of easing her discomfort. Despite her initial diagnosis, Sophie's tumor shrank dramatically with chemotherapy. Sophie turns five years old this year and is starting school. She is on track with her developmental milestones, "thriving, healthy, and happy," her mother says.

Tracy Ryan, meanwhile, has founded CannaKids, a company that offers cannabis oil-based products for people of any age but with a focus on pediatric conditions. That business, she says, is "booming."

Ryan's is just one of many young businesses

Demand for chemists and specialized instruments grows as range of products expands

operating in the new world of medical marijuana, where products may have to be tested for purity and potency but do not have to go through the approval process of the U.S. Food & Drug Administration (FDA). In other words, this is a new "gray area" of medical products, unlike the approval processes for typical prescription medications or overthe-counter treatments. The Grand View Research market-research and consulting company estimates the market for medical marijuana to reach \$55 billion by 2025. The range and number of marijuana products is also growing. Producers have branched out from the highly popular dried flowers, extracts, and vape pens to include a wider range of products. CannaKids, for example, has expanded its product line from syringes of oil delivered by mouth to tinctures, topicals, and nasal spray. Testing these products is fueling demand for chemists and analytical instruments specifically for the medical marijuana market.

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This new market was born of several trends: The public is increasingly accepting marijuana as a recreational drug, many of the medical conditions it is used for are otherwise untreatable, and anecdotes abound about its efficacy. "Why not?" seems to be the reasoning. As the market expands and evolves, "What's next?" seems to be the looming question.

#### **FDA-APPROVED PRODUCTS**

Besides the gray-area dispensaries, there are businesses aiming at the traditional drug market. Axim Biotechnologies CEO George Anastassov and his business partner got involved with cannabis while looking for novel analgesics to treat chronic pain. "We could see the opioid epidemic evolving," he explains, "and being surgeons, we knew there was a critical need for new, powerful pain relievers that could be used on a long-term basis without the side effects that opioids have."

Axim has nine cannabis-based products in development, including chewing gums, suppositories, ophthalmic formulations, and skin creams. These treatments target conditions including smoking, glaucoma, dry eye, psoriasis, eczema, vitiligo, restless legs syndrome, loss of appetite, chemotherapy-induced vomiting, and postherpetic neuralgia. One of the company's flagship products is MedChew Rx, which is in preclinical trials for pain and spasticity associated with multiple sclerosis. A trial of CanChew, meanwhile, was just completed in people with irritable bowel syndrome.

Several other companies are also working on pharmaceutical-grade cannabis-based products, all of which will follow the stringent FDA-review path to approval.



Those companies include Corbus Pharmaceuticals, GW Pharmaceuticals, Insys Therapeutics, and Zynerba Pharmaceuticals. "There are some wonderful products headed to the market from us and our competitors," Anastassov says.

The progress is happening despite the massive legal and regulatory hurdles that

have long hamstrung developers of cannabisbased products. The U.S. federal government has listed cannabis as a Schedule 1 drug (that is, it is deemed to have the highest level risk of abuse and so is among the most tightly regulated substances). As a result, simply being able to do research on cannabis is a major undertaking. It can take years to get approval, and transporting the plant, its extract, or even seeds across state lines to get it into a laboratory is another headache.

## MORE OF EVERYTHING

Researchers and entrepreneurs are keeping up with surging demand for medical marijuana by expanding their operations and finding new uses for the cannabis plant, its extracts, and the hundreds of compounds it contains. Thanks to advances in instrumentation, it is now fairly easy to extract those compounds and identify them. The real challenge is figuring out which ones have medicinal effects and what those are. The barriers to research on the plant have resulted in a paucity of peer-reviewed data and a plethora of anecdotal accounts.



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The two star compounds in cannabis that have been well studied so far are tetrahydrocannabinol (THC) and cannabidiol (CBD). THC has intense psychogenic effects; CBD does not. Some people have claimed that CBD has analgesic, anti-inflammatory, antianxiety, and other properties, so manufacturers are using CBD to make medicinal marijuana-based products that are nonpsychogenic. Some researchers in this field also believe the terpenes and other cannabinoids in the plant have healing properties. "Identifying safe ingredients that synergize with the cannabinoids is really important," says Christian Sweeney, director of science and technology at Cannabistry Labs, which provides services from production through marketing to marijuana producers. But such synergy is hard to confirm both because the plant itself is so complex and because of the rules for its use and study.

The only cannabis-related pharmaceutical-grade products currently on the U.S. market—Marinol, Syndros and Cesamet all contain synthetic THC. Detractors claim synthetic THC is not as effective as the botanical version. GW's Sativex for multiple sclerosis spasticity has been approved in at least a dozen countries, though not the U.S. yet. It contains botanically derived THC and CBD as well other cannabinoids and cannabis-related compounds.

Axim intends to be next to market, and with a slew of products. It has been a tough slog, to say the least. Anastassov points out that only one company in the world, Bedrocan, is allowed to produce flowers for pharmaceutical-grade cannabis extract, a crucial ingredient for these products. "It took 30 years for Bedrocan to get that approval," he says. Axim uses such flowers to make its FDA-approvable products. Those flowers come from the Netherlands, and the Dutch ministry of health controls production. The strict regulations for transporting cannabis-related ingredients add to the challenges. Further, "THC is very volatile and oxidizes easily," Anastassov says. Even the extraction process for FDA-approvable cannabis-based products from the plant is complex. Axim has proprietary intellectual property on its entire extraction process.

A key challenge is that there are many different cultivars of cannabis, and they all have different mixtures of the many compounds found in the plant, says Mark Scialdone, principal consultant at BetterChem Consulting. "There is now inexpensive [polymerase chain reaction] technology that makes it possible to do rapid testing to determine whether a cultivar is enriched with CBD or THC," he says. Companies are also moving toward purification by shortpath distillation to isolate pure cannabinoids from solvent extracts for accurate doses in products such as vape pens. The processing of the plant material into cannabinoid isolates, such as THC distillate or crystalline CBD, requires high volumes of starting material and extraction solvent.

That's one of the reasons Heidolph North America has developed the automated Distimatic module for continuous, unattended solvent recovery. Distimatic pairs with the Heidolph rotary evaporator to remove bulk solvents that are added to the cannabis oil during earlier processing steps, thereby turning it into a higher purity extract.

The free form of the medical marijuana market has also led to a lot of variation in the quality of product. "We went out and grabbed some products from dispensaries. We found that the best product was 90% accurate with the labeled claim and the worst had 0% THC," says Neil Spingarn, chief science officer of Nebula Management, which operates manufacturing facilities for cannabis-based products. "How could you even do a clinical study with products like that?"

Many states require that companies perform third-party testing to validate dose level and detect unwanted contaminants. Spingarn and others recommend that producers do rigorous testing on their own. "If someone questions your product, you want to have your own documented results," he explains.

To do this type of analysis, most labs use high-performance liquid chromatography with an ultraviolet detector, says Bob Clifford, general manager of marketing at Shimadzu Scientific Instruments. But he adds, "If you want to know the molecular structure of the compounds you are seeing, you will go to a mass spectrometer." Scialdone of BetterChem recommends that his clients who need to know the purity of their extracts and isolates obtain their own HPLC and gas chromatography/ mass spectrometry instruments as well as "a real chemist who has expertise" to run the instruments and troubleshoot. The analysis process has gotten easier as companies such as Shimadzu have developed cannabis-analysis-specific instruments. Shimadzu's systems include everything clients need, including a software overlay "to get up and running in a single day," Clifford says. "Shimadzu and others are stepping up to the plate," Scialdone says.

Although a lesser-used technique for routine quality assurance and quality control, nuclear magnetic resonance spectroscopy is also useful for analyzing organic components of cannabis extracts. Benchtop NMR spectrometers, such as the Nanalysis NMReady-60, improves efficiency for routine cannibinoid detection and quantification in extracts. "The NMReady provides high resolution spectroscopy in a compact, affordable instruments," says Susanne Riegel, NMR Product Manager at Nanalysis. "Given the inherent quantitative nature of NMR and our simplified software packages, a wide range of professionals can use NMR spectroscopy to quickly

We found that the best product was 90% accurate with the labeled claim and the worst had 0% THC."

> Neil Spingarn chief science officer of NebulaManagement

and easily extract quantitative data, including parameters such as THC and CBD content" in cannabis extracts.

#### **GOING FORWARD**

Today's cannabis product developers often say that the medical marijuana business started in people's garages and that there was not much attention to chemistry or evidence-based medicine at that time. But that's over. "Most customers want lab-tested medicines they can trust. "None of us would be here without those guys who started it," CannaKids' Ryan says. "But today there are lots of serious people in this business, including very big players. Some even have quality control, marketing departments, and expert scientists on their advisory boards." Those companies seeking FDA approval for their products are tied to much tighter regulatory standards.

Companies such as Heidolph North America are trying to advance the science. Heidolph North America recently sponsored a scholarship in conjunction with the American Chemical Society Cannabis Chemistry Subdivision in the Division of Chemical Health & Safety. Heidolph North America has committed \$50,000 over five years to support the participation at ACS national meetings of chemists doing research on cannabis. (C&EN is published by ACS.) "People working in this field have limited opportunity to present their findings to their peers," says Michael Bishop, director of applied markets at Heidolph North America. "The scholarship is a great opportunity for cannabis chemists around the world to come together annually to

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recognize excellence and advance the field."

Regulations will continue to be a challenge. The rules and qualifying conditions vary from state to state. Ohio, for example, allows the use of medical marijuana for more than 20 conditions, including hepatitis C and HIV-positive status. Mississippi allows only the use of CBD oil, and only for debilitating seizure disorder. Even within a single state, regulations can vary. "In California, the laws depend on the municipality," Spingarn says. "You literally face different regulations from town to town."

Despite some warning from the current U.S. Administration about possible crackdowns, the range and number of these products continue to grow at a dizzying rate. It now appears that medical marijuana is here to stay.

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# A whole new world for rare earths

How the technologically important metals rose from obscurity to ubiquity

#### STEPHEN K. RITTER, C&EN WASHINGTON



Rare-earth oxides (clockwise from top center): praseodymium, cerium,

# In brief

The rare earths, a collection of 17 elements including the lanthanides—lanthanum to lutetium along with scandium and yttrium, have become indispensable components in many essential technologies of modern life, including smart phones, LEDs, and medical imaging. But not much was known about rare-earth chemistry until the 1960s. Since then, researchers have uncovered the elements' abundant magnetic. luminescent. electrochemical. and other properties. The Rare Earth Research Conference, held recently in Ames, Iowa, brought together researchers who discussed the evolution of rare-earth chemistry. new research trends. and the need for sound natural resource management to ensure their sustainable use for future technologies.

Not much was known about the chemistry of the rare earths in the 1940s, or even by the 1960s. This group of 17 elements, which include the lanthanides—lanthanum to lutetium—along with scandium and vttrium. seemed to consist of fairly unreactive metals that all behaved similarly. Most of the research and development involving the elements was metallurgical, not chemical. Until 1965, the major applications for the rare earths included using mixtures of rare-earth oxides for polishing lenses and mirrors, using cerium and lanthanum oxides as promoters in zeolite catalysts for petroleum refining, and using "mischmetal" rare-earth alloys with iron as flints for lighters.

Erbium

HO

Holmium

Terbium

Dysprosium

69

Flash forward to this past June, and rare earthers were back in Ames for the first time since 1965, for the 28th RERC. The Holiday Inn sign is long gone from the still-cozy midwestern college town, and the world of rare earths has changed.

In 1965, the "counterculture revolution" was under way, and many of the world's young adults were protesting in favor of peace over nuclear power and the nuclear weapons of the Cold War. At the same time, they were falling in love with modern conveniences, driving demand for microwave ovens, early versions of personal computers and video games, and televisions. Coincidentally, 1965 witnessed the launch of the first major commercial use for a highly purified rare-earth material: Europium-doped yttrium salts began to be used as red phosphors in the picture tube of color television sets.

Now 52 years on, the internet rules nearly everyone's lives, and handheld devices have greater capabilities than those early

# 'elcome Rare Earthers."

In 1965, this message appeared on a Holiday Inn sign in Ames, Iowa, to greet the attendees of the 5th Rare Earth Research Conference (RERC). Rare-earth chemistry was at a fulcrum point in its history. Previously, during World War II, chemists working in Ames at Iowa State University had played a critical role in rare-earth technology. As part of the Manhattan Project in 1942, the researchers developed methods to remove traces of rare-earth metals from the uranium used to create the first nuclear chain reaction and to make the first nuclear bombs.



bulky computers and televisions. Much of the technology evolution since the 5th RERC has come about as researchers discovered that rare earths have abundant magnetic, luminescent, electrochemical, and thermal properties that have made possible smart phones, electric cars, light-emitting diodes, wind turbines, medical imaging, and more. This year's RERC served as a grand review of this rare-earth chemistry, highlighting how adding a dash of rare-earth metals to materials is like adding a bit of magic fairy dust—the metals help everything perform better.

"The remarkable properties of the rare earths have long engaged the imagination of the scientific community," said rare earther Ana de Bettencourt-Dias of the University of Nevada, Reno, one of this year's conference organizers. She marveled at the metals' importance in applications as varied as automobile starter motors, audio speakers, lasers, and colored glass.

The conference revealed new research trends showing that rare-earth chemistry is still very much a scientific frontier of the periodic table, with further technological developments to come. The discussion in Ames also turned to the need for better environmental stewardship of rare-earth element resources to ensure their sustainable, socially responsible use in existing and future technologies.

Although labeled as a "rare earth" conference, scientists in Ames included the actinides such as uranium on the agenda. given the kinship between lanthanides and actinides as fellow f-block elements. The actinides are increasingly being used in

nuclear medicine and as catalysts.

The f-element relationship is actually how rare-earth chemistry got started. For the Manhattan Project, scientists needed pure uranium, lots of it, fast and at a low price. Rare-earth impurities in uranium could prevent a nuclear reactor from working by absorbing the neutrons needed to keep the chain reaction going. So the rare earths had to be removed. Yet the chemical similarity of the lanthanides makes it extremely difficult to isolate them from one another and to separate them from uranium and other actinides. Iowa State chemistry professor Frank H. Spedding, an expert on rare earths, helped guide solution processing efforts to make tons of pure uranium oxide and a new high-temperature smelting methodcalled the Ames process-to make tons of pure uranium metal.

After WWII, in 1947, Spedding helped create and became director of Ames Laboratory, a U.S. Department of Energy national laboratory with a mission to further develop rare earths, initially for military uses and space exploration. Building on their earlier work, Spedding and his team developed an ion-exchange method to extract rare earths from minerals, enabling better separation of the rare-earth metals on a larger scale.

"Rare-earth research became commonplace after the groundbreaking work performed in Ames in the 1940s and 1950s," explained materials scientist Vitalij Pecharsky of Iowa State and Ames Laboratory, another RERC organizer. "Spedding and his colleagues made pure rare earths available in quantities required for broad chemistry and physics research and applications for the first time."

Pecharsky said his own research developing new rare-earth magnetic materials was made possible by those pioneering efforts. For example, his work with one of those pioneers, Karl A. Gschneidner Jr., who passed away last year and was memorialized at the conference, led to the invention of Gd<sub>5</sub>Si<sub>2</sub>Ge<sub>2</sub>. This material's temperature, Pecharsky explained, can be altered by exposing it to a changing magnetic field. Such magnetocaloric materials are being developed for high-efficiency refrigeration that uses a quarter of the energy of current systems.

"Rare earths remain a favorite playground for both basic and applied science," Pecharsky said, "driven by the potential for their everyday applications."

Kenneth N. Raymond of the University of California, Berkeley, another rare-earth-playground leader, was recognized during the conference as this year's



#### A new term, "rare earthers," was created for attendees of the 5th Rare Earth Research Conference when the Holiday Inn welcomed them to Ames, Iowa, in 1965.

Spedding Award winner, a prize that honors outstanding achievement in rare-earth research and education. Raymond's award lecture, "Lanthanides in Bondage: From Basics to Business," which led off the conference, reviewed his 40-plus-year career studying lanthanide luminescence and developing biomedical applications for the rare earths.

Starting out, Raymond worked with other leading researchers of the day—UC Berkeley's Glenn T. Seaborg and Andrew Streitwieser—to determine crystal structures of new lanthanide and actinide complexes. "Although there were a number of these compounds known, there was almost no structural information about them," Raymond said. "So I set about to change that." Raymond developed predictive models for the structure and bonding of lanthanide and actinide compounds based on the ionic radii of the metals.

Subsequent studies have enabled chemists to better understand the electronic transitions possible in lanthanide complexes when they are excited by light, and helped researchers design sequestering agents for plutonium and other heavy elements used to prepare and reprocess nuclear fuels.

Although lanthanides are weaker light emitters than organic dyes such as rhodamine B and fluorescein, Raymond said, they provide a technical advantage because their luminescence lasts longer, which allows better detection. Understanding the photochemistry of these lanthanide complexes when they are attached to drugs, proteins, and antibodies has proved valuable for developing new types of diagnostic assays and medical imaging.

In 2001, Raymond cofounded Lumiphore to commercialize terbium, europium, and other lanthanide luminescent complexes. These complexes are now used in assay kits sold by other companies to test saliva, blood, or tissues for drugs of abuse, hospital bacterial infections, and fetal and neonatal diseases. The technology is also being developed for biological imaging—for example, to study protein-protein interactions in living cells.

"We have learned a lot about the fundamental coordination chemistry of lanthanides over the years, and it's still an interesting subject for research," Raymond said. "Maybe the biggest thing for me is that if you put these metals in bondage, that is, incorporate them inside chelating ligands, the chemistry can be used to practical effect."

William J. Evans, another rare earther, agrees. Evans and his coworkers at the University of California, Irvine, are one of several research groups who have been designing new metal complexes that are shaking up the conventional wisdom about rare-earth element oxidation states. Their findings point to new approaches for manipulating the magnetic, optical, and catalytic properties of rare earths.

"When I started working with rare-earth metals in the 1970s, they were considered an exotic part of the periodic table—people had to stop and think about



Gd<sub>5</sub>Si<sub>2</sub>Ge<sub>2</sub>, a material created at Ames Laboratory, exhibits a giant magnetocaloric effect: Its temperature can be altered by exposing it to a changing magnetic field, a property that could be used in high-efficiency refrigeration.

## Rare earths at a glance

NAME	SYMBOL	ATOMIC NUMBER	ELECTRON CONFIGURATION <sup>a</sup>	ETYMOLOGY	NOTABLE APPLICATIONS
Scandium	Sc	21	3d <sup>1</sup> 4s <sup>2</sup>	Scandia (Latin for Scandinavia)	Aluminum alloys, lighting
Yttrium	Y	39	4d <sup>1</sup> 5s <sup>2</sup>	Ytterby, Sweden <sup>b</sup>	Yttrium-aluminium-garnet lasers, red phosphors, cancer drugs
Lanthanum	La	57	4f <sup>0</sup> 5d <sup>1</sup> 6s <sup>2</sup>	Lanthanein (Greek, meaning to lie hidden)	Refinery catalyst, camera lenses, lighter flints
Cerium	Ce	58	4f <sup>1</sup> 5d <sup>1</sup> 6s <sup>2</sup>	Ceres, the dwarf planet, and Roman goddess of agriculture	Car catalytic converters, glass polishing agent, lighter flints
Praseodymium	Pr	59	4f <sup>3</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Prasios and didymos (Greek, meaning leek-green twin)	Magnets, lighter flints, greenish-yellow glass and ceramics
Neodymium	Nd	60	4f <sup>4</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Neo and didymos (Greek, meaning new twin)	$Nd_2Fe_{14}B$ magnets, lasers, violet glass and ceramics
Promethium	Pm	61	4f <sup>5</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Greek Titan Prometheus	Radioactive; luminous paint, pacemaker batteries
Samarium	Sm	62	4f <sup>6</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Vasili Samarsky-Bykhovets <sup>c</sup>	SmCo5 magnets, cancer therapy, nuclear reactor control rods
Europium	Eu	63	4f <sup>7</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Europe	Red phosphors for lighting and color displays
Gadolinium	Gd	64	4f <sup>7</sup> 5d <sup>1</sup> 6s <sup>2</sup>	Johan Gadolin <sup>d</sup>	Refractive glass, MRI contrast agent, nuclear reactor shielding
Terbium	Tb	65	4f <sup>9</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Ytterby, Sweden <sup>b</sup>	Green phosphors for lighting, magnetorestrictive alloys
Dysprosium	Dy	66	4f <sup>10</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Dysprositos (Greek for hard to get)	Stabilizing additive in magnets, lasers
Holmium	Ho	67	4f <sup>11</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Holmia (Latin for Stockholm)	Lasers, magnets
Erbium	Er	68	4f <sup>12</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Ytterby, Sweden <sup>b</sup>	Lasers, fiber optics, nuclear reactor control rods
Thulium	Tm	69	4f <sup>13</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Mythological land of Thule	Portable X-ray source, light filaments, lasers
Ytterbium	Yb	70	4f <sup>14</sup> 5d <sup>0</sup> 6s <sup>2</sup>	Ytterby, Sweden <sup>b</sup>	Lasers, chemical reducing agent, stainless steel additive, cancer therapy
Lutetium	Lu	71	4f <sup>14</sup> 5d <sup>1</sup> 6s <sup>2</sup>	Lutetia (Latin for the city that became Paris)	PET scan detectors, refractive glass, refinery catalyst

a Ground shells, NIST data. b One of four new elements in the first discovered rare-earth ore found near Ytterby, Sweden, credited to Carl Arrhenius. c Mining engineer who discovered samarskite, a mineral containing samarium, the first element named after a person. d Gadolinium is named in honor of this rare earther who first identified yttrium in a sample sent from Carl Arrhenius.

where those metals are positioned," Evans told C&EN. "My research advisers thought I was crazy to go to work in this area, because there was no demonstrated importance in the chemistry of these elements." But Evans said the dearth of work on lanthanides was their allure.

Today, the attitude toward rare earths is much different, Evans said, because people have heard of their many uses. "So now when I say I am a rare-earth chemist, people have an idea that these are useful, interesting, and strategically important metals."

Conventional wisdom among chemists until recently held that most rare earths exist only in the +3 oxidation state in molecular complexes. Each of the 17 elements in the rare-earth collection have three ionizable electrons-two s electrons and one d electron. Moving across the row of lanthanides from lanthanum to lutetium, each element has an additional electron that takes up a position in a 4f orbital. Because the 4f orbitals don't extend far enough from the atom, they tend not to directly participate in bonding, yet they still influence the elements' magnetic and optical properties. That's a broad, simplistic view; the real situation "is complicated," Evans said.

Researchers found early on with rare earths that cerium readily assumes a +4 oxidation state in compounds, and later researchers began to find that other elements could take on +2 or possibly +5 oxidation states. By the late 1990s, chemists had isolated lanthanide(II) complexes for six of the elements. At the time, the researchers rationalized their results by noting the ions were stabilized by having filled, nearly filled, half-filled, or nearly half-filled 4f orbitals.

But as researchers continued to investigate, they discovered that ligands with the right electronic properties could provide additional stability, leading to additional +2 complexes. In 2013, Evans and Matthew R. MacDonald in his group reported complexes for the final seven elements, completing the lanthanide(II) series to show that it could be done. The team actually didn't make the promethium complex, because the element is radioactive and doesn't occur naturally. But the researchers expect it should follow suit and form a +2 complex.

The lanthanide(II) complexes are especially interesting, Evans noted, because they are kind of a hybrid between transition metals and lanthanide metals. They don't appear to have a 6s electron, but rather a 5d electron like a transition metal, in addition to any 4f electrons. And they display one-electron redox chemistry, which is not always typical for transition metals. "It's like they are a new type of metal," he said.

Evans and his colleagues have since found that the dysprosium(II) and holmium(II) complexes exhibit the highest magnetic moments reported to date for any single metal ion complex. They haven't figured out how to use this breakthrough practically yet, Evans said. One idea is that these complexes could function as single-molecule magnets and be used in thinfilm coatings for computer hard drives to increase the density of data storage.

As for what's next with rare-earth chemistry, Evans asked: Why not try to make +1 rare-earth complexes? He thinks as chemists continue to tinker with new electron configurations, they should be able to further elaborate on rare-earth technologies. "Hopefully, future research will allow us to use these metals more efficiently and reduce the tremendous demand on them for their special properties."

As Evans alluded, the demand for rare earths could lead to their commercial demise. Access to the metals has always been tenuous, leading to worries that one day demand for them may outstrip supply.

To head off that scenario, Gisele Azimi of the University of Toronto, another rare earther speaking at the conference, sees an opportunity for developing better strategies to ensure sustainable supplies of rare earths. These include finding new sources of the metals, developing better extraction technology for them, improving the efficiency of rare-earth-metal usage in products, and closing the loop on their use with better recycling.

Despite their name, rare-earth elements are not rare. All the metals except radioactive promethium are actually more abundant in Earth's crust than silver, gold, and platinum. When the first rare earths were discovered in the late 18th century, they were found as complex mixtures of metal oxides in various minerals. The minerals were initially, and incorrectly, classified as "earths," a geological term denoting nonmetallic substances that are insoluble in water and resistant to chemical change by heating. Furthermore, because of their geochemical properties, rare-earth elements don't concentrate in ore deposits but are widely dispersed, so they only seemed to be scarce.

Global rare-earth reserves, at more than 130 million metric tons, appear to be ample, Azimi noted. However, most of those reserves either are too low in concentration to be extracted economically, or they are not readily accessible, such as metals locked away in deep-sea manganese-based nodules or hydrothermal deposits.

"Currently, the demand for rare earths is increasing at a rate of about 5% annually," Azimi said. Some rare-earth applications require large amounts of the metals: Wind turbines use some 600 kg of rare-earth metals apiece. Some uses need intermediate amounts: Electric vehicle batteries use 5 to 10 kg of rare earths each. And some uses require small amounts: Phosphors in lighting may use a fraction of a gram per bulb.

The key issue at the moment is that China is home to about 25% of the world's rare-earth reserves, yet economic forces have aligned so that China now accounts for roughly 90% of the global supply. This situation has made sourcing rare earths precarious, subject to price and supply swings that are disruptive to product manufacturers.

That leaves mining companies outside China caught in an industrial catch-22: If they want to grab a larger piece of the market, the companies must ramp up production of rare earths, but they must do so without saturating the market with supply to avoid lowering prices. While companies deal with those economic conditions, they are also increasingly being judged for their environmental stewardship and their social responsibility to the communities they operate in.

The U.S., Australia, Brazil, and Canada have large reserves of rare earths, Azimi said, but little active mining is currently going on in those countries because of the cost. The real challenge going forward, she said, is going to be scaling up supply at a rate that matches increases in demand. "Opening new mines takes time—a decade



Ames Laboratory scientist Ikenna Nlebedim holds samples of neodymiumiron-boron magnets sourced and manufactured entirely in the U.S. The magnets are the result of the lab's Critical Materials Institute's role in supporting American manufacturing and national security interests.

or more—for prospecting, permitting, and construction. It's expensive and has environmental downsides." From digging in the ground to producing pure rare-earth oxides and pure metals, the process uses a lot of water, acids, organic solvents, and extraction chemicals.

One solution Azimi is promoting is to rescue rare-earth metals from existing stockpiles of mining wastes. For example, she is working with residue called red mud from bauxite mining to produce aluminum, and leftovers called phosphogypsum from phosphate rock mining that makes fertilizer. These materials contain 300 to 500 ppm of rare-earth metals, which is more concentrated than the roughly 0.2 to 60 ppm levels of the elements found in natural mineral deposits. With millions of tons of these waste materials piled up globally, thousands of tons of rare-earth metals could be procured, she said. Other researchers at the conference discussed coal ash and spent nuclear fuel from power plants as additional secondary sources of rare earths.

Rare earths are also plentiful in electronic waste, Azimi explained. Used fluorescent lights, computer hard drives, large permanent magnets, and batteries tend to end up in landfills. "Only 1% of their rare-earth content is being recycled," Azimi said. "It is absolutely imperative to develop recycling processes to address the sustainability challenges associated with these critical materials." That's a big challenge for e-waste because most consumer products aren't designed to be recycled. In addition, the metals are often used in combination for specific applications and need to be separated again. For example, neodymium-based permanent magnets (Nd<sub>2</sub>Fe<sub>14</sub>B) contain some dysprosium to improve thermal performance.

Azimi's group is working toward a designer acid-leaching process to recover rare earths from red mud and phosphogypsum. At RERC, she described how her team is further using the metals to design rare-earth-containing materials for new commercial uses. For example, the researchers are working on rare-earth oxide ceramics as transparent waterproof coatings for applications such as heat exchangers, airplanes, and solar panels. These materials use a minimal amount of rare earths and they are thermally stable, so they last longer than other types of hydrophobic coatings, which could help address the rare-earth supply challenge, she said

Other methods being used or tested to recycle e-waste include traditional coordination and chelation chemistry, ionic liquid extraction, metal-adsorbing bacteria, and the Ames high-temperature metallurgical process. For example, Eric J. Schelter of the University of Pennsylvania and his group have been developing a new type of targeted metal separation process that uses tailored nitroxide ligands to efficiently separate mixtures of rare-earth metals when recycling magnets and lighting phosphors.

"Rare earths have become indispensable and, in many cases, irreplaceable components of materials that are essential in modern life," said Schelter, one of the conference organizers. "Moving forward, I'm excited to see the magnetic properties of rare-earth molecules and molecular clusters reach their potential, for f-element complexes to catalytically drive multielectron transformations, and for the realization of highly efficient chemistries for recycling rare earths from consumer materials."

Technical solutions to the long-term sustainable use of rare earths undoubtedly will come from further research and design of new materials, such as coreshell nanoparticles that use just a dash of rare earths or even thin films of single molecules that achieve the same magnetic, optical, and other magical rare-earth properties as bulkier materials. Some researchers are looking to rare earths as a guide to exploit transition- and maingroup metals to mimic rare-earth properties. Those developments might be on the agenda the next time rare earthers reunite in Ames. ■

COMMENT

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more employment-related services from the society. PROF has a similar vision to that of YCC, most recently defined as "empowering chemical professionals for success in a diverse world." In this light, PROF is a unique technical division within ACS; it is a home for all chemists and includes focused subdivisions, such as the Younger Chemists subdivision. As such, it's not surprising that over the years YCC and PROF have been close collaborators.

### The ACS of today

Today, YCC and PROF still work closely to support the society's efforts toward their common goals. YCC is tasked with advising and providing information on topics relevant to younger chemists, both internal and external to ACS. However, our YCC core team is focused and small,

**Connecting younger chemists** 

with only 33 members

be a founding member of the newly established International Younger Chemists Network (IYCN). An organization envisioned during the International Year of Chemistry in 2011, IYCN aims "to create a unified global network of young chemists to communicate, collaborate, educate, and mentor."

With official support from the Interna-

It's impossible to consider building a network today that limits interactions by engaging chemists only within the U.S.

and associates who meet

in person at each ACS national meeting. So we look to our partnership with PROF and the Younger Chemists subdivision to help build a network of younger chemists with which to engage. This work is closely in line with PROF's mission of "creating inclusive communities, resources, and programming for the benefit of chemical professionals throughout their careers."

When you join ACS as a younger chemist, I encourage you to include membership in the PROF Younger Chemists subdivision. This will ensure that you stay up to date on the most recent resources, events, and programs related to career development, science policy, and networking that PROF and YCC offer. Then, please stop by and visit with members of PROF and YCC at regional and national meetings. By coming together in person and virtually, we are building a community that can teach and learn from each other: a network of engaged, passionate scientists.

#### Growing internationally

As valuable as the ACS younger chemists networks are, it's impossible to consider building a network today that limits interactions by engaging chemists only within the U.S. As such, YCC is proud to tional Union of Pure & Applied Chemistry, IYCN met for its inaugural meeting as part of the 2017 World Chemistry Congress in São Paolo, Brazil, this July. The full governance meeting was broadcast internationally via Facebook Live. You can find the recording and other news on the IYCN Facebook page: facebook.com/ IYCN.global.

The world is vast, but through both virtual and physical interactions, IYCN will unite young and early-career professionals who may not have the opportunity to connect otherwise. By participating, younger chemists across the world can broaden their horizons and engage in conversations that are most relevant and powerful on a global scale.

#### How to stay connected

If you're a young or early-career chemist and you want to keep up to date with what's happening in chemistry in your local section, in ACS nationally, and across the world, consider becoming an active member of your local section YCC, the PROF Younger Chemists subdivision, IYCN, or all three networks. There's no limit to what we can learn from each other.

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







NATALIE LAFRANZO, CHAIR, ACS YOUNGER CHEMISTS COMMITTEE

he ACS Younger Chemists

in 1974, with much of the

laid in the late 1960s and early 1970s, a

time of great unrest. The environment,

the Vietnam War, Watergate, and wom-

en's rights were all controversial issues

for society, and chemists

The world continues to be both challenging

and exciting for chemists. Politics, science,

and technology are all evolving at a rapid pace, and this trans-

formation is creating many opportunities for

chemists to make an impact on the changing

Since its inception,

YCC has been serving the needs of young-

er chemists, advocating and providing

professionals in the chemical scienc-

es to enable them to contribute to the

chemical industry and to society as a

whole. YCC serves as a voice for younger chemists within ACS and addresses

specific issues they face. Not all younger

chemists follow the same career path, so

Around the same time that YCC was

formed, the Division of Professional Rela-

tions (PROF) was also conceived. In fact,

Younger Chemists Task Force (which pre-

ceded YCC) were involved in the forma-

tion of PROF; these members pressed for

several of the founding members of the

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ACADEMIC POSITIONS

## PROFESSORS IN CHEMISTRY, OPEN AREA

The Department of Chemistry at Indiana University invites applications for two positions in any area of chemistry to begin August 2018 at the rank of Assistant or Associate Professor. Candidates with research interests related to biological problems are encouraged to apply. A Ph.D. in chemistry, biochemistry, or a related field and postdoctoral experience are required. Successful candidates will be expected to develop or already have a visible, externally funded research program. Primary teaching responsibilities will be consistent with the expertise of the successful candidate and will include both graduate and undergraduate courses. Applications completed by Oct. 15. 2017 will receive full consideration, but the review will continue until the position is filled. Interested candidates should submit a complete curriculum vitae, a summary of future research plans and arrange to have three letters of recommendation to be sent to (https://indiana.peopleadmin.com). Questions regarding the position or application process can be directed to: Professor David Giedroc, Chair, Faculty Search Committee, Department of Chemistry, Indiana University, 800 E. Kirkwood Ave., Bloomington, IN 47405, chemchair@indiana.edu. The Department of Chemistry and College of Arts and Sciences are committed to building and supporting a diverse, inclusive, and equitable community of students and scholars.

Indiana University is an equal employment and affirmative action employer and a provider of ADA services. All qualified applicants will receive consideration for employment without regard to age, ethnicity, color, race, religion, sex, sexual orientation or identity, national origin, disability status, or protected veteran status.

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# O UNIVERSITY OF OREGON

Two tenured or tenure-track positions at the University of Oregon in the area of Energy and Sustainable Materials

The University of Oregon (UO) continues a cluster hire initiative in Energy and Sustainable Materials (https:// provost.uoregon.edu/energy-and-sustainable-materials). Target areas include: electronic and energy devices, advanced/in-situ characterization, computational materials chemistry/physics, solid-state and materials physics/chemistry, surface science and catalysis.

Appointments may be made in or across any academic department(s), at any rank, and continue UO's long-term commitment to grow the basic and applied sciences. The hires will join an innovative and highly collaborative team in the Materials Science Institute. Exceptional candidates with backgrounds in chemistry, physics, chemical/electrical/mechanical engineering, and materials science, as well as leaders in industrial research and development, are encouraged to apply. The positions will remain open until filled. Salaries and start-up packages will be highly competitive.

The successful candidate will work effectively with faculty, staff and students from a variety of diverse backgrounds. She/he will maintain a high-profile, internationally prominent and externally funded research group, while contributing to the teaching mission at the UO.

The initiative builds upon the established excellence of Materials Science at UO. Recent investments include over \$30 million in equipment for the CAMCOR materials analysis, characterization and nanofabrication facility, which is managed by professional staff and housed in two new buildings along with state-ofthe art laboratory space. Oregon is home to the new Knight Campus for Accelerating Scientific Impact, a \$1B initiative to fast-track scientific discovery and innovation (http://accelerate.uoregon.edu/). Faculty and student experiences are further enhanced by unique graduate-education programs, industry partnerships and innovation activities.

Inquiries/nominations can be sent to materialscluster@uoregon.edu. Upload application materials here: https://academicjobsonline.org/ajo/jobs/9449

Applicants at the Senior level (Associate or Full Professor) should include a cover letter and curriculum vitae.

Applicants at the Junior level (Assistant Professor) should include, in addition to the cover letter and vitae, a statement of research plans and objectives (typically approx. five pages in length) and a brief statement of teaching philosophy or interests. Junior candidates should also arrange for three letters of recommendation to be uploaded directly by the recommenders.

Review of applications will begin October 1, 2017 and continue on a rolling basis until the positions are filled.

The University of Oregon is an equal opportunity, affirmative action institution committed to cultural diversity and compliance with the ADA. The University encourages all qualified individuals to apply, and does not discriminate on the basis of any protected status, including veteran and disability status.

UO prohibits discrimination on the basis of race, color, sex, national or ethnic origin, age, religion, marital status, disability, veteran status, sexual orientation, gender identity, and gender expression in all programs, activities and employment practices as required by Title IX, other applicable laws, and policies. Retaliation is prohibited by UO policy. Questions may be referred to the Title IX Coordinator, Office of Affirmative Action and Equal Opportunity, or to the Office for Civil Rights. Contact information, related policies, and complaint procedures are listed on the statement of non-discrimination.

#### THE UNION COLLEGE DEPARTMENT OF

**CHEMISTRY** invites applications for two faculty positions beginning in Fall 2018.

**PHYSICAL CHEMIST.** The candidate for this tenure-track position (pending final administrative approval) will have teaching responsibilities principally in physical chemistry and general chemistry courses. The candidate is expected to have a Ph.D. in physical chemistry, biophysical chemistry or a related sub-discipline, postdoctoral experience and the potential for excellence in undergraduate teaching and research.

Candidates whose research program would contribute to the College's ongoing interdisciplinary activities are especially welcome. Union College is an equal opportunity employer and strongly committed to student and workforce diversity. Increasing diversity and inclusiveness is a critical priority for Union and we invite applicants to share how they can further this goal in their applications. Applications must include a CV, a statement on the applicant's background and interests in teaching, an outline of research interests (three-page maximum), and a list of required instrumentation and equipment.

LECTURER/INSTRUMENTATION SPECIALIST. The candidate for this non-tenure-track position should have a Ph.D. in chemistry or closely related field, significant breadth of experience with chemical instrumentation, and the potential for excellence in undergraduate teaching. Teaching responsibilities will be principally in laboratory courses in introductory chemistry, organic chemistry, and chemical instrumentation. Co-curricular responsibilities include maintenance of the department's instrumentation for teaching and research, training of faculty members and students in the use of instrumentation, and working with other faculty to develop new instrumentation-based experiments for laboratory courses. Union College is an equal opportunity employer and strongly committed to student and workforce diversity. Increasing diversity and inclusiveness is a critical priority for Union and we invite applicants to share how they can further this goal in their applications. The initial appointment will be for a three-year period with the possibility of renewal. Applications should include a CV, a statement of teaching interests, and a statement of experience with chemical instrumentation.

For both positions, the required materials should be e-mailed as a single pdf file to chemsearch@union.edu c/o Professor Laurie Tyler, Chair, Department of Chemistry, Union College Schenectady, NY. In addition, we require both graduate and undergraduate transcripts and three letters of recommendation (originals) that can be sent separately. The application deadline is October 6, 2017, but review of completed applications will begin immediately and continue until the positions are filled. Union College is a small, highly selective undergraduate institution with particular strengths in science and engineering. Union offers an exceptional benefits package that includes medical, dental, vision insurance, and life and disability coverage.

For more information, visit our web site http://www.union.edu.

#### **ACADEMIC POSITIONS**

#### METABOLISM INVESTIGATOR

The **Morgridge Institute for Research**, a premier private, nonprofit research institute affiliated with the University of Wisconsin–Madison, seeks outstanding early– to mid–career scientists to lead vibrant metabolism–focused research programs based in biochemistry and/or chemical biology. We are particularly interested in interdisciplinary and collaborative–mind– ed scientists passionate about exploring the basic molecular and mechanistic underpinnings of primary cellular metabolism, and how essential biological processes are linked to the metabolic state of a cell.

The Morgridge Institute serves as a central hub for investigators to work collaboratively on fundamental biomedical questions, and as such offers an extraordinary interdisciplinary work environment. Our recruitment of investigators into the new Metabolism Theme is part of our larger Metabolism Initiative that aims to enhance the pace, productivity, and international profile of metabolism-related research in Madison. The metabolism community in Madison includes hundreds of scientists spanning diverse areas of organismal biology, biochemistry, genetics, nutritional sciences, and medicine, and is home to world-class capabilities in proteomics, metabolomics, and computational biology.

Candidates must have a proven track record of high quality research related to metabolism, have outstanding communication skills, and embrace the collaborative and interdisciplinary culture of the institute. Successful candidates will be eligible for appointment to a tenure track or tenured position in the UW-Madison Biochemistry, Biomolecular Chemistry, or Chemistry departments. The institute provides an attractive salary and benefits package and offers generous start-up support.

**To Apply:** Applicants should submit electronic copies of their curriculum vitae, a two-three-page description of research vision and future research plans, a one-page description of teaching experience and future teaching plans, and should arrange for at least three referees to submit letters of recommendation. All materials should be sent to **metabolism@morgridge**. **org.** Applications will be accepted until December 1, 2017, and will be considered on a rolling basis. Morgridge Institute for Research promotes and supports a diverse and inclusive environment.

#### PHYSICAL CHEMISTRY

The Department of Chemistry and Biochemistry invites applications for a tenure-related position in experimental physical chemistry to begin Fall 2018 or later at the anticipated rank of Assistant Professor. A PhD is required and postdoctoral experience is preferred.

We seek individuals studying problems of fundamental importance to experimental physical chemistry, which may also be applied uniquely to advance related chemical disciplines. We are especially interested in scholars who will enhance the department's existing strengths in biophysical chemistry, materials related physical chemistry, spectroscopy, statistical mechanics and quantum chemistry. The potential for establishing a vigorous independent research program in experimental physical chemistry and active participation and excellence in teaching at the undergraduate and graduate levels will be the most important criteria for selection. In addition to membership in the Department of Chemistry and Biochemistry, the successful candidate will have the opportunity to pursue research in a variety of interdisciplinary institutes (see https:// chemistry.uoregon.edu/research/institutes/).

We particularly welcome applications from scholars from populations that are historically underrepresented in the academy, and/or who have experience working with students from diverse backgrounds.

Please apply here **https://academicjobsonline.org/ ajo/jobs/9374.** To ensure full consideration, candidates should submit application materials by October 3, 2017 and upload a curriculum vitae, a statement of research plans (maximum 10 pages), and a brief statement of teaching philosophy or interests (onetwo pages). Candidates should also arrange for three letters of recommendation to be submitted directly by recommenders via the AcademicJobsOnline portal. The position will remain open until filled.

The University of Oregon is an equal opportunity, affirmative action institution committed to cultural diversity and compliance with the ADA. The University encourages all qualified individuals to apply and does not discriminate on the basis of any protected status, including veteran and disability status.

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#### **ACADEMIC POSITIONS**

#### TWO TENURE TRACK FACULTY POSITIONS IN

CHEMISTRY. The Department of Chemistry & Biochemistry in the College of Science & Health at the University of Wisconsin-La Crosse (UWL) http:// www.uwlax.edu/Chemistry-and-Biochemistry/anticipates hiring two dynamic teacher-scholars at the Assistant Professor level to join its top-rated program on August 27, 2018. Our new colleagues will teach General and Organic Chemistry lecture and laboratory courses along with advanced elective courses in their areas of expertise, develop an active research program involving undergraduates, and be engaged in university, professional, and public service. Special consideration may be given to individuals with additional expertise in the areas of materials science and/or industrial/ nuclear/energy chemistry. Our department and college maintain a large array of modern instrumentation resources, and we will move into a brand new, state-ofthe-art laboratory sciences facility in 2018.

Qualifications: An earned Ph.D. degree in organic chemistry or related discipline, a commitment to excellence in teaching and scholarship at the undergraduate level, and demonstrated excellence in oral and written communication are required. Preference will be given to candidates with post-doctoral research experience and those whose professional expertise complements that of the existing faculty. To apply for this 100% academic year (nine-month) appointment, please submit a cover letter, CV, teaching philosophy, statement of research plans, and unofficial undergraduate and graduate transcripts through the UWL employment portal at https://employment.uwlax. edu/. The cover letter should explicitly emphasize both an interest in this position and a commitment to teaching effectiveness and student engagement and mentoring. Applicants also must arrange to have three professional references upload their letters of recommendation through the portal by the application deadline, which is Friday, October 27, 2017. UW-La Crosse is an AA/EO employer encouraging excellence through diversity. Employment will require a criminal background check.

## ASSISTANT PROFESSOR

Massachusetts Institute of Technology (MIT) The Massachusetts Institute of Technology Department of Chemistry, located at 77 Massachusetts Avenue, Cambridge, MA 02139-4307, invites applications for tenure-track positions at the assistant professor level beginning July 2018 or thereafter. Outstanding applicants with research interests in all areas of chemistry are encouraged to apply. MIT Chemistry has interest in appointments of faculty to teach in all areas of chemistry, broadly defined. Faculty duties include teaching at the undergraduate and graduate levels. Appointments are at the rank of assistant professor, but outstanding senior applicants may be considered. Requirements: Applicants must hold a Ph.D. in chemistry or a related field by the start of employment and must demonstrate ability to excel in teaching. To Apply: Applications are being accepted at Academic Jobs Online. (https://academicjobsonline.org/ajo/jobs/9498). To receive full consideration, completed applications must be received by October 1, 2017. A complete application must include a curriculum vitae, a one-page summary of research plans, two or more research proposals, a brief statement of teaching interests, and three letters of recommendation. Search Contact: Ms. Michele Harris, Human Resources Coordinator, Department of Chemistry, Room 18-392, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139-4307 (mharris@mit.edu). MIT is an equal employment opportunity employer. All qualified applicants will receive consideration for employment and will not be discriminated against on the basis of race, color, religion, sex, sexual orientation, gender identity, national origin, veteran status, or disability.

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# Newscripts

# Curating quirky science since 1943

This week, the Newscripts gang has some suggestions for how to create pizzazz in the kitchen by adding a portion—or three—of scientific know-how.

# Shape-shifting pasta

To start, add an extra dimension to your cooking by using two-dimensional pasta that becomes 3-D when cooked. Scientists at Massachusetts Institute of Technology's Tangible Media Group have engineered flat sheets of gelatin or starch to make a type of pasta that instantly springs into predetermined 3-D shapes when

The shapes are

One layer of gelatin

is denser and able

to absorb more wa-



#### Edible transformers: MIT scientists combine gelatin sheets and 3-D-printed cellulose to control pasta shape.

ter than the loosely packed gelatin of a second layer, so the sheet arches.

To control the angle at which the pasta bends, MIT researchers led by Wen Wang and Lining Yao applied 3-D-printed strips of edible ethyl cellulose onto the denser layer of gelatin. The cellulose limits the amount of water that can reach the adjacent gelatin. The design of the 3-D-printed pattern determines the pasta shape.

The technology works for a broad range of shapes, including traditional tube-shaped macaroni. But you could also use the technology to cook up something crazy; Wang and Yao have created an online interface that allows users to design their own pasta shapes.

Engineering pasta sheets so that they ship flat could also lessen packaging costs, Wang says. Wang and his colleagues calculate that for tube-shaped macaroni pasta, 67% of the package's volume is air even when the pasta packs perfectly. Reducing the space needed for the pasta could markedly curb pasta packaging, the scientists say.

# Beer from air

eople often have a glass of red wine with their pasta. To mix things up a little, though, Newscripts recommends a craft beer named CleanEscape made by San Diego-based Ballast Point Brewing. CleanEscape is one of the most unusual and potentially sustainable beers because it is made with water drawn from air. Ballast Point uses a water generator developed by Washington state company Ambient Water to extract moisture from the sometimes foggy air that rolls into San Diego.



Sustainable sip: Ballast Point Brewing makes beer using water extracted from air.

The generator chills air to its dew point. Moisture

condenses onto patented stainless-steel or specially coated coils before being channeled through filtering chambers. The system is energy intensive, consuming 600 kWh of energy in a day to capture about 1,500 L of potable water.

But for Ballast, capturing water from air is cheaper than other sources, such as tapping seawater via reverse osmosis, because it allows the brewery to skip a purification step. The water's high purity also has taste benefits. It's a "perfect canvas" for exploring new styles and flavors, says Julia Cain, Ballast's director of R&D.

# Nonmelting ice cream

or dessert, the Newscripts team suggests melt-resistant ice cream. Typical ice cream might start to drip after a minute or so on a hot summer day. Scientists at Japan's Kanazawa-based Biotherapy Development Research Center Co., in collaboration with Kanazawa University, think they have a cool solution: an additive that slows down the melting process so that the first drips don't appear for five minutes, even on a hot and sunny day.

To stifle the melting process, the center's scientists added polyphenol liquid sourced from strawberries to the ice cream. "Polyphenol liquid has properties to

make it difficult for water and oil

Ota, president of the company and

professor emeritus of pharmacy at

Kanazawa University, told Japanese

Ota and colleagues reportedly

tested polyphenol-rich ice creams in

Kanazawa under the heat of a hair dryer and found that they retained

their original shape after a full five

The researchers accidentally

made the discovery when they

daily newspaper Asahi Shimbun.

to separate," enabling ice cream

to stay intact longer, Tomihisa



Slow melt: Adding polyphenol from strawberries makes ice cream drip-free for five minutes.

hired a chef to create a new type of confection using the polyphenol. The chef realized that cream hardened when it came into contact with polyphenol.

minutes.

The research center's idea has attracted solid commercial interest. Melt-resistant ice creams are already on the streets of the Japanese cities of Osaka and Tokyo.

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





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