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CHEMICAL & ENGINEERING NEWS

NOVEMBER 28, 2016

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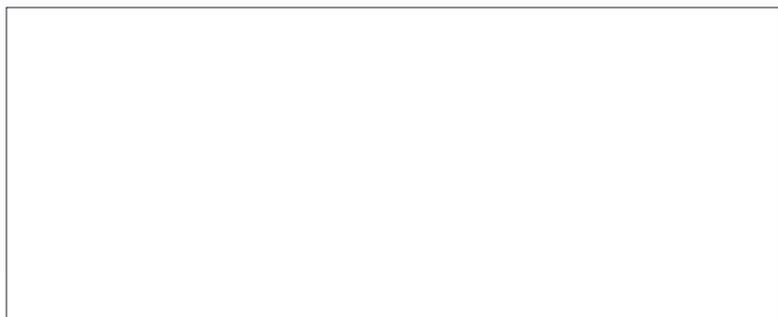


**CAUTION: ASBESTOS IS
STILL A GLOBAL THREAT**



Regulators consider
banning the material, while
researchers get a better
handle on its effects

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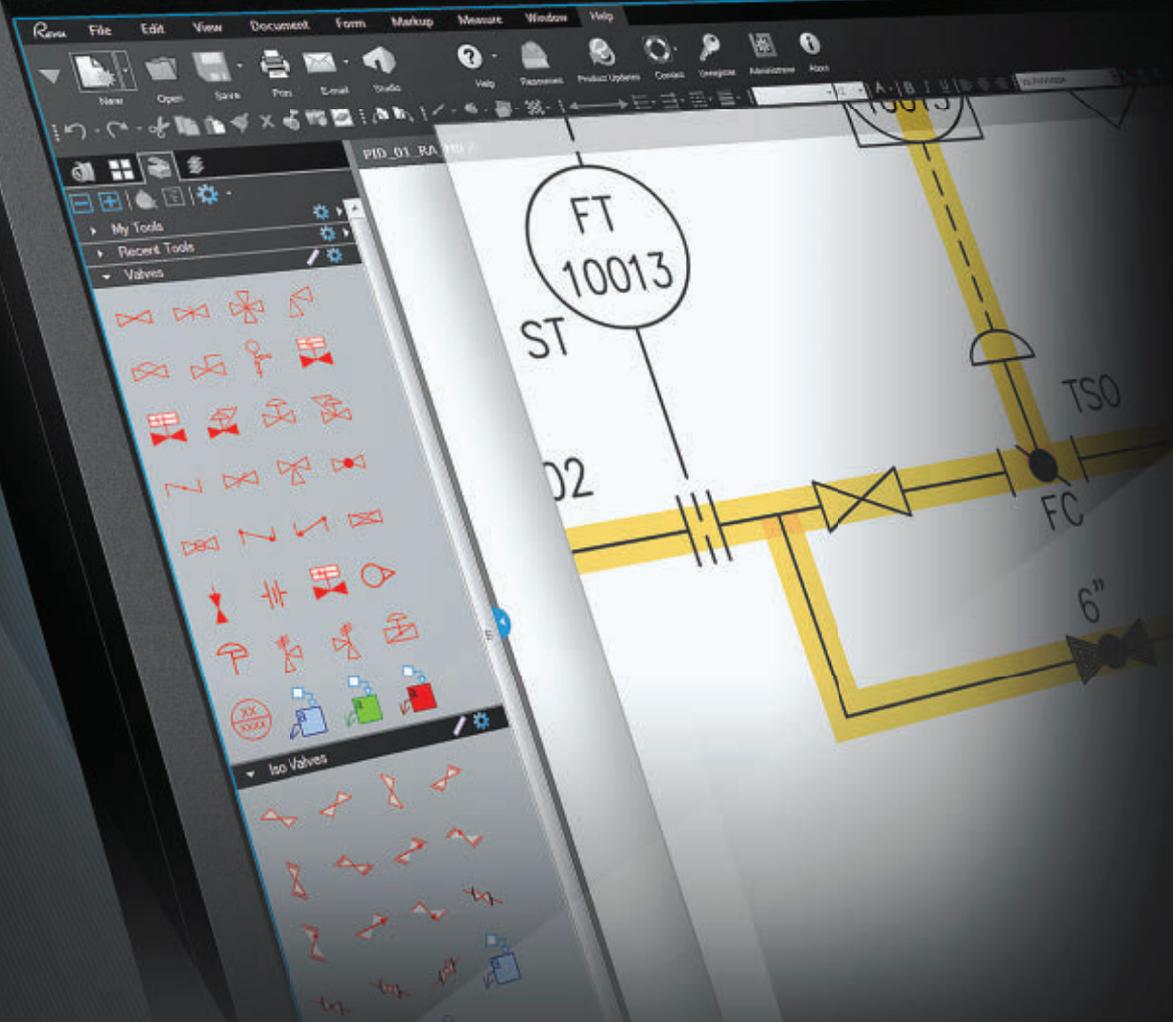


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Asbestos: Still a global menace

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Chrysotile asbestos, also known as white asbestos. Photo illustration by Science Stock Photography/Science Source/C&EN

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“The black middle class is bigger and better off, but on average, the gap between the rich and poor is bigger.”

—Gert Kruger, pharmaceutical sciences professor, University of KwaZulu-Natal, on economic inequality in South Africa
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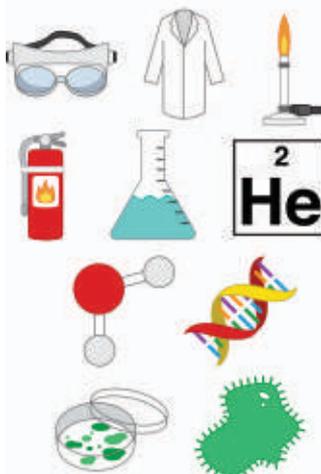
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▶ *Letters to the editor*

Cold fusion

The article “Cold Fusion Lives On” does readers a disservice when it says that the term “low-energy nuclear reactions” (LENR) is simply a rebranding of the term “cold fusion” (C&EN, Nov. 7, page 34). The distinction is, in fact, crucial because the data, as my book “Hacking the Atom” shows, do not look anything like fusion. They never have.

It was a mistake to label this research “fusion” 27 years ago, and it is a mistake to continue doing so. LENR is non-fu-

sion-based nuclear reactions that occur at or near room temperature. Cold fusion is the incorrect hypothesis of nuclear fusion reactions that occur at or near room temperature. Even Robert Park, a former spokesperson for the American Physical Society, recognized this distinction in 2009 in his newsletter. This year, the Library of Congress recognized the distinction when it created a new subject-matter heading for LENR. Martin Fleischmann, part of the duo who announced fusion in a test tube in 1989, conceded that he and Stanley Pons made a mistake by calling it fusion. Of course, as C&EN found, there are scientists who still believe that LENR might be the result of room-temperature fusion, but science should not cater to believers.

Low-energy nuclear reactions most likely are explained by the creation of ultra-low-momentum neutrons followed by subsequent neutron-capture processes, not deuterium-deuterium nuclear fusion. Regardless of the possible explanation, such experimentally observed phenomena are, understandably, difficult for many scientists to accept. For the past 100 years, nuclear effects without the use of radioactive sources, high-energy accelerators, or nuclear reactors have been considered impossible. Be that as it may, researchers have observed isotopic shifts, elemental transmutations, melting of metals, and a variety of other anomalies that offer new understanding of nature. In fact, some of these anomalies were observed 100 years ago, as my book “Lost History” reveals.

Beyond the smoke and noise created by hucksters and believers, there is valid research and credible data in the LENR field. C&EN would do well to explain the distinction between the terms and to help its readers see the mystery behind an unfolding new field of science with unknown possibilities.

Steven B. Krivit
Publisher, *New Energy Times*
San Rafael, Calif.

I read with interest C&EN’s article on cold fusion. When Stanley Pons and Martin Fleischmann made their original announcement in the popular press in 1989 and technical details were initially absent, I assumed it had something to do with muon-catalyzed fusion. Muons are a massive

Correction

▶ **Oct. 31, page 25:** In C&EN’s feature on 10 start-ups to watch, the founders of two companies were presented incorrectly. The founders of Kyulux are Chihaya Adachi, Junji Adachi, Akira Minakuchi, and Christopher J. Savoie. The founders of NuMat Technologies are Omar K. Farha, Benjamin Hernandez, and Christopher Wilmer.

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relative of the electron and can be produced by high-energy collisions in particle accelerators. Their short half-life—somewhat in excess of two microseconds (although quite long as compared with some other subatomic particles)—and difficulty and expense of production make muon-catalyzed fusion highly uneconomic.

But perhaps the type of cold fusion announced by Pons and Fleischmann actually does have its roots in muon catalysis. Cosmic rays striking the upper atmosphere generate a particle shower producing, on average, about 10,000 muons per square meter per minute arriving at Earth's surface. By chance, an occasional muon must strike a given cold fusion apparatus, catalyzing the process. This would account for the reproducibility and variability issues.

This also suggests a potential experimental verification. Victor Hess, in 1912, found that what was later shown to be cosmic ray shower particle density increases with altitude. He observed a fourfold increase at 5300 meters in a free balloon flight. A cold fusion apparatus operated at altitude should then likely show an increased probability of "excess energy" production. Similarly, an apparatus operated deep in an underground mine should hardly ever work at all.

Greg Konesky
Hampton Bays, N.Y.

Regarding C&EN's story on cold fusion, consider Lord Kelvin's quote "X-rays will prove to be a hoax." Within about a year of Wilhelm Röntgen's 1895 discovery, a thousand confirming papers were published and the phenomenon commercialized. In contrast, cold fusion/low-energy nuclear reactions/hydrinos and Randell Mills's efforts regarding the latter have nothing (as in zero) to show after a quarter-century.

It is one thing to note that advocates "had no generally accepted theory to guide them," but another more germane issue is that they had no way of explaining why several existing, well-established physical theories had to be trashed to accept otherwise inexplicable observations of excess energy generation. Citing that Mills's "ideas seem less far-fetched when compared with ... muonium ... [a] short-lived exotic entity made of an antimuon particle ... and an electron," is a curious misdirection. There are multiple thousands of peer-reviewed scientific papers on muonium and applications of muonium in chemistry, physics, and materials science.

Quoting my former colleague Ludwik Kowalski's view that "social stigma" against the phenomena was the problem is nonsense. The initial scientific response was complaints about the poor experimental

design followed by a flood of independent investigations, probably 90% of which were never published because of the clearly negative results. Why is C&EN flogging a dead horse?

Paul J. Karol
Palo Alto, Calif.

ACS and politics

I was in no way surprised to read about the politicization and potential misuse of power by Rep. Lamar Smith (R-Texas), chair of the House of Representatives Science, Space & Technology Committee (C&EN, Oct. 24, page 20). His track record of questionable science policy leadership is now well-established, and as stated in C&EN's article, "Smith has been stirring up controversy in the Science Committee almost since the moment he took over in January 2013." His leadership in this position has been criticized by members of Congress from both parties.

Yet, in 2013, I remember being shocked to read in C&EN that the American Chemical Society had awarded Smith ACS's 2013 Public Service Award for "vision and leadership in public policy that benefits science, engineering, and innovation" (April 29, 2013, page 8) despite the fact that many

of his actions run contrary to ACS's own statement to "promote science and sustainability in public policy." I remember feeling that this was political gamesmanship by ACS back in 2013.

Now, three years later, what has that recognition of Smith gotten ACS members and the broader scientific community? It appears the representative's "vision and leadership" remains unchanged and that he is still as much a threat to transparent and responsible leadership in science policy as he was three years ago. I hope ACS will learn from these past actions by ensuring all future honors are based on merits and achievements, rather than politics and pandering.

Name withheld upon request

Election 2016

Rather than adopting a doomsday outlook regarding the results of the 2016 U.S. election (C&EN, Nov. 14, page 5), think about the "regulatory changes" Walmart made within a short five or so years. During this time, the retail giant orchestrated a marriage with Proctor & Gamble to make laundry soap "greener." The partnership resulted in new and innovative packaging, waste reduction, space savings, and a reduction in consumer (retail) costs—all without any

regulatory umbrella.

Other enterprise projects should yield the same type of research and innovation. So rather than focus on loss of regulation—which might just be good—the enterprise communities should come together themselves to make the world a better place, taking the lead from Walmart.

Martha G. K. Dibblee
Portland, Ore.

ACS 2015 IRS Form 990 available

The American Chemical Society's 2015 IRS Form 990 is now available on ACS's website. To access the information, go to www.acs.org and follow these instructions: Click on "About ACS," and then click on "Financial," which brings you to the "ACS Financial Information" page. Under the heading "ACS IRS Form 990," click on "2015 IRS Form 990."

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Concentrates

Chemistry news from the week

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BIOCATALYSIS

Protein provides new route to carbon-silicon bonds

Bacterial cytochrome *c* demonstrates first example of biologically catalyzed organosilicon chemistry

Silicon is the second most abundant element in Earth's crust after oxygen, but carbon-silicon bonds are unheard of in nature: Neither biological organosilicon compounds nor biosynthetic pathways to create them have been identified. But when given the right starting materials, some heme proteins can stereospecifically form carbon-silicon bonds, report researchers from Caltech (*Science* 2016, DOI: 10.1126/science.aah6219).

"Nature's iron heme chemistry just jumps on this opportunity because we provided it with the right precursors," says Frances H. Arnold, who led the work with S. B. Jennifer Kan. "It's a profound demonstration of how easily nature can innovate."

"This closes a crucial gap between biological and chemical catalysis," writes Martin Oestreich of the Technical University

of Berlin in a commentary accompanying the paper. "The impact is unforeseeable, but it seems that we are a big step closer to potentially facilitating industrially relevant reactions such as alkene hydrosilylation with biomolecules."

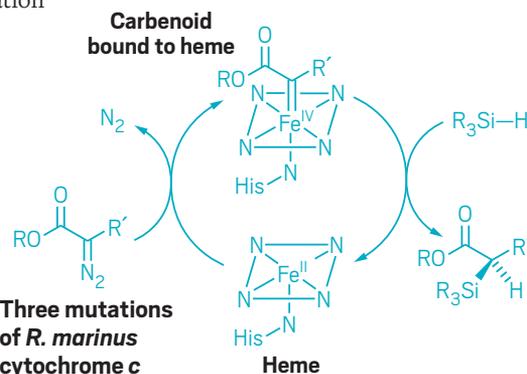
Chemists have experimented for decades with forming chiral organosilicon compounds by carbenoid insertion into Si-H bonds, but the reactions typically require halogenated solvents and catalysts made of precious metals coordinated with chiral ligands. The catalysts also have low turnover—each catalyst complex survives fewer than 100 reactions before it inactivates.

Prior work in Arnold's lab and elsewhere had demonstrated that heme proteins can catalyze nonnatural carbene transfer reactions through insertion into N-H and S-H bonds. In the new experiments, the researchers screened a panel of heme proteins to find ones that could catalyze insertion of ethyl 2-diazopropanoate into the Si-H bond of dimethyl(phenyl)silane. Cytochrome *c* from the bacterium *Rhodothermus marinus*, which is found in submarine hot springs in Iceland, catalyzed the reaction with 97% enantiomeric excess, although the catalytic turnover was still low.

Cytochrome *c* proteins normally don't catalyze chemical reactions; instead they transfer electrons between biomolecules in cells. But that did not stop Kan, Arnold, and colleagues from pushing the *R. marinus* cy-

tochrome *c* to improve its newfound ability to perform organosilicon catalysis.

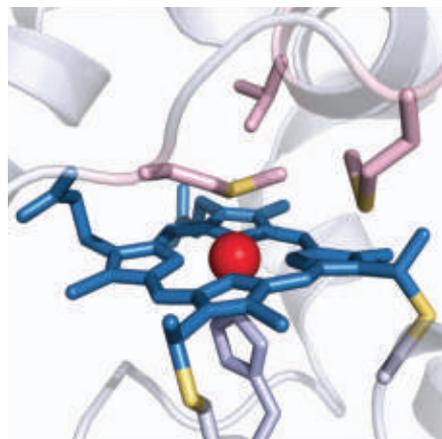
The researchers used directed evolution to come up with a set of three mutations that together increase the new enzyme's enantioselectivity to greater than 99% and turnover to greater than 1,500. One of the mutations involved a methionine residue that



Three mutations of *R. marinus* cytochrome *c* turn the protein into an enzyme that produces organosilicon compounds with greater than 99% enantiomeric excess.

provides an axial ligand to the protein's iron center. A change from methionine to aspartic acid possibly provided more substrate access for the formation of an iron-carbenoid intermediate.

The "evolved" cytochrome *c* performs stereoselective carbene insertion into Si-H bonds using a variety of silicon and diazo reagents, without competing cyclopropanation. And when given 4-(dimethylsilyl)aniline, which can accommodate insertion at both N-H and Si-H bonds, the enzyme formed the organosilicon product with 97% chemoselectivity. Arnold thinks that the partially exposed active site promotes substrate promiscuity but that there's also some characteristic of the heme pocket that prefers silicon chemistry.—JYLLIAN KEMSLEY



The heme group (blue) of *R. marinus* cytochrome *c* catalyzes carbenoid insertion into Si-H bonds.

CLIMATE CHANGE

Cement could be a helpful carbon sink

Model suggests cement reacting with CO₂ can offset part of the emissions from its production

Making cement requires a lot of heat and releases large amounts of carbon dioxide. The heat helps transform limestone (calcium carbonate) into clinker, which is largely calcium oxide. This process, called calcination, is responsible for about 5% of global human-based CO₂ emissions.

Cement plants are major emitters of carbon dioxide.



But the cement itself may help offset some of those climate-changing emissions, according to a new study. A team of researchers estimate that 43% of the CO₂ released by cement calcination between 1930 and 2013 was reabsorbed by the cement created during that period (*Nat. Geosci.* 2016, DOI: 10.1038/ngeo2840).

Removing CO₂ from the atmosphere, not just emitting less of it, is a significant part of what many climate scientists think we must do to avoid major consequences from climate change. “What is interesting about this study is that part of that requirement of removing CO₂ from the atmosphere may already be happening by the unintended carbonation of cement,” says Phil Renforth, who studies carbon sequestration at Cardiff University.

Carbonation is the process by which

cement takes up CO₂: Hydrated minerals in cement react with CO₂ in the air to form carbonates. Based on modeling by a team led by Zhu Liu of the Resnick Sustainability Institute at Caltech, this carbonation process has sequestered about 4.5 gigatons of carbon since 1930. And the annual sequestration rate has been increasing overtime, reaching 0.25 gigatons of carbon in 2013. The 2013 carbonation rate is equivalent to 22.7% of the average annual carbon uptake of global forests and about 2.5% of global human-based carbon emissions in 2013.

But Thomas Gasser, who works on climate models at the International Institute for Applied Systems Analysis, stresses that cement isn’t exactly a conventional carbon sink because making the material releases CO₂. The best way to summarize the new study, he says, “is to say that cement production actually has a lower impact on climate than previously thought, since it emits less CO₂ in total.”—MICHAEL TORRICE

BIOCHEMISTRY

Young blood may not cure aging ills

New method for mouse blood exchange might clear up conflicts in past experiments

A new blood transfusion method may help resolve confusion over past experiments on the effects of giving young mouse blood to old mice and vice versa. In those experiments, the rodents’ circulatory systems were connected surgically.

A team at the University of California, Berkeley, including bioengineer Irina M. Conboy and her husband, researcher Michael J. Conboy, used computer-controlled microfluidic pumps to exchange blood between young and old mice, so that each received 50% of the other’s blood (*Nat. Comm.* 2016, DOI: 10.1038/ncomms13363). After the transfusion, the mice were disconnected.

Past studies that surgically connected old-young mice pairs have produced sometimes controversial evidence that seemed to point to young blood’s power to reverse age-related ills such as impaired cognition and cardiac function.

The new work is “very interesting”

and “raises significant questions about the original experiments,” says Michael Rudnicki, director of the regenerative medicine program at the University of Ottawa.

The Conboy team points out that those past studies that surgically connect mice involved the sharing of more than blood: The old mice benefited from having access to the

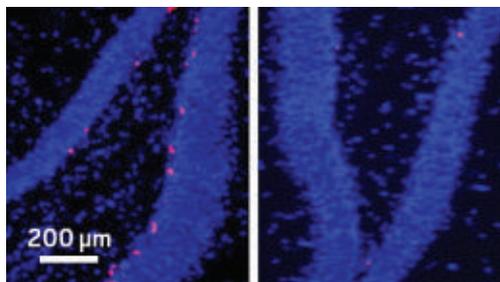
young animals’ organs to help carry out processes like blood oxygenation and filtration.

Irina Conboy says this complication has led to results that could be misinterpreted. “The research is valid, but it is not just about results, it’s how you draw conclusions,” she tells C&EN. Blood transfusions, she says, eliminate these confounding variables.

The team found that effects of young and old blood transfusions on the mice were complex. Old mice were better able to

recover from muscle tissue injury when given young blood. But the young blood did not improve neuron regeneration in the old mice; and more important, neuron and liver cell regeneration was inhibited in young mice that received blood from elderly animals. This implies that old blood contains substances that cause health decline, the team says.

Identifying the substances and figuring out ways to remove them from old blood may be a more successful approach to thwarting the aging process than a dose of young blood, the researchers say.—ELIZABETH WILSON

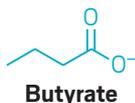
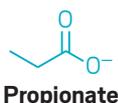
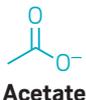


In these micrographs, new brain cells (red) form in the hippocampus of a young mouse with young blood (left), but when a young mouse receives old blood, brain cell formation slows (right).

MICROBIOME

Microbiome modifies epigenetics

Over the past decade, scientists studying the human microbiome have found that the microorganisms inhabiting our bodies can influence our propensity for obesity, cardiovascular disease, diabetes, inflammatory bowel disease, and many other ailments. Although the precise mechanisms by which our microbiome alters our health—for good and bad—have mostly eluded researchers, many increasingly believe that the short-chain fatty acids produced by our microbes, including acetate, propionate, and butyrate, are likely involved.



Now a team of researchers led by Federico E. Rey and John M. Denu at the University of Wisconsin, Madison, reports that short-chain fatty acids produced by a mouse's gut microbiome can affect the epigenetics in the animal's cells: The compounds change the activity of enzymes that help add acetyl and methyl groups to histone proteins, thereby altering the availability of nearby DNA for transcription (*Mol. Cell.* 2016, DOI: 10.1016/j.molcel.2016.10.025). Although they found a direct connection between short-chain fatty acids and histone acetylation, the connection with histone methylation was less straightforward, suggesting that other microbiome metabolites are likely involved in modifying mouse epigenetics.

Furthermore, the team found that feeding mice a high-fat Western diet suppressed production of short-chain fatty acids by their gut microbes as well as the epigenetic modifications that would normally occur with a healthier fiber-rich diet.—SARAH EVERTS

DRUG DELIVERY

A step toward mitochondrial gene therapy

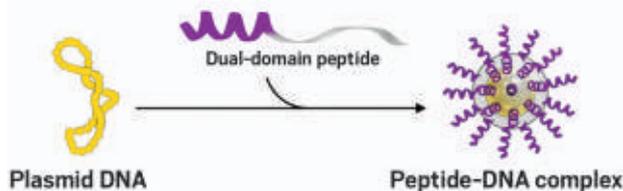
Peptide-based system delivers DNA into mitochondria

Mutations in DNA that resides in cells' energy-producing mitochondria underlie many diseases, including cancer, diabetes, heart disease, and age-related neurodegenerative disorders. But a safe, reliable method to deliver therapeutic DNA to mitochondria to correct these mutations doesn't currently exist.

Now, Keiji Numata of Japan's RIKEN research institute and colleagues have developed a peptide-based system that delivers a functional gene to human mitochondria without toxic effects. The system could pave the way to gene therapy for mitochondrial diseases (*Biomacromolecules* 2016, DOI: 10.1021/acs.biomac.6b01056).

Earlier attempts to develop mitochondria-targeted gene delivery systems posed limitations. Many were toxic, and although researchers had shown that mitochondria took up peptides used in various delivery systems, no one had shown whether mitochondria actually expressed the genes delivered.

Numata's team built and tested a dual-domain peptide designed to penetrate cell membranes and then trigger transport receptors on the surface of mitochondria. The peptide is made of a subunit of a yeast enzyme, cytochrome *c* oxidase (Cytcox), fused to another peptide containing only lysine and histidine residues. The residues enable the peptide to pass through a cell's mem-



A mitochondrial gene delivery system uses a self-assembling, dual-domain peptide to bundle DNA into a spherical particle.

brane, while the Cytcox helps trigger the mitochondrial transporters. The researchers packaged DNA with this modified Cytcox by mixing plasmid DNA encoding a green fluorescent protein (GFP) with the modified peptide and allowing the components to self-assemble into spherical particles.

To see if the system could deliver the DNA, the researchers added the peptide-DNA complexes to human embryonic cells whose mitochondria they stained with red fluorescent dye. Confocal microscopy revealed that the glow from the GFP and the red dye overlapped, indicating that 82% of the mitochondria had taken up and expressed the plasmid DNA. The researchers observed gene expression for about a week and saw that the cells remained viable throughout.

But the system requires further analysis, experts say. Michael A. Teitell of UCLA says successful delivery of a gene involved in mitochondrial disease would confirm the system's clinical usefulness.—MELISSA PANDIKA, special to C&EN

BY THE NUMBERS

7.07 million km²

Area covered by ice in the Arctic at the end of October, according to the National Snow & Ice Data Center. This is the lowest recorded area for that time of year since scientists began monitoring arctic ice via satellite. Between 1981 and 2010, arctic ice on average covered about 9.5 million km² at the end of October. Scientists partially blame record-high arctic temperatures—about 20 °C greater than average earlier this month, according to the Danish Meteorological Institute—for the new record low.

DRUG DISCOVERY

► **Nanobody blocks inflammation target**

Researchers have identified a mini antibody that blocks signaling by a disease-related ion channel protein potently and selectively. When the P2X7 channel senses ATP from damaged cells, it sends signals that can lead to conditions such as nerve inflammation, multiple sclerosis, and rheumatoid arthritis. Several drug companies are developing small-molecule P2X7 inhibitors, but the agents have had poor target selectivity, a factor that can cause side effects. Friedrich Koch-Nolte of University Medical Center Hamburg-Eppendorf and coworkers have now identified a minimal antigen-binding domain, called a Nanobody, that selectively inhibits human P2X7 (*Sci. Transl. Med.* 2016, DOI: 10.1126/scitranslmed.aaf8463). In endotoxin-treated human blood, the Nanobody was 1,000 times as potent at preventing cytokine release, a harbinger of inflammation, as small-molecule P2X7 antagonists in clinical development. Nanobodies are often species-specific, making animal testing difficult, and they tend to have trouble crossing the blood-brain barrier, which could limit their use for neurological indications, comments P2X7 expert Ronald Sluyter of the University of Wollongong. Nevertheless, the new study does suggest that Nanobodies “provide an exciting, novel therapeutic approach to targets P2X7,” Sluyter says.—STU BORMAN

REAGENTS

► **Deoxyfluorinations continue to evolve**

Once upon a time, carrying out a deoxyfluorination reaction to replace an alcohol group with fluorine required using brutish reagents such as sulfur tetrafluoride gas or the sulfur fluoride-based liquids DAST or Deoxo-Fluor. In time, chemists have developed milder crystalline reagents, such



as XtalFluor, Fluolead, PhenoFluor, and PyFluor. While the solid reagents are easier to handle, the compounds each have limitations, including low thermal and moisture stability, poor functional group selectivity, and the need for an auxiliary reagent such as a base. Researchers led by Tobias Ritter of Harvard University and the Max Plank Institute for Kohlenforschung have now reported a new reagent, called AlkylFluor, that resolves many of the problems (*Org. Lett.* 2016, DOI: 10.1021/acs.orglett.6b03086). Ritter’s group initially developed PhenoFluor, a difluoroimidazolium reagent, which works

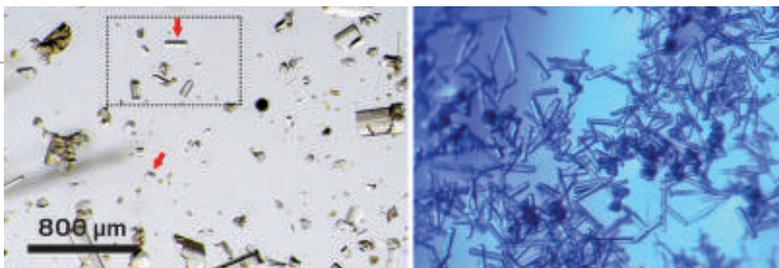
well for deoxyfluorination of phenols and aliphatic alcohols but is sensitive to moisture and requires special handling. The researchers subsequently made an imidazolium chloride derivative, PhenoFluorMix, which is

stable in air but limited to arene deoxyfluorinations. AlkylFluor is a monofluoroimidazolium borate derivative that’s stable to air and moisture and geared toward deoxyfluorination of primary and secondary aliphatic alcohols. Using the deoxyfluorination of testosterone as a test case, the researchers found that AlkylFluor outperformed other reagents.—STEVE RITTER

EPIGENETICS

► **Glutamic acids get chromatin to loosen up**

The DNA-packaging material chromatin is made of DNA wrapped around protein spools called histones. These histones control access for copying and transcribing the DNA. Modifying histones with the



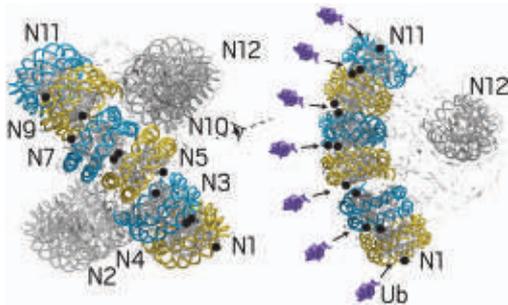
Crystals grown via batch process (top) form in a range of sizes and shapes. Those grown in multiwell microplates (bottom) have a more consistent shape and size (about 100 μm long)—good for soaking up guest molecules.

ANALYTICAL CHEMISTRY

Making the ‘crystalline sponge’ more user-friendly

In 2013, when University of Tokyo’s Makoto Fujita reported a way to determine a complex molecule’s X-ray crystal structure without having to actually crystallize the molecule in question, the technique was hailed as a breakthrough for structural determination. But the technique, known as the “crystalline sponge” method because guest molecules soak into a metal-organic framework crystal where they orient themselves in a way that their structure can be determined via X-ray analysis, has yet to be adopted as a routine characterization tool. The technique, as originally reported, takes a significant amount of trial-and-error. Only about 5% of the crystals prepared are suitable for soaking, and it can take up to 16 days to create a single guest-soaked crystalline sponge. Seeking a way to shorten and improve this process, University of Illinois, Chicago, researchers Bernard D. Santarsiero, Neal P. Mankad, and Greyson W. Waldhart made some tweaks to existing protocols (*Org. Lett.* 2016, DOI: 10.1021/acs.orglett.6b03119). Rather than grow crystalline sponges in a batch process as the original protocol indicates, the UIC researchers used multiwell microplates and layered a drop of ZnI₂ in methanol with a drop of the sponge ligand 2,4,6-tris(4-pyridyl)-1,3,5-triazene in nitrobenzene. This step produces crystals, 90% of which are suitable sponges, in only 10 hours. Because it takes seven days for this step under the original protocol, this improvement dramatically cuts down on experiment time.—BETHANY HALFORD

protein ubiquitin is known to be one way of loosening the chromatin structure to provide access to the DNA. But the mechanism by which ubiquitin achieves this loosening has remained unknown. Tom W. Muir, Galia T. Debelouchina, and Karola Gerecht of Princeton University have reported using cross-linking experiments and hydrogen-deuterium exchange with NMR spectroscopy to figure out what in ubiquitin interacts with chromatin (*Nat. Chem. Biol.* 2016, DOI: 10.1038/nchembio.2235). Their findings suggest that two glutamic acids on ubiquitin's surface are the key drivers. The researchers observe that many more cross-links form between ubiquitin and histone proteins when those glutamic acids are present than when they are replaced by other amino acids. In addition, the cross-linking experiments revealed that ubiquitin interacts both with histone



In this 12-mer nucleosome array, ubiquitin (purple) binds at locations (black spots) between neighboring nucleosomes (blue/gold, labeled N1-N12).

proteins and with other copies of itself. The Princeton team proposes that ubiquitin forces chromatin to loosen up by acting as a wedge between neighboring nucleosomes, the repeating unit of chromatin. In addition, the researchers suggest that the ubiquitin-ubiquitin interactions further promote loosening by preventing chromatin fibers from associating with one another.—CELIA ARNAUD

INORGANIC CHEMISTRY

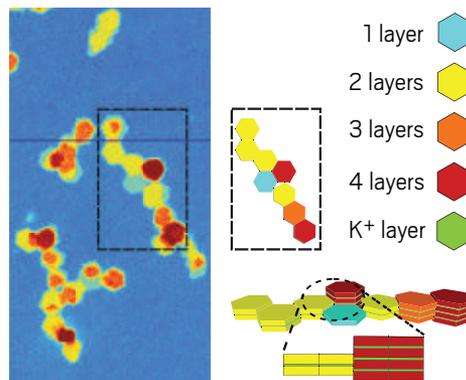
► Chemoctopus has superlative redox powers

An octasilsesquioxane grafted with redox-active metallacarborane arms—we'll call it a chemoctopus—could prove to be a versatile material for a host of sensing, catalytic, and biomedical applications (*Inorg. Chem.* 2016, DOI: 10.1021/

2-D MATERIALS

A flaky solution for 2-D materials

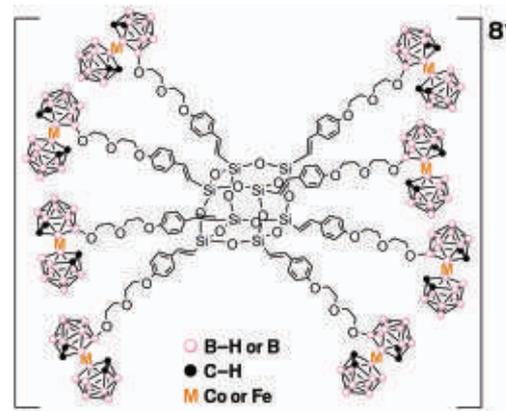
There's a new solution afloat for coating large swaths of substrates with two-dimensional materials—and that solution is ionic. Chemists have previously investigated ways to dissolve 3-D crystals that exist naturally as stacks of atomically thin 2-D sheets. A famous example is 3-D graphite with its 2-D graphene layers. Liquids filled with 2-D flakes could help scientists cover macroscopic areas with these materials, which have attractive optical, electronic, or mechanical properties. But researchers have struggled with using existing solutions to liberate uniform, single sheets from their parent crystals. A team led by Christopher A. Howard of University College London has overcome this problem with help from alkali metals and organic solvents. The researchers soaked 10 dif-



Single sheets of bismuth telluride, about 100 nm across, were deposited using an ionic solution of the 2-D material and electroplating.

ferent layered materials, including graphite and molybdenum disulfide, in liquid ammonia sprinkled with lithium or potassium. The baths enable metal atoms to work themselves between the sheets of a layered material. Once removed from the ammonia, a metal-loaded material is given a dip in aprotic organic solvents. Here, negatively charged single layers of the stacked material, such as molybdenum disulfide, flake off, leaving alkali-metal cations (*Nat. Chem.* 2016, DOI: 10.1038/nchem.2650). The 2-D flakes can then be transferred to a substrate by simply letting the liquid dry or by electroplating.—MATT DAVENPORT

acs.inorgchem.6b02394). Octasilsesquioxanes are intriguing Si_8O_8 cubes that are favorites of materials researchers because they are easy to make. The cagey framework ensures mechanical and thermal stability, and the easily functionalized silicon atoms give rise to tunable properties. Researchers have previously prepared electroactive metallodendrimers by attaching ferrocene units to silsesquioxane cores. But these compounds haven't always been soluble in common solvents or exhibited uniform redox activity. In the new example, a team led by Rosario Núñez of the Institute of Materials Science of Barcelona grafted metallacarboranes to the silicon atoms of octavinylsilsesquioxane via olefin metathesis. The resulting octopus-like molecules exhibit high solubility in organic solvents, the researchers note, but in addition their pendant metallacarboranes act as inde-



pendent, one-electron redox units that can transfer eight electrons at essentially the same potential. Developing such molecules that can uniformly store and transfer many electrons is an ongoing challenge in developing molecule-based electronics.—STEVE RITTER

CHEMISTRY IN PICTURES

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Selections from cen.chempics.org, where C&EN showcases the beauty of chemistry



Curly crystals

Brian E. Love has kept this flask for more than 20 years. Love, an associate professor at East Carolina University, develops new organic reactions in his lab. One of his projects in the 1990s centered around modifying camphor, a compound that can be used as a starting point for synthesizing small molecules used in many fragrances and skin care products. In this beloved flask, Love made an imine by reacting camphor and 2-aminobiphenyl, but he couldn't bring himself to break up these eye-catching branched crystals. He ran the reaction again so that he could preserve the crystals and has held onto them ever since.—MANNY MORONE

Submitted by Brian E. Love, East Carolina University

Light-bearer

Stefan Schramm works in a truly illuminating field of chemistry. To create this photo, the postdoc dissolved just 5 mg of a 2-coumaranone derivative in a flask with a strong base. The 2-coumaranone reacted with oxygen in the air, creating an excited intermediate molecule, which then released energy in the form of bright blue light as it relaxed to its ground state. Schramm, who works with Panče Naumov at New York University, Abu Dhabi, carries out research focused on making these 2-coumaranones, a group of molecules that haven't been studied much but could be useful for the detection of diseases such as HIV and various cancers.—MANNY MORONE

Submitted by Stefan Schramm, New York University, Abu Dhabi



DRUG DEVELOPMENT

Vanderbilt neuroscience drug advances to clinic

In a first for an academic drug discovery group, the Vanderbilt Center for Neuroscience Drug Discovery has received FDA approval to put a treatment for brain disorders into the clinic without any help from the pharmaceutical industry. A study assessing the safety of the compound, a positive allosteric modulator of muscarinic acetylcholine receptor 1 (M1) for Alzheimer's disease and schizophrenia, will begin early next year.

Academic drug discovery centers such as VCND D typically focus on generating early-stage compounds that are spun off into companies or licensed to partners with the cash and experience to push them into clinical studies. Since it was established in 2008, VCND D has secured several drug discovery partnerships with big pharma firms for pre-clinical compounds developed in its labs.

But with many drug firms exiting neuroscience research, some of those programs have stalled. Big pharma's waning commitment to neuroscience prompted a shift in strategy at VCND D. For the past two years, the academic team has focused on putting molecules through early clinical studies in the hope that they will have a better chance of getting to patients.

"We rarely see companies license a clinical-stage asset and then back out of it for non-science-based reasons," notes VCND D Director P. Jeffrey Conn. "We felt that if we partnered at a later stage, it gives programs a better chance of going the distance."

NIH funded much of the basic science on the M1 receptor, and in 2014 the William K. Warren Foundation kicked in \$5 million to support the preclinical studies. Those data allowed VCND D to get grants from the Alzheimer's Association and Alzheimer's Drug Discovery Foundation to support the Phase I trials.—LISA JARVIS



Conn

FINANCE

DuPont readies a pension freeze

DuPont intends to overhaul its pension plan as it merges with Dow Chemical and the new firm, DowDuPont, splits up into three separate companies.

DuPont will freeze its defined benefit pension plan for current employees on Nov. 30, 2018, or when the first of the new companies breaks off from DowDuPont, whichever comes first. When a company freezes a pension, benefits stop accruing in employees' accounts.

Additionally, the firm will cut off retiree medical, dental, and life insurance benefits for active employees who are less than 50 years old.

The pension changes impact 13,000 out of the 133,000 participants in DuPont's pension program. Some 4,500 employees will be affected by the insurance benefits changes.

DuPont closed its defined benefits pension plan to new participants in 2007 and shifted toward an enhanced 401K system. This summer, the company launched a buyout program aimed at 18,000 former employees who were vested in the pension program but not yet receiving benefits.

DuPont estimates that the pension freeze will reduce its long-term employee benefits obligation by about \$550 million. At the end of 2015, DuPont's pension obligations totaled about \$26 billion.

"The changes will reflect another step in our multiyear analysis and bring us closer to the practices of our global peer set," Benito Cachinero-Sánchez, DuPont's senior vice president of human resources, wrote in a letter to employees.

Defined benefits pensions are becoming rare. According to a survey from the consulting firm Willis Towers Watson, only 20% of Fortune 500 firms offered some form of defined benefits pension in 2015, down from nearly 60% in 1998.—ALEX TULLO

NEUROSCIENCE

Lilly Alzheimer's drug fails

In yet another blow to the amyloid hypothesis, Eli Lilly & Co. disclosed that its Alzheimer's treatment solanezumab failed in a Phase III study. Shares of Lilly fell about 10% on the news on Nov. 23.

For more than a decade, Alzheimer's drug developers have focused their efforts on trying to prevent or remove the amyloid plaques coating the brains of people with the disease. Solanezumab, which binds to soluble, monomeric forms of amyloid-β, had already tanked in two Phase III studies. But Lilly decided to push on with a third trial based on signs that people with early-stage Alzheimer's benefited from the drug.

In this latest study, the drug failed to

slow down the cognitive decline seen in the disease. Lilly said it would no longer file for regulatory approval for the drug, which, if approved, would easily have enjoyed multi-billion-dollar sales.

"This result will no doubt cast a shadow over Lilly's Alzheimer's disease pipeline portfolio, which is heavily based on the beta-amyloid hypothesis," Leerink stock analyst Seamus Fernandez told clients. The news also hit Biogen, which has an antibody targeting aggregated amyloid-β in late-stage trials.

The solanezumab failure adds to a graveyard of Alzheimer's disease treatments. Indeed, Lilly already had plots



A Lilly researcher in New York City.

there: Solanezumab is the third Alzheimer's drug the firm has dropped from its pipeline. In 2010, Lilly pulled the plug on semagacesat, a γ-secretase inhibitor, and in 2013 ended development of the BACE inhibitor LY2886721.—LISA JARVIS

CREDIT: VCND D (CONN); LILLY (LAB)

INVESTMENT

► Butene-1 plant planned for Baytown

SBE Chemical Partners has secured the financial, customer, and engineering commitments it says it needed to go ahead with a butene-1 plant in Baytown, Texas. The plant will use Axens' AlphaButol process to dimerize ethylene into butene-1, used mainly as a polyethylene comonomer. The plant will cost about \$200 million and have 100,000 metric tons per year of capacity when it starts up in 2018. SBE is a joint venture between Evonik Industries and Stonebridge Energy Partners. Evonik is a major butene-1 producer in Marl, Germany, and Antwerp, Belgium. The Baytown site is a former Evonik carbon black plant.—ALEX TULLO

INORGANIC CHEMICALS

► BASF to divest inorganic specialties

BASF has agreed to sell its inorganic specialties business to the private equity firm Edgewater Capital Partners for an undisclosed sum. The business includes a site in Evans City, Pa., that makes specialty alcohols, boranes, and alkali metal products. About 80 employees are involved. The site is the former Callery Chemical, which BASF acquired in 2003 for \$65 million. Edgewater acquired another BASF business, the polymer additives service firm PolyAd Services, in 2014.—MICHAEL MCCOY

PETROCHEMICALS

► PTT still considering Ohio ethylene cracker

PTT Global Chemical continues to review plans to build an ethylene cracker complex in Mead County, Ohio, in light of what it sees as uncertainty in U.S. tax and energy policy, which could influence the availability of feedstock ethane from cheap shale gas. The Thai chemical company says the project would have a 1 million-metric-ton-per-year ethylene cracker, plus downstream polyethylene, ethylene oxide, and ethylene glycol plants. PTT is evaluating engineering bids and preparing documentation for potential lenders. However, the firm is still looking for

FOOD INGREDIENTS

DIC expands natural blue food color

Earthrise Nutritionals, a California-based subsidiary of Japan's DIC Group, will spend \$13 million to expand its production of a natural blue food coloring made from Spirulina, a corkscrew-shaped cyanobacteria used mostly as a dietary supplement. In 2013, the confectionary company Mars obtained FDA approval to use phycocyanin, a blue extract from Spirulina, to color foods. Earlier this year, Mars vowed to phase out the use of synthetic colors over the next five years. DIC claims to have 90% of the global market for natural blue color from Spirulina and says it expects demand to grow 50% annually through 2020. Earthrise cultivates the cyanobacteria in an 180,000 m² outdoor facility that currently yields about 500 metric tons per year. DIC is exploring ways to extract other pigments from Spirulina and use the remaining proteins in food and animal feed.—MELODY BOMGARDNER



Mars plans to phase out use of artificial colors, including blue.

partners. Marubeni had been mentioned as a partner when the project was unveiled a year ago but not recently.—ALEX TULLO

MATERIALS

► Evonik expands specialty polymers

Evonik Industries will expand production of poly-lactic-glycolic acid (PLGA), used to make biodegradable polymers, at its facilities in Birmingham, Ala., and Darmstadt, Germany. The firm will open a PLGA lab for medical device customers in Darmstadt by year-end. A lab for polymer contract research projects is planned for Birmingham. Evonik will also increase capacity for its Rohacell brand of rigid polymethacrylimide foam in Darmstadt by 20% in the second half of 2017. The firm expects sales to continue to rise at a double-digit rate.—ALEX SCOTT

AWARDS

► Kramvis is the 2017 Industry Medalist

The American Section of the Society of Chemical Industry has named Andreas C.



Kramvis

Hotel in New York City. The award recognizes his performance at Honeywell and as a thought leader in management methodology.—MARC REISCH

Kramvis its 2017 Chemical Industry Medalist. Kramvis, who is vice chair of Honeywell and former CEO of the firm's performance materials and technologies unit, will receive the award at a dinner in his honor on March 7, 2017, at the Plaza

INSTRUMENTATION

► Rutgers gets Thermo drug making tool

Thermo Fisher Scientific and Rutgers University's engineering research center for structured organic particulate systems will work together on continuous drug manufacturing techniques. Under the agreement, the center has acquired a Pharma 11 twin-screw extruder/granulator from Thermo Fisher. The center, in Piscataway, N.J., will use the tool to test hot-melt extrusion

and wet granulation processes for making tamper resistant and sustained release oral-dose drugs.—MICHAEL MCCOY

ONCOLOGY

► Grant from Texas prompts biotech to move

The biotech firm Ruga Corp. has changed its name to Aravive Biologics and moved from Palo Alto, Calif., to Houston after receiving a \$20 million grant from the Cancer Prevention & Research Institute of Texas (CPRIT). The product of a 2007 state constitutional amendment, CPRIT has to date awarded \$1.7 billion to Texas researchers. Aravive will be based at the Texas Medical Center, where it will develop Aravive-S6, a fusion protein designed to block a signaling pathway active in acute myelogenous leukemia.—MICHAEL MCCOY

PHARMACEUTICALS

► Novartis opts to buy Selexys Pharma

Novartis has acquired Selexys Pharmaceuticals, a specialist in hematological and inflammatory disease. The deal comes after successful Phase II clinical trials of

Selexys' SelG1, an antibody that treats vaso-occlusive pain in patients with sickle cell disease. The value of the deal could amount to \$665 million, including an undisclosed up-front payment and milestone payments. Novartis obtained the exclusive right to acquire Selexys and SelG1 in 2012.—RICK MULLIN

RARE DISEASE

► Shire to augment Cambridge presence

Shire will expand its operations in Cambridge, Mass., by establishing a rare disease "innovation hub" in Kendall Square. The firm has leased a 32,000 m² building at 500 Kendall Street, adjacent to space it currently occupies at 650 Kendall Street. Last year, Shire closed a facility in Pennsylvania and set up its U.S. headquarters in Lexington, Mass. The British company says it employs more than 3,000 people in Massachusetts and has nearly 400 job openings in the state.—MICHAEL MCCOY

INFORMATICS

► Broad, Intel team on genomics data

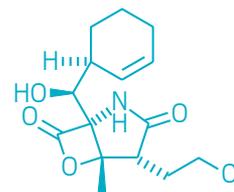
The Broad Institute and Intel have formed a five-year, \$25 million pact to develop in-

formation technology tools for processing genomics data. The Intel-Broad Center for Genomic Data Engineering aims to identify hardware and software that will make it possible to use data resident in private and public cloud storage. The partners say the venture will combine Intel's data analytics and artificial intelligence expertise with Broad's experience in genomics data generation and health care research.—RICK MULLIN

ONCOLOGY

► Celgene acquires a myeloma treatment

Celgene has acquired the proteasome inhibitor marizomib from Triphase Accelerator for an undisclosed sum plus future milestone payments. Triphase has completed Phase I clinical trials of marizomib as a treatment for glioblastoma and multiple myeloma. Celgene already markets the multiple myeloma treatments Revlimid and Thalomid. Triphase, a spin-off from the Ontario Institute for Cancer Research, granted Celgene the option to buy the drug in 2014.—MICHAEL MCCOY



Marizomib

Business Roundup

► **Showa Denko** has agreed to acquire GMM, a manufacturer of nonstick coating chemicals used by makers of frying pans and other cookware. With plants in India and China, GMM supplies Asian cookware companies that export to the U.S.

► **Stahl**, a Dutch maker of process chemicals for leather, coatings, and polymer dispersions, has acquired Calhoun, Ga.-based Eagle Performance Products. The purchase adds water-based flame retardants to Stahl's products for automotive, aeronautics, and home furnishings customers.

► **Honeywell** has launched a new business, Honeywell Research Chemicals, that includes its existing research chemicals plus the solvents and inorganic chemicals it acquired from Sigma-Aldrich late last year. The firm is also launching a purchasing website for research chemicals.

► **The American Cleaning Institute** has named Melissa Hockstad as its president and CEO, effective Jan. 1, 2017. Hockstad, now an executive with the American Fuels & Petrochemical Manufacturers trade group, will replace Ernie Rosenberg, who announced

in May his intention to step down.

► **Frutarom**, an Israeli flavors and fragrances maker, is buying 75% of Mexico's Grupo Piasa for \$20.5 million. The savory ingredients producer has 300 employees and annual sales of \$45 million. The acquisition is Frutarom's eighth this year.

► **Arysta LifeScience**, an agricultural chemicals firm, will license a biostimulant from Beem Biologics that reduces the impact of stress on crops while promoting vigorous plant growth, according to the companies. Beem develops isoprenoid compounds from desert, mountain, and sea plants.

► **Sekisui Medical**, a Japanese drug ingredients producer, has received a warning from FDA for failing to maintain comprehensive manufacturing records. An inspection revealed that the company had been retesting batches and selectively recording results.

► **Autolus**, a spin-off from University College London, is the first tenant of the U.K.'s Cell & Gene Therapy Catapult, a 7,200 m² cell therapy manufacturing center set to open next year in Stevenage, England. The \$68 million center features 12 lab, office, and manufacturing modules for cell therapy companies.

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POSTDOCS

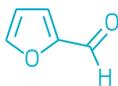
► Obama's overtime rule blocked by judge

A federal judge has stalled an Obama Administration overtime rule that would mean significant raises or overtime pay for millions of employees, including chemistry postdocs, starting on Dec. 1. The rule, put forward in May, requires overtime pay for workers who work more than 40 hours a week if they make less than \$47,476, up from the previous limit of \$23,660 set 12 years ago. Universities had been hit hard by the change. Although employees who teach were exempt, postdocs in the sciences and other nonteaching staff were included. That means the institutions would either have to pay them more or track their overtime, which many do not currently do. Some critics argued that the rule might end up hurting postdocs by making universities push them further away from regular employment. Many already do not get healthcare and other benefits that regular employees receive. The judge, ruling in Texas on Nov. 22, issued a temporary injunction against the rule, saying the White House had exceeded its authority with such a large pay increase. Obama's Department of Labor indicated that it will appeal, though there is little time left for the Administration to push it through.—ANDREA WIDENER

CONSUMER PRODUCTS

► EU proposes to limit furfural in cosmetics

The European Union is considering a plan to limit the concentration of furfural in cosmetic products to 0.001%, citing carcinogenicity concerns. The substance is used as a scent in oral care products, perfumes, shampoos, soaps, and other toiletries, according to the European Commission, the executive branch of the EU. As part of its safety program, the industry group International Fragrance Association already requires its members to restrict the amount of furfural to 0.001% in products designed for contact with skin and to 0.05% in other products. The government's proposal would give companies nine months to stop placing cosmetic



Furfural

RESEARCH FUNDING

Federal backing for university research continues decline

For the fourth straight year, federal support for R&D at U.S. universities fell in 2015, says an NSF report on how much universities spent and the sources of that funding. This inflation-adjusted decline of 13% over four years marks the longest fall in academic research funding since NSF began collecting data in 1972. The \$37.9 billion in federal support accounted for 55.2% of R&D spending at universities in 2015, down from 62.5% in 2011. However, the overall picture for science isn't all bleak. Spending is up from \$65.3 billion in 2011 to \$68.7 billion in 2015, including a 2.2% jump from 2014 to 2015. That is driven primarily by growth in spending from businesses, which was up 7.5%; nonprofit organizations, up 6.9%; and the universities themselves, up 5.9%. Research spending in many individual science disciplines in 2015 matched that trend, with a 2.2% increase from 2014 in all science spending by universities. Chemistry was up 2.0% to \$1.8 billion in 2015, and chemical engineering was up 0.9% to \$915 million.—ANDREA WIDENER

products on the EU market with furfural concentrations greater than 0.001% and 12 months to withdraw noncompliant products. The EC says the transition periods are necessary "as any modification of a fragrance composition is a complex process, which requires sufficient time for obtaining a satisfying olfactory result." The commission is seeking comments from the public about its proposal until early next year.—CHERYL HOGUE

FOOD

► FDA prohibits outdated food wrapper chemicals

Two grease-repelling perfluorinated chemicals that were formerly used in paper-based food packaging are no longer allowed in the U.S. in such products, under a Nov. 22 regulation from FDA. The two chemicals, once used in microwave popcorn bags, pizza boxes, and fast-food wrappers, are no longer made or used in the U.S., says 3M. The company claims to have been the only producer and user of the substances in the country. FDA's action is aimed at stopping companies from using the two chemicals in food packaging in



FDA has banned two more perfluorinated chemicals once used in paper packaging for greasy food such as pizza.

the future, and makes it illegal to import such products into the U.S. The agency's decision to ban the two chemicals was not based on safety considerations. Rather, it rested solely on the fact that they are no longer used. Earlier this year, FDA banned three other perfluorinated chemicals from such uses, claiming "there is no longer a reasonable certainty of no harm from the food-contact use" of the substances. Environmental and public health groups claim perfluorinated chemicals are linked to cancer and birth defects.—BRITT ERICKSON



Formulators are increasingly concerned about microbial contamination in cosmetics.

CHEMICAL REGULATION

Restrictions ramp up on cosmetic preservatives

With fewer preservatives in use, chemists worry about protecting consumer products from contamination

MARC S. REISCH, C&EN NEW YORK CITY

It has been a slow war of attrition. For the past decade, environmental groups have called out a growing number of cosmetic preservatives as suspected endocrine disruptors, cancer-causing agents, and skin irritants. Regulators have examined the claims and in some cases enacted restrictions on widely used preservatives.

Now the list of useful preservatives is down to a handful, say cosmetic formulators and suppliers. And because of the high cost of developing new preservatives and strictures against animal testing, few qualified alternatives are in the offing.

Without a preservative, often used at less than 1%, skin creams, makeup, and shampoos can become contaminated with mold, fungi, and bacteria. Some contaminants can spoil the appearance and smell of cosmetics. Others can lead to skin, scalp,

and eye infections, or even worse.

Bad actors include *Staphylococcus aureus*, a gram-positive bacteria that can cause skin infections, and *Escherichia coli*, a gram-negative bacteria that can cause stomach cramps and diarrhea when people share cosmetics. “Consumers assume that preservatives are bad without understanding how necessary they are,” says Janet Blaschke, chief executive officer of the consulting firm International Cosmetics & Regulatory Specialists.

Preservatives are meant “to keep cosmetics safe throughout their useful life from production until the last bit is used at the bottom of the jar,” Blaschke says. She fears that, over time, bacteria will build up resistance to the diminishing number of options now available. She doesn’t see alternatives such as single-use or aseptic packaging as realistic—both because of the additional cost and because of the increased packaging waste.

When it comes to preservatives, the most important regulator is the European Union. The EU has a list of allowable preservatives, known as Annex V, that not only governs preservative use in the 28-nation alliance but also influences regulations in many other countries. Although the list contains more than 50 approved ingredients, often only two or three options are appropriate for a particular formulation, formulators and preservative suppliers say.

Among the preservatives European authorities have restricted are methylisothiazolinone and the mixture of methylisothiazolinone and methylchlorisothiazoli-

none for use in cosmetics, such as lotions, that remain on the skin. The restrictions, effective earlier this year for the combination and in 2017 for the single ingredient, were widely expected. Most everyone, including their maker, Dow Chemical, agreed the ingredients can irritate skin.

An unfavorable review by the Scientific Committee on Consumer Safety (SCCS), an EU panel of experts, judged one widely used preservative, poly(hexamethylene) biguanide hydrochloride (PHMB), not safe for use at a maximum concentration of 0.3% because of mutagenic and cancer concerns. SCCS is now considering whether PHMB is safe for use at concentrations of up to 0.1%, says PHMB maker Lonza. That opinion is expected in December.

Insiders also say EU authorities may soon ban chloroacetamide. French authorities banned it in 2012, but it still appears on the Annex V list of allowable preservatives. The U.S. Cosmetic Ingredient Review, a government-sanctioned industry organization, determined in 1991 that the ingredient is “a potential human sensitizer” and thus not safe for cosmetic use.

EU authorities have examined other preservatives on Annex V and found them acceptable but sometimes at reduced allowable use levels. The widely used preservative phenoxyethanol received a clean bill of health earlier this year. In 2015, phenylphenol got a passing grade but at reduced use levels. SCCS said it did not have enough data to judge safe use of sodium *o*-phenylphenate and potassium *o*-phenylphenate.

A 2013 SCCS review of parabens, compounds the advocacy organization Environmental Working Group has targeted as endocrine system disruptors, found they were safe to use. SCCS did recommend new, lower concentration limits for propylparaben and butylparaben, both of which it judged to have “a weak endocrine-modifying potential.”

Rob Taalman, director of research and science at Cosmetics Europe, which represents European cosmetics makers, says the parabens recommendation reflects the EU’s risk-based assessment process for cosmetic ingredients. An ingredient “may have an intrinsic undesirable property, but EU authorities don’t automatically ban it,” he says. Preservatives are used in cosmetics to ensure public safety, he notes.

Yet for companies, a government stamp of approval isn’t always

“Consumers assume that preservatives are bad without understanding how necessary they are.”

—Janet Blaschke, CEO, International Cosmetics & Regulatory Specialists

enough. Following criticism from outside groups, some consumer product formulators have banned what they consider chemicals of concern. For example, Johnson & Johnson removed formaldehyde-releasing preservatives, which might evoke an allergic response, from all its products. It also removed parabens from baby products.

Andrea Mitarotonda, chief scientific officer of Neal’s Yard Remedies, a U.K.-based cosmetics retailer and formulator, notes that any suspicion, even if undeserved, can prompt corporate action. Without waiting for the outcome of an investigation, companies often reformulate entire ranges of products so they don’t have to face “the

detrimental consequence of a possible ban later,” he explains.

Questioning old standby preservatives is not necessarily a bad thing, Mitarotonda observes. “What was considered safe 20 years ago, tested using methods and protocols available at that time, needs to be reviewed in light of the knowledge and technologies available now,” he says.

Neal’s Yard Remedies draws on the ingredients from the Annex V list, but Mitarotonda is also interested in using them in combination with natural alternatives not on the list. “Very few formulators will be aware of the chemistry of essential oils or plant extracts, which is obviously a shame as they may be missing out on opportunities to use substances to enhance the preservation profile of their products.”

Some industry players are leery of essential oils and plant extracts, which are often called “nonpreservative preservatives.” Oils and extracts can vary in quality and consistency, notes David Steinberg, a cosmetic formulation consultant. “How do you guarantee the purity of extracts compared with the purity of synthetic preservatives like parabens?” he asks.

Steinberg also wonders about the efficacy of alternative preservatives, noting that they don’t have the long history of use and characterization that backs the traditional sort. Recalls of contaminated cosmetics are dwarfed by those of clothing, toys, and other consumer products on the EU’s Rapid Alert recall database, he says. But he notes a subtle rise in cosmetic recalls in the past few years, which he attributes to lower levels of effective preservatives and the use of alternatives.

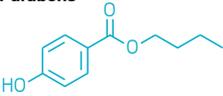
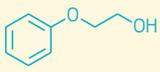
Some products that are primarily added as emollients or conditioners, for instance, can also have preservative qualities, notes Rick Strittmatter, global microbial control R&D director at Dow. Like plant extracts, they also fall into the category of nonpreservative preservatives and “can clearly play a preservation role,” he says.

Under fire

European authorities have banned three preservatives and reviewed four others over the past five years.

INGREDIENT	DATE	ACTION
BANS		
Chloroacetamide	June 2012	French regulatory ban
Methylisothiazolinone 	February 2017	EC disallows for leave-on products
Methylisothiazolinone & methylchloroisothiazolinone mixture	April 2016	EC disallows for leave-on products

RECENT EU REVIEWS

Parabens 	May 2013	SCCS rules safe with some restriction on propyl- and butylparaben
Butylparaben		
Phenoxyethanol 	October 2016	SCCS rules safe for all uses
<i>o</i> -Phenylphenol	December 2015	SCCS rules safe at prescribed levels
Poly(hexamethylene) biguanide hydrochloride	July 2015	SCCS rules says not safe at 0.3% by weight or higher

EC = European Commission. SCCS = Scientific Committee on Consumer Safety, which advises EC on the safety of preservatives.

Sources: European Commission, Agence Nationale de Sécurité des Médicaments et des Produits de Santé

But the assessment of such preservatives “also must be subject to the same risk-based approach that traditional preservatives have been subject to,” Strittmatter says. “If it is being used as a preservative, it needs to be assessed on a level playing field.”

Companies are pursuing all preservative options to combat the shrinking arsenal of traditional products. Niall D’Arcy, project manager for the Ireland-based consulting firm Biocide Information, sees a business opportunity because the new products are generally more expensive than parabens and other traditional ingredients. He says the \$1 billion-a-year global market for preservatives of all types is growing 4 to 5% annually.

Of the more than 50 preservatives listed on Annex V, only about one-third are in regular use, says Andrea Wingenfeld, a technical marketing manager at the specialty chemical maker Ashland. Temperature sensitivity, pH sensitivity, and antimicrobial activity all play a role in the choice a formulator makes. In addition, formulators may avoid using a preservative approved in Europe or other regions if that preservative has been the subject of negative publicity, she says.

For leave-on products such as sunblock or makeup, the choice of preservatives is especially limited, Wingenfeld says. Since the bans on use of isothiazolinones, formulators rely mostly on phenoxyethanol, benzyl alcohol, and organic acids, she notes.

Although they do not like the attacks on what they view as beneficial ingredients, preservative suppliers acknowledge market realities. Lonza, for instance, just revamped its FormulaProtect online preservative selector tool, which allows users to avoid controversial products such as formaldehyde donors and instead choose “less controversial products,” says Phil Hindley, Lonza Consumer Care’s global marketing head for preservation.

Lonza is also interested in developing new preservatives that are acceptable to regulators, formulators, and environmental groups. Hindley says he is open to working with all stakeholders to develop such alternatives (see sidebar). But only a “robust solution” with performance, safety, and cost benefits will work in the long run, he says.

Other challenges to the development of new preservatives are the time, cost, and effort required to win regulatory approval. Ashland’s Wingenfeld says it took eight years from the time authorities received a dossier on the most recent addition to Annex V, citric acid/silver citrate, until it appeared in 2014. Given that timetable, “most companies will not see a business case in

commercializing new preservatives,” she says.

The ban on animal testing for cosmetics, in place in Europe since 2009, makes it difficult for developers to submit required safety data on a new preservative, Wingenfeld adds. Cosmetics Europe’s Taalman says member companies are working with regulators to qualify new skin exposure and risk-assessment models.

However, at the moment, it’s not easy to

qualify a new preservative, Taalman says. “We are basically stuck,” he says, at least until new testing protocols are approved, and that is at least a few years off.

Cosmetic products today are by and large safe, Blaschke, the consultant, emphasizes. By worrying about preservative options now, formulators and suppliers “are trying to keep up their good record,” she says, and keep crises from occurring down the road. ■

Contest will offer cash for new preservatives

A group of consumer product formulators, preservative makers, retailers, and nongovernment organizations is coming together under the banner of the Green Chemistry & Commerce Council (GC3) to stage a crowdsourcing competition for new preservative technologies.

Details on the competition, to be managed by the open innovation expert InnoCentive, are still being worked out. But when the competition gets under way in about six months, it’s expected to offer up to 10 prizes of \$5,000 to \$10,000 apiece for early-stage ideas and \$20,000 to \$25,000 for more advanced preservative concepts, according to Monica Becker, codirector of GC3, an organization of chemical makers, product manufacturers, and retailers.

The goal, Becker says, is to accelerate commercialization of safe and effective preservative systems. Contest-judging criteria, now being developed, are likely to echo a “need statement” GC3 developed with a number of formulators about a year ago. The statement called for preservatives that are biodegradable, free of carcinogen and endocrine disruption concerns, and not likely to build microbial resistance.

The contest backers don’t want intellectual property rights, Becker says. Instead, their goal is “to bring promising technology to light” and connect innovators to companies with which they can partner to develop, test, register, and manufacture inherently safer preservatives.

“We want to help academic researchers or small companies

who don’t have the resources to get new ‘green’ preservatives to market,” she says.

In all, 17 entities are backing the contest. Among them are retailers Walmart and Target. Both firms have pressured suppliers to reduce or eliminate ingredients in household goods that they deem harmful to human health and the environment.

Consumer goods makers such as Johnson & Johnson, which pledged to eliminate certain chemicals of concern from its products in 2012, are among the backers. Additional contest underwriters include the advocacy group Environmental Defense Fund and large preservative makers such as Dow Chemical, Lonza, and Schülke & Mayr.

The preservation project has been two years in the making, Becker says. An executive at J&J got the ball rolling when he watched a webinar on open innovation at which Becker was a speaker.

When they talked, Becker and the J&J executive realized that many companies in the personal care and household products space share a need for new, safe, and effective preservatives, Becker

recounts. “We thought we could make it a collaborative effort,” she says.

After gathering an initial group of formulators, Becker also drew in preservative makers. Though not initially involved, large retailers heard about it and asked to join, she says.

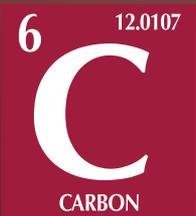
Becker says she is hoping the challenge will attract a large number of entries. “We’ve never done anything like this before. I’m cautiously optimistic,” she says.

Backers

A list of contest supporters that agreed to be named:

- ▶ Babyganics
- ▶ Beiersdorf
- ▶ Dow Chemical
- ▶ Environmental Defense Fund
- ▶ Johnson & Johnson
- ▶ Lonza
- ▶ Method
- ▶ Schülke & Mayr
- ▶ Seventh Generation
- ▶ Target
- ▶ Walmart

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LOOKS LIKE

Organic
LETTERS



Students gathered at a University of the Witwatersrand campus in Johannesburg on Oct. 4 to protest tuition increases.

EDUCATION

Chemists at South African universities endure campus violence

Students protest tuition increases amid continuing racial and economic inequities

JYLLIAN KEMSLEY, C&EN WEST COAST

Violence flared for several weeks this fall at university campuses in South Africa as students objected to proposed tuition increases of as much as 8%. The #FeesMustFall movement began in 2015 when the government proposed a similar fee increase, which was later rescinded. Although the demonstrations started to protest these tuition increases, students quickly switched to demanding free higher education.

The protests have disrupted deliveries to laboratories and canceled classes. Protesters have torched buildings and police have used stun grenades and rubber bullets to subdue demonstrators. Overall damage is estimated to be \$50 million. After police crackdowns, campuses are quieter now and students are writing their final exams, but it's unclear what will happen when a new academic year begins in February.

The roots of the movement lie in continued racial and economic inequality in the country, more than two decades after apartheid ended and Nelson Mandela was elected president in South Africa's first election with universal suffrage. "The black middle class is bigger and better off, but on average, the gap between the rich and poor is bigger," says Gert Kruger, a pharmaceu-

tical sciences professor at the University of KwaZulu-Natal (UKZN). More than 26% of the workforce is unemployed, and the government still struggles to provide basic necessities such as clean water, electricity, housing, and health care, as well as quality primary and secondary education. The African National Congress (ANC), which has ruled South Africa since apartheid ended, is now plagued by allegations of corruption.

"Most of our students were born after 1994," the year Mandela took office, says Charles de Koning, a chemistry professor at the University of the Witwatersrand and the chair of the South Africa international chapter of the American Chemical Society. ACS publishes C&EN. "Society had high expectations of post-apartheid South Africa, including increased access to higher educa-

tion. Progress toward this and other goals has been slow, and this has led to frustration that is being played out at the universities."

University enrollment has roughly doubled to nearly 1 million since 1994. But racial inequalities persist: Black South Africans make up roughly 80% of the population, but only about 16% of black people ages 20 to 24 are enrolled in higher education. White people make up about 9% of the population, but 55% of white 20- to 24-year-olds enroll in university. The racial composition of university academic staff is about 34% black and 51% white.

The South African government does have a National Student Financial Aid Scheme to provide funding for poor students to attend universities. Edwin Mmutlane is the son of a mine laborer and a housewife, and he received both scholarship money and a loan through the program. He is now a senior lecturer in chemistry at the University of Johannesburg. "I would not be where I am today if it was not for this scheme," Mmutlane says. But the program is underfunded and a "missing middle" class of students—children of people in professions such as teaching, nursing, and police work—often don't qualify for aid and struggle to pay tuition, sources tell C&EN.

Meanwhile, neither government funding for universities nor faculty and staff hiring has increased proportionately with student

enrollment. "It's put a strain on the whole system," Kruger says. At UKZN, "in chemistry, we now have something like 2,000 first-year undergraduates. I'm convinced that the overall quality of the degree has not decreased much, but to teach such large classes is a huge burden administratively."

The protests themselves have not had huge effects on chemistry departments, however. Although classes were interrupted on some campuses, they did finish eventually.

As for research, graduate students and faculty were largely able to get to their labs and offices when they wanted. "Personally, I have been able to come to campus nearly every day, although I had to leave early" when protests were happening, says a chemistry graduate student who asked to be identified only by her first name, Memory. "Our main problem was delivery of chemicals or services—we didn't have any chemicals delivery during the protests."

The fallout from the protests, however, has strained funding. When tuition increases were rescinded last year, the government

Inequality in South Africa continues

Black people are underrepresented in higher education and earn significantly less than white people.

	BLACK	MIXED RACE	INDIAN/ASIAN	WHITE
Percentage of total population	80%	9%	3%	9%
Percentage of public university undergraduate enrollment	70	6	5	17
Percentage of students ages 20 to 24 enrolled in higher education	16	14	47	55
Percentage of academic staff	34	5	8	51
Median annual earnings	\$4,389	\$5,705	\$13,166	\$17,555

Note: Data are for 2013 except median annual earnings, which are for 2012. Median annual earnings were converted from South African rands to U.S. dollars using the average of monthly exchange rates for 2012.

Sources: South Africa Council on Higher Education, the University of the Witwatersrand

made up only some of the shortfall. Campuses had to absorb the rest. "We wanted to get a new mass spectrometer," de Koning says. "We have a program called the national equipment program that provides two-thirds of funding for major equipment. The university did come up with its one-third share, but it was quite a struggle."

What happens from this point is an open question. In January, current South Africa President Jacob Zuma set up a commission to examine the feasibility of eliminating

university fees. The commission's report is currently expected in June of 2017.

People who spoke with C&EN were skeptical that fee-free higher education is possible. "For a country like South Africa to have free university education now would be very destructive to the economy," Memory says. "We should be doing more to stimulate the economy so that we have more people working, more middle-class people, and more disposable income. That will, in turn, reduce the burden on the government." Others suggest that basic services and improved primary and secondary education perhaps should be tackled before university tuition.

"Why are universities being targeted?" asks Grant A. Farred, who grew up in South Africa and is now a professor of Africana studies at Cornell University. "The black working poor have been served badly by the ANC. Why are people not mobilizing against all of the inequities produced by a government that is corrupt, nepotistic, and primarily responsible for the failure to deliver services to black areas?" ■



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C&EN talks with Wei Yang, president of China's National Natural Science Foundation

Funding agency head strives to raise quality of Chinese research and curb misconduct

MITCH JACOBY, C&EN CHICAGO

Wei Yang is a man on a mission. As president of the National Natural Science Foundation of China (NSFC), one of the nation's main science funding organizations, Yang is setting the bar high for China's scientific research enterprise. He's also not afraid to tell it like it is.

He wants to boost the quality of his nation's basic scientific research and raise the significance and applicability of that research. At the same time, Yang is waging a campaign to persuade Chinese scientists to adhere to a high level of research integrity.

China already has a great head start: The nation's scientific research output has risen dramatically in recent years, Yang says. He notes, for example, that the country's share of research papers worldwide, according to Elsevier's Scopus database, grew from 2.5% in 1997 to 18.8% in 2015.

"But that does not necessarily mean our contributions are original and significant," he asserts. Yang, who also serves as a professor of engineering mechanics at Zhejiang University, explains that research institutes' traditional emphasis on publication numbers often leads scientists in China to write numerous "incremental papers rather than a few good ones." As a result, some observers say China's universities have become "paper mills" that are driven to value quantity over quality.

Yang sees some truth in that criticism. He points out that few chemical reactions or processes are named for Chinese chemists, even though chemists in China author large numbers of scholarly papers. He also notes that citations of Chinese publications lag behind those of other countries, according to citation indexes. And thus far, only one mainland Chinese scientist has been honored with a Nobel Prize in science.

Still, by many measures, the quality of China's research output is improving, Yang says. For example, the Scopus index shows that China's share of high-impact papers—the top 0.1%, judging by number of citations—measured less than 1% in 1997. Now the value stands at nearly 20%.

That trend holds true for chemistry. In the early 1990s, researchers at Chinese institutions published very few papers in the *Journal of the American Chemical Society*. Now China has grown to become the largest JACS contributor outside of North America.

In Yang's view, however, that progress is insufficient to put Chi-



Vitals

- ▶ **Age:** 62
- ▶ **Education:** B.S., 1976, Northwestern Polytechnical University, Xi'an, China; M.S., 1981, Tsinghua University; Ph.D., 1985, Brown University
- ▶ **Career highlights:** president, Zhejiang University, 2006–13; member, Chinese Academy of Sciences, 2003– ; president, National Natural Science Foundation of China (NSFC), 2013–
- ▶ **Current job:** overseeing NSFC's funding of basic research, set at \$3.7 billion in 2016
- ▶ **Technical areas of expertise:** fracture and failure mechanics

na on track to meet the goals enumerated by the nation's central government this past spring. "China wants to become a global powerhouse in science and technology over the next 35 years," Yang says. The aim is to meet various milestones along the way.

By 2020, China seeks to become "an innovative country and important player" in science and technology, producing research that scientists elsewhere adopt broadly. China is headed in that direction, but is not yet there, Yang says. "We want to achieve 'global powerhouse' status by 2050."

To get there, Yang says, China needs to stimulate its researchers to make scientific breakthroughs by investing heavily in important fundamental research. It also will require research independence for investigators who show promise and originality.

Regarding the level of support, NSFC's research grant allocations have grown 300-fold since the agency was founded in 1986. In that year, NSFC doled out \$12 million for basic research. In 2016, allocations reached \$3.7 billion. "I'd like us to grow even faster and maintain double-digit increases every year," Yang says.

It's not so clear his wish will come true. As Yang notes, it's hard in China—as it is in most nations—to convince government officials and the people alike that investigations in areas of fundamental science are valuable to society. "Some people see the value in basic research, but not most people. They think cell phones are useful. Not number theory."

Also, it'll take more than just increasing NSFC's allocation budget to put China on a path toward meeting its goals. The agency must divvy up research funds in the way

that best stimulates Chinese scientific innovation.

With that goal in mind, NSFC currently appropriates some 70% of its funds to support “blue-skies research,” Yang says. These kinds of research projects are driven by curiosity and not necessarily aimed at commercial applications or products. Also, they’re proposed by working scientists, not government committees. Another 10% of the budget supports “talent,” meaning the funds are given to promising scientists with impressive research track records to use as they see fit. The remaining 20% goes to major projects and research facilities.

Regardless of the size of the funding pot and the way in which grant money gets distributed, Yang argues that the success of China’s research enterprise also depends on the integrity of the nation’s scientists.

That’s why Yang has focused attention on combatting scientific misconduct in China. Such misconduct comes in many forms, Yang says, and may be unintentionally encouraged by institutions relying too heavily on quantitative rather than qualitative measures of merit. Violations include plagiarism and fabrication and falsification of data. There are also less severe infractions, such as needlessly dividing studies into multiple pieces to inflate publication

numbers, unwarranted self-citing to boost citation ratings, and colluding with colleagues for mutual citations.

During his seven-year tenure as president of Zhejiang University, Yang dealt with more than 20 cases of research ethics violations. He earned a reputation for leading a crusade to curb scientific misconduct and for developing training programs to promote scientific integrity.

China’s Ministry of Education and leading science organizations, including the China Association for Science & Technology and the Chinese Academy of Sciences, all embrace strict codes of research ethics now and broadly support scientific ethics education for faculty, students, and postdocs.

“Ethics violations hinder China’s growth in original science and dampen the impact of science developed in China,” Yang says. “Quality needs to matter more than quantity, and integrity is the best way to ensure quality.”

Looking back on the winding path that brought Yang to the helm of NSFC, he says he never expected China to explode onto

the world science scene as it has in recent years. At age 14, Yang, a Beijing resident, got caught up in China’s tumultuous Cultural Revolution. Along with many urban youngsters, he spent five years in China’s countryside doing hard manual farm labor.

Like some of his fellow laborers, Yang was determined to get a formal education. He studied on his own while doing farm work and mastered enough high school material to be accepted to an engineering college. The chaos of that era delayed Yang’s education, but he eventually pursued graduate studies. He received a master’s degree in China, and then went to the U.S. and completed a Ph.D. at Brown University in 1985 at age 31.

Science in China has come a long way since Yang was a student. “We couldn’t have had any idea 30 years ago what things would be like here today,” he says. Without the benefit of a crystal ball, Yang also doesn’t know what the next 30 years will bring, but he’s doing his part to move science in China forward. “China has made a lot of progress, but we still have a long way to go.” ■

“Quality needs to matter more than quantity, and integrity is the best way to ensure quality.”



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The case for science emoji

Chemists who find meaning in the symbolic characters seek greater representation for their field

JESSICA MORRISON, C&EN WASHINGTON

You're firing off a punchy text about your day to a friend or colleague—but wait, there's no petri dish emoji. You scroll through your phone's keyboard looking for a flask or a lab coat. No luck. The nerd face, sweat droplets, and microscope emoji will have to do until a set of science emoji arrive.

Emoji have been around since the late 1990s, starting as graphical renditions of earlier emoticons, such as :-) and :-(. In recent years, the expressive icons have grown in popularity thanks in part to the ubiquity of smartphones, which contain dedicated keyboards for the characters. Some chemists disparage emoji as “illiteracy-promoting drivel,” while others view them as a way to express sentiment that transcends linguistic, cultural, and generational barriers.

The faces, gestures, and trove of digital objects that now comprise nearly 1,100 emoji characters have made their mark on popular culture. In 2015, the “face with tears of joy” emoji had the highest global usage of any emoji, and Oxford Dictionaries named it word of the year.

Emoji have broad appeal, says Jennifer 8. Lee, organizer of Emojicon, the first emoji-themed conference, and cocreator of the dumpling emoji that is expected to come to keyboards in 2017. “We're all communicating with the same vocabulary.”

The limited number of emoji creates constraint and the possibility for various interpretations, Lee says. That makes communicating with emoji interesting, she adds.

The options for communicating science by emoji are currently limited. Fewer than a dozen explicitly represent science. Among these are equipment: a microscope, a telescope, and an alembic (an alchemical still used for distillation). A lab-coat-wearing scientist emoji, proposed by a team at Google, will come out in 2017 in a set of career-focused emoji that includes a farmer, a cook, a teacher, a mechanic, and an artist.

Symbols of science

Unicode currently contains nearly 1,100 emoji, a handful of which represent science, including:



Microscope



Telescope



Alembic



Comet



Rocket



Milky Way



Atom symbol



Radioactive symbol



Biohazard symbol

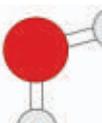
More could be on the way. These are a few of those that have been proposed:



Goggles



Lab coat



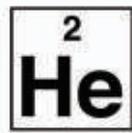
Molecule



Bunsen burner



Petri dish



Helium element tile



Fire extinguisher



Erlenmeyer flask



DNA



Microbe

Rose Yen, a chemist at San Francisco-based Rigel Pharmaceuticals, says an appreciation and understanding of how symbolic imagery reflects culture can have broad impact.

“Science emoji can convey that science is more than just” a career, Yen says. Science can be powerful, but also fun, she adds. “I would like to see that representation assimilated more into our culture.”

About 1,000 people showed up at Emojicon, held in San Francisco earlier this month. Yen and I were among them. I saw

emoji balloon animals and poop emoji-themed soap dispensers. I even competed in an emoji spelling bee. But the main reason I was at Emojicon was to participate in a hackathon—an event where people get together to work on digital projects that sometimes lasts multiple days and continues around the clock.

During that hackathon, our team of scientists and designers proposed a set of science emoji. They include laboratory science mainstays such as goggles, a lab coat, a petri dish, a Bunsen burner, and an Erlenmeyer flask.

But don't expect to see them anytime soon. Proposals for new emoji must be reviewed and approved by the Unicode Consortium, a nonprofit that develops and maintains software standards used internationally. The process for proposing new emoji can be lengthy. Even if accepted, a new emoji may not appear in phone keyboards for years.

The proposal to include more science in the Unicode emoji builds on other efforts to inject more emoji into science. Last year, the American Chemical Society, which publishes C&EN, created ACS Chemoji, a set of chemistry-themed digital stickers. And in late 2014, General Electric launched Emoji Science, a campaign that includes a periodic table of emoji and a series of videos that explain science concepts using emoji.

“We began the campaign as a way to demystify science through the language of emoji,” says Nancy Briscoe, audience development manager for GE, which was a corporate sponsor for Emojicon. Science emoji—like those proposed at Emojicon—would boost science's role in modern conversation, she adds.

C&EN wants to know about the creative ways that you use emoji to describe your work and experiences. Go online to tell us more in the comments or on social media using the hashtag #ACSSchemoji. ■

More
online



Can't wait for science emoji? Get our chemistry-themed ACS Chemoji stickers today at cenm.ag/chemoji.

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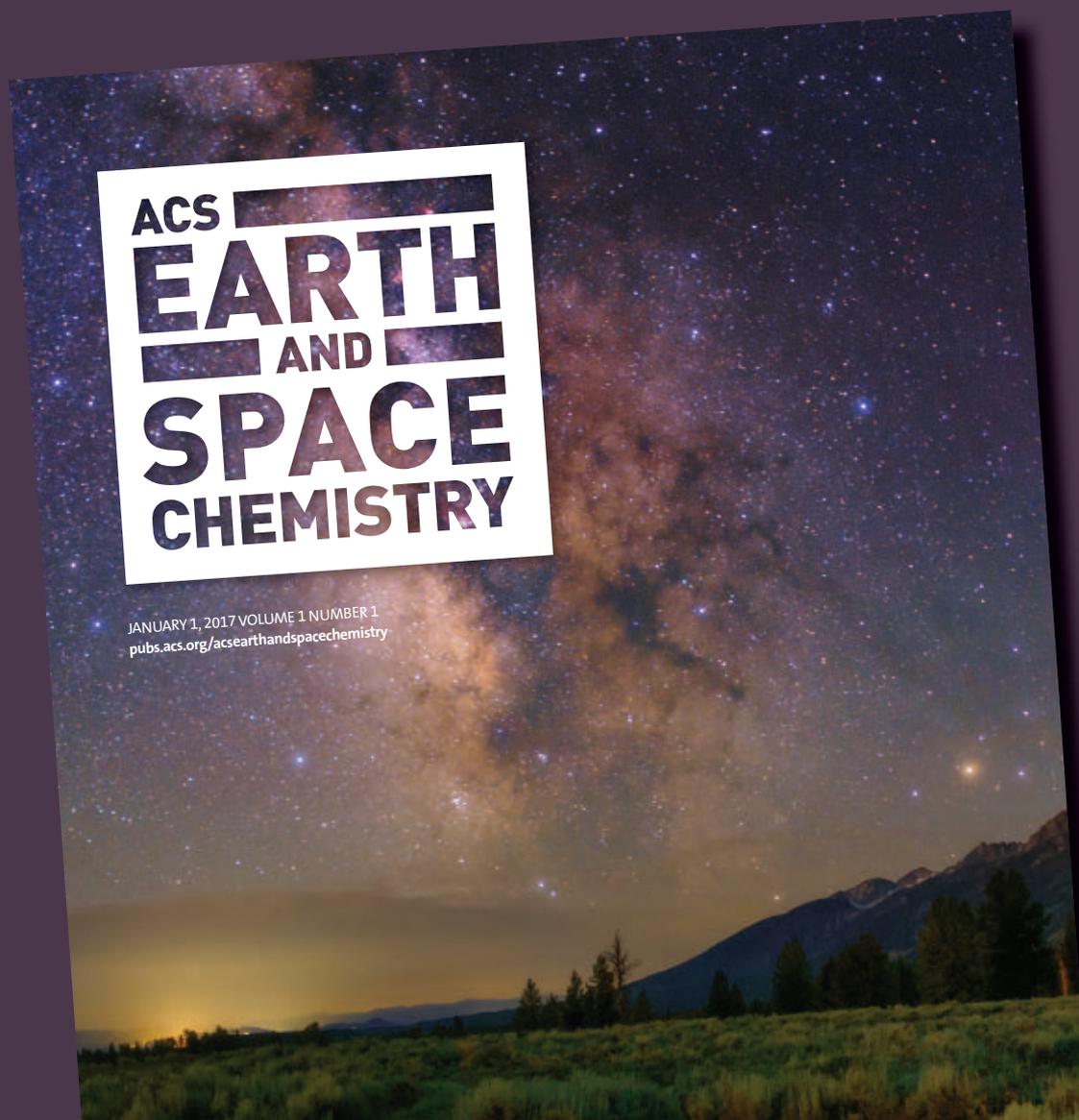


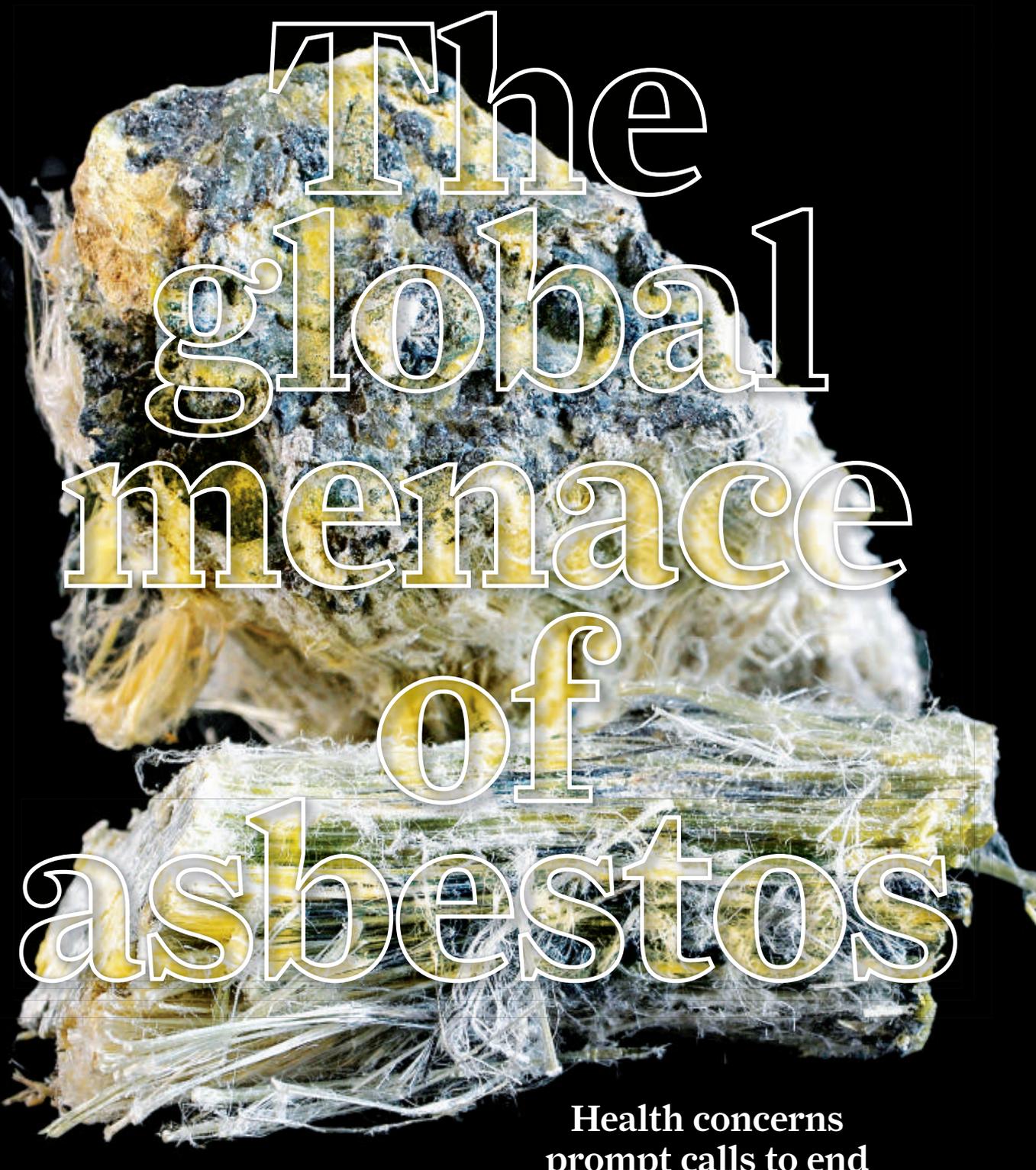
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The global menace of asbestos

BRITT E. ERICKSON,
C&EN WASHINGTON

**Health concerns
prompt calls to end
production and use of
deadly substance in
the U.S. and beyond**



As a 7-year-old child in suburban Sydney, Australia, Serafina Salucci recalls playing with white wall sheeting material leftover from her dad's renovation of the family's garage. She used it like chalk to draw on the

driveway, and threw chunks of it back and forth with her brothers. Little did anyone know at the time that the sheeting contained carcinogenic asbestos fibers that would later be blamed for giving Salucci mesothelioma, an incurable cancer attacking the lining of her lungs.

Salucci was diagnosed with mesothelioma in 2007, 30 years after her likely exposure to asbestos. She has outlived her doctor's prognosis and now spends her time raising awareness about the disease and the threat of asbestos in older buildings like houses, hospitals, and schools. If asbestos fibers become airborne, there's a risk of exposure, she says. "We must safely get rid of it."

Salucci joined hundreds of other people seeking to eradicate asbestos exposure around the world at an Australian government conference earlier this month. Production and use of asbestos was banned in Australia in 2003, but approximately one-third of all homes in the country contain the substance. Australia had the highest per capita rate of asbestos use in the world from the 1950s to the 1970s.

Salucci, now 47, is one of hundreds of Australians diagnosed with mesothelioma every year. Like many other kids that grew up during the 1960s and 1970s, she never worked around asbestos nor did any home renovations herself. She was exposed to asbestos while playing as a child.

While Australia, like many other countries, faces huge challenges related to its former use of asbestos, more than 100 countries face even greater problems because they have yet to ban the fibrous material. The U.S., Canada, and many countries in the Asia-Pacific region, for instance, still allow some use of asbestos, despite the substance's known adverse health effects.

That could all be about to change, however, as regulators face mounting calls from trade unions, patient advocacy groups, and environmental activists to cut off any further use of the material. Such groups are urging the liberal Canadian government, which took office last year, to keep its campaign promise and ban all uses of asbestos. In the U.S., recent changes to the law that governs commercial chemicals have prompted ac-

tivists to intensify pressure on the Environmental Protection Agency to do the same.

The problem with asbestos

Asbestos is defined by regulators worldwide as a group of six naturally occurring fibrous silicate minerals—actinolite, amosite, anthophyllite, chrysotile, crocidolite, and tremolite (see page 30). More than 90% of all asbestos used historically and nearly all of it used today is chrysotile, according to the World Health Organization (WHO).

The substance was once mined and used extensively throughout the world in a wide range of construction materials and other consumer products, including thermal insulation, vinyl floor tiles, cement sheeting, brake pads, gaskets, and roofing materials. Although these products are now banned in many countries, they still remain as so-called legacy sources in homes and other buildings or lurk in hazardous waste sites.

Asbestos is known for its high tensile strength, flexibility, and resistance to heat and chemicals. But those same properties make it deadly when its fibers get lodged within the human lung. Inhalation of asbestos has been linked to the mesothelioma that Salucci battles, as well as lung cancer and asbestosis, which is a severe scarring of the lungs.

Worldwide, more than 100,000 people die each year from occupational exposure to asbestos, and hundreds more die each year from nonoccupational exposures, according to WHO.

Iceland became the first country to ban the production and use of all types of asbestos in 1983. Since then, more than 50 countries have followed suit, according to the International Ban Asbestos Secretariat, an advocacy group founded in 1999 that seeks to prohibit production and use of asbestos worldwide.

In brief

More than 50 countries around the world have banned the use of asbestos, a known human carcinogen linked to lung cancer, mesothelioma, and other diseases. But two Western industrialized countries—the U.S. and Canada—have not taken such steps. Anti-asbestos activists are ramping up pressure on regulators in the U.S. and elsewhere to stop the production and use of the fibrous material. Meanwhile, scientists would like to better understand the basic science of the substance in order to deal with remediation at hazardous sites and to treat those who are susceptible to asbestos-related diseases. An NIH-funded research center at the University of Pennsylvania is leading the charge (see page 32).

Asbestos and U.S. law

The U.S. EPA banned most uses of asbestos in 1989 under the Toxic Substances Control Act (TSCA). Industry sued, however, and in 1991, a federal appeals court overturned the regulation.

Now that TSCA has been revised, an action that was signed into law on June 22, EPA faces renewed pressure to use its new authority to ban all uses of asbestos in the U.S. Pushing the agency to do so are federal lawmakers, environmental and public health groups, and the motor equipment manufacturing industry. Many observers view asbestos as the poster child for why this year's congressional overhaul of TSCA was needed.

"EPA spent more than a decade developing a rule to ban existing uses of asbestos," recalls Richard Denison, a lead senior scientist at the Environmental Defense Fund, an advocacy group. In the 1980s, it sunk millions of dollars into the effort and compiled nearly 100,000 pages of documentation showing why the ban was needed. Nonetheless, the court ruled that EPA had not demonstrated what was legally required under TSCA to justify regulation. Denison says EPA is likely to have an easier time justifying a ban on asbestos under the revised TSCA.

That's because under TSCA as it was originally passed in 1976, EPA had to show that the benefits of regulation outweigh the costs. The agency also had to show that restriction of each use was the least burdensome way to reduce the risk. The new law forbids EPA from considering costs when determining whether a chemical poses an "unreasonable risk." It also strikes the "least burdensome" requirement, allowing EPA to restrict a chemical "to the extent necessary" to reduce the risk.

The chemical industry is anxiously waiting to see whether EPA will include asbestos in the first group of chemicals it reassesses under the revised TSCA. Under that new law, Congress gave EPA until Dec. 22 to choose 10 high-risk chemicals that are currently on the market for further risk evaluation. Those 10 must be taken from a list of about 90 chemicals that EPA has already designated as high-priority substances. Asbestos is one of those 90.

Chlor-alkali industry and asbestos

Although asbestos use in the U.S. has declined by 99% since the 1970s, when there was extensive litigation around its adverse health effects, the chlor-alkali industry still uses asbestos diaphragms to produce chlorine. The process involves passing an electric current through a NaCl solution in

Asbestos 101

Asbestos is a group of six fibrous silicate minerals known for their high tensile strength, flexibility, and resistance to heat and chemicals.



Chrysotile: $Mg_3(Si_2O_5)(OH)_4$. Has been used more than any other type of asbestos. Accounts for most of the asbestos found in U.S. and Canadian buildings.



Amosite: $Fe_7Si_8O_{22}(OH)_2$. Mined predominantly in South Africa.



Crocidolite: $Na_2(Fe^{2+}3Fe^{3+}_2)Si_8O_{22}(OH)_2$. Often referred to as blue asbestos. Considered the most hazardous form of the six minerals.



Tremolite: $Ca_2(Mg_{5.0-4.5}Fe^{2+}_{0.0-0.5})Si_8O_{22}(OH)_2$. Typically found as a contaminant in vermiculite, chrysotile, and talc. Responsible for asbestos-related ailments in Libby, Mont.



Anthophyllite: $Mg_2Mg_5Si_8O_{22}(OH)_2$. Formerly mined in Finland and Japan.



Actinolite: $Ca_2(Mg_{4.5-2.5}Fe^{2+}_{0.5-2.5})Si_8O_{22}(OH)_2$. Formerly mined in Australia.

125 million

The number of people worldwide who are exposed to asbestos in the workplace each year.

>100,000

The number of people who die each year from asbestos-related diseases linked to occupational exposures.

2.0 million metric tons

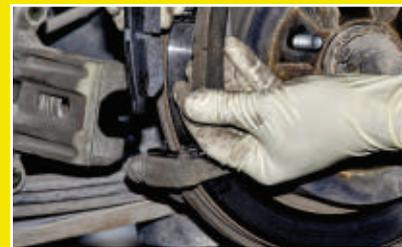
The amount of asbestos mined globally each year. The U.S. stopped mining asbestos in 2002 because of public health concerns.

Sources: World Health Organization, U.S. Geological Survey

Despite health concerns, asbestos is still found in many places.



For example, many buildings throughout the world still have corrugated roofing materials made with asbestos.



Meanwhile, countries that have banned certain asbestos-containing products, such as brake pads, still struggle to control illegal imports.

an electrolytic cell. The diaphragm separates the anode from the cathode, preventing OH⁻ generated at the cathode from reacting with the chlorine gas generated at the anode.

The chlor-alkali industry is phasing out the use of asbestos-based diaphragms. Newer industrial plants have replaced them with ion-exchange membranes, which require less energy and have less environmental impact. But such technology is more expensive to replace than asbestos-based diaphragms, so much of the industry has been reluctant to switch.

About 60% of the U.S. chlor-alkali industry still uses asbestos diaphragms, according to the American Chemistry Council's Chlorine Chemistry Division, which represents chlorine manufacturers.

Chemical companies were successful in getting EPA to make an exception for the chlor-alkali process in the agency's now-defunct 1989 ban of asbestos. So too were they successful in getting an exemption when asbestos was banned in the European Union in 2005.

The chlor-alkali industry uses most of the asbestos sold in the U.S.—about 90%, according to the U.S. Geological Survey. USGS figures show approximately 360 metric tons of asbestos was imported and consumed in the U.S. in 2015.

Today, as EPA is under pressure to revisit the safety of asbestos under the revised TSCA, the U.S. chemical industry is once again urging regulators not to impose restrictions on chlor-alkali manufacturers.

“Because the use of asbestos in the chlor-alkali industry is confined in the

production process, worker exposure risk is essentially eliminated,” ACC claimed in an August letter to EPA. In its 1989 rule, the agency concluded that “a ban on this product category would result in only minimal benefits because asbestos exposure is limited,” the lobbying group noted.

Anti-asbestos activists double down

Meanwhile, activists who want EPA to ban all uses of asbestos are ramping up their efforts to persuade the agency to include asbestos in the first group of chemicals it reassesses under the revised TSCA.

In a Nov. 9 letter to EPA Administrator Gina McCarthy, international trade unions, patient advocacy groups, environmental activists, and others who want to rid society of asbestos urged EPA to act quickly to ban all uses of the substance. The groups, led by the Asbestos Disease Awareness Organization (ADAO), are concerned that President-Elect Donald Trump will eviscerate EPA and hamstring the agency's efforts to ban dangerous chemicals.

Trump has “made clear, time and time again, his affinity for continuing the use of asbestos,” says Linda Reinstein, cofounder of ADAO. Reinstein began raising awareness about the dangers of asbestos after her husband, Alan, was diagnosed with mesothelioma in 2003. “Trump's Administration could well usher in a resurgence in rampant use of this known human carcinogen by encouraging development and further deregulating industry,” she says.

Some U.S. lawmakers, including Sens. Barbara Boxer (D-Calif.), Dianne Feinstein (D-Calif.), Dick Durbin (D-Ill.), and Jon Tester (D-Mont.), are also pushing EPA to act swiftly to ban asbestos. “Now that the impediments in the original TSCA law are gone, completing the job started by EPA in 1989 would send a strong signal that the new law can be effective in addressing the most dangerous chemicals in commerce,” Boxer writes in an August letter to EPA. Boxer's letter also raises concerns about asbestos-containing products being imported into the U.S. at various ports.

There have been reports of asbestos-containing brake pads and insulation tiles being imported into the U.S., Denison says. Because of these imports, at least two states, California and Washington, have banned asbestos-containing brake pads, he says.

Imports of asbestos-containing products are a growing problem worldwide, said several participants at the conference Salucci attended in Australia. During that meeting, trade unions representing workers across Australia posted on Twitter about the need for more action to stop illegal asbestos imports. “E-commerce and complex supply chains make testing for asbestos at our borders a nightmare,” tweeted Australia's Electrical Trades Union, which represents electrical and communications workers.

To prevent more people from being exposed to asbestos, governments around the world need to stop the production of asbestos, Salucci warned during a panel discussion at the meeting. “We need to tackle the global problem,” she said. ■

Asbestos in the wild

In the past, most concern about asbestos was related to exposure on the job or from buildings that contain the fibrous material. But in some places, such as parts of the western U.S., asbestos and asbestos-like minerals in the environment can be just as worrying. These minerals, which are found in the rock and soil, can become airborne by construction-site digging or even wind.

As commercial development expands in areas where the soil geology permits the formation of asbestos, human exposure to this substance increases, says Christopher Weis, toxicology liaison at the National Institute of Environmental Health Sciences. Such development, he says, includes hydraulic fracturing operations in North Dakota and highway construction in the Las Vegas area.

Rodney Metcalf and Brenda J. Buck, geologists at the University of Nevada, Las Vegas, are mapping the distribution of asbestiform minerals in that state, where such minerals are part of the bedrock. Through wind and water erosion,

asbestos is distributed across the landscape in soil and dust.

“Out here, you don't need a big bulldozer to disturb it. You just need a windy day,” Buck says. “Sand, silt, gravel, dust—it all has asbestos in it.”

In their mapping project, Metcalf and Buck have found areas with unexpectedly high levels of asbestiform minerals.

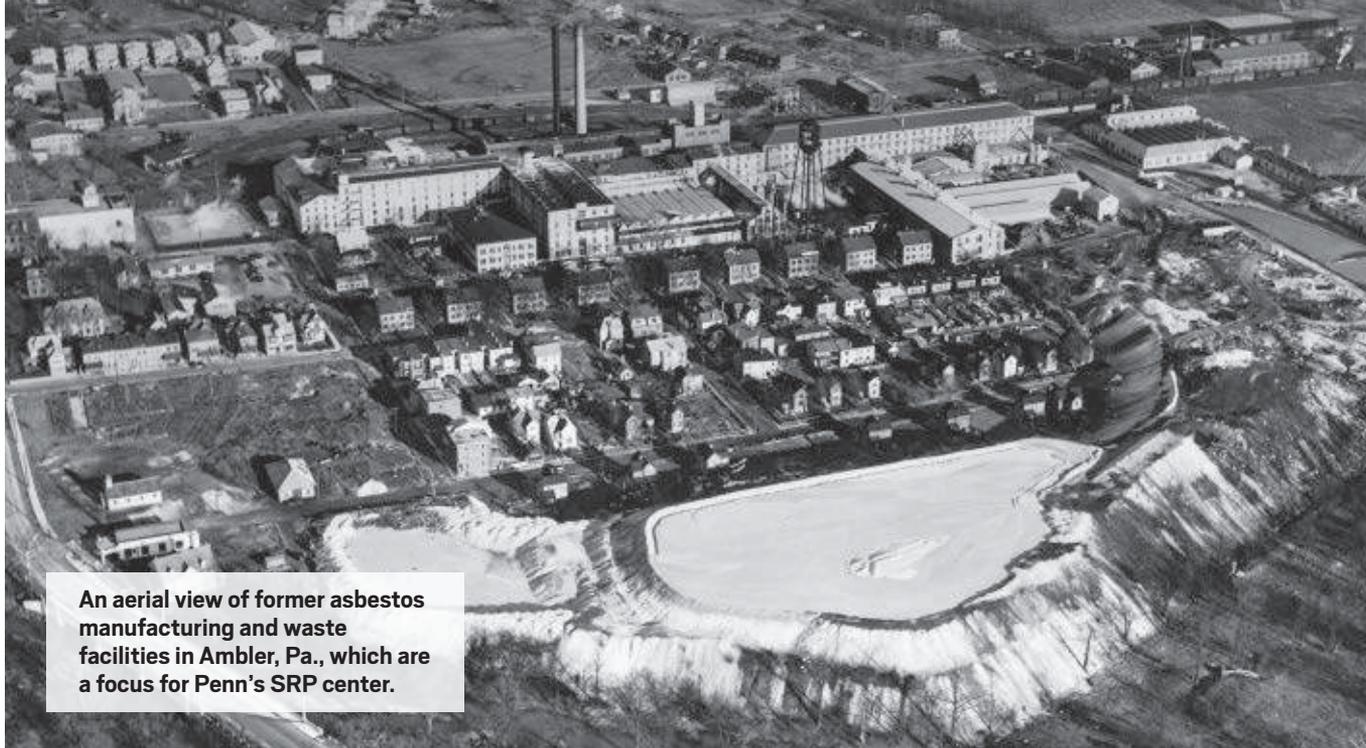
“The old models for geologic predictions about where we would find it wouldn't have predicted this,” Metcalf says. Those models were designed to locate concentrations high enough to support mining. The levels researchers are now finding aren't that concentrated, but they represent “a fairly sizable footprint of low-concentration asbestos.”

And some areas have the potential to affect people who might not otherwise be exposed to asbestos. “There's a dry lake bed that's a favorite place for driving off-road vehicles that has quite a bit of asbestos in it,” Buck says.

People can protect themselves by avoiding those areas. “If you're an off-road driver, don't drive on that lake bed. Go to a different one where asbestos hasn't been found or isn't predicted to occur.”—CELIA ARNAUD



In arid regions of the western U.S., asbestos can be carried by wind in dust storms. Shown here is a view looking south from the University of Nevada, Las Vegas.



An aerial view of former asbestos manufacturing and waste facilities in Ambler, Pa., which are a focus for Penn's SRP center.

PUBLIC HEALTH

Attacking asbestos from all angles

University of Pennsylvania research center addresses aspects from environmental containment to health effects

CELIA HENRY ARNAUD, C&EN WASHINGTON

Ads in which a lawyer talks about compensation for asbestos exposure and mesothelioma have been a television mainstay in the U.S. for a long time. Watching those, one might assume that the science of asbestos—how it's formed, how it's transported in the environment, and how it causes lung cancers—is a closed book. It turns out, however, there's still lots to learn about the long, thin fibrous material.

Prized for its flame and heat resistance, asbestos was used for decades in products such as floor and ceiling tiles, wallboard, electrical insulation, and brake linings. Once the mineral's link to mesothelioma was established, the use of asbestos in the U.S. plummeted but never completely stopped. Many other countries banned new uses of asbestos minerals (see page 28).

Still, asbestos waste lingers at various sites across the globe, and buildings con-

Penn's SRP center at a glance

- ▶ **Year founded:** 2014, with a four-year grant from NIEHS
- ▶ **Number of affiliated researchers:** 16
- ▶ **Budget:** \$10 million

The center is structured around these six questions:

- ▶ Can asbestos be remediated?
- ▶ Is asbestos transported by water?
- ▶ What types of asbestos exposure played into the high incidence of mesothelioma seen in a former asbestos factory town?
- ▶ Is there a genetic predisposition to asbestos-induced mesothelioma?
- ▶ Can asbestos-induced mesothelioma be prevented?
- ▶ Can blood tests for asbestos exposure or mesothelioma be developed?

taining the material continue to age and decay. By some estimates, as many as 35 million homes in the U.S. harbor it.

"Asbestos kills at least 10,000 people a year in this country and many, many more worldwide," says Christopher Weis, toxicology liaison at the National Institute of Environmental Health Sciences (NIEHS). "There's ongoing exposure to asbestos that needs to be measured and studied—both general exposures in the ambient environment and specific areas of exposure."

Enter the Penn SRP center, an NIEHS-funded research program that focuses exclusively on the challenges still posed by asbestos. Its lengthier, formal name, the Superfund Research & Training Program at the University of Pennsylvania: Asbestos Fate, Exposure, Remediation & Adverse Health Effects, describes its purpose. The largest NIH-funded program dedicated to studying asbestos, Penn's SRP center aims to answer a multitude of scientific questions about the fibrous material, including how it is transported in the environment, how best to remediate it, and how exposure causes health effects.

The center grew out of a relationship between professors at Penn's Center of Excellence in Environmental Toxicology and the

CREDIT: DALLIN AERIAL SURVEY COMPANY/HAGLEY MUSEUM AND LIBRARY

Community Advisory Group for the BoRit Superfund Site in Ambler, Pa. That site and the nearby Ambler Piles Superfund Site are the largest industrial waste sites for asbestos in the U.S. Another site in Libby, Mont., is larger, but it was a vermiculite mine that happened to contain large amounts of asbestos rather than being a designated asbestos manufacturing facility.

The Ambler sites, located just north of Philadelphia, were dumps for asbestos-containing waste from nearby facilities that manufactured asbestos-containing construction materials such as tiles, shingles, and pipes. The type of asbestos used there is chrysotile, a member of the curvy-shaped serpentine class of minerals. The last of the factories closed in 1987. The defunct facilities left behind huge piles of asbestos-containing materials that had accumulated over decades. At the Ambler Piles site, the color and height of some of the heaps earned them the nickname “White Mountains.”

Edward Emmett, an occupational medicine expert at Penn and onetime director of community outreach at Penn’s environmental toxicology center, is a member of the community advisory group for the BoRit site. In this role, he hears a lot about the community’s concerns about cleanup and remediation efforts. He realized there were scientific questions in those concerns.

“Communities can identify the issues, but they’re not good at identifying the precise scientific questions that need to be answered to help,” Emmett says. “We took those issues and formulated them into questions.” Six of them to be precise. The SRP center is organized around those questions. The goal is to make its findings relevant to Ambler and to other asbestos-contaminated sites around the world.

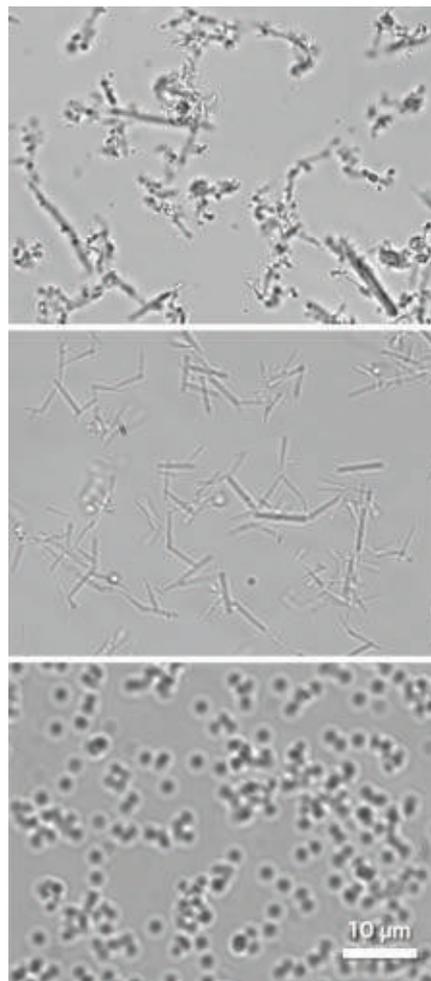
One of the SRP center’s six projects, led by plant biologist Brenda Casper, aims to figure out how best to revegetate the Ambler site. The asbestos piles are capped with a thick layer of soil intended to contain the asbestos. The right plants can help hold that soil in place. “The question is what types of soil additives to use and what types of plants to plant,” Casper says.

Rocky outcrops that contain serpentine minerals related to the chrysotile asbestos occur throughout the eastern U.S. “The first thing we did was go to serpentine sites to see if the plants that grew there would be better at growing on asbestos.”

Casper’s team planted seeds from grasses growing on the serpentine rocks in asbestos-containing soil. “We expected these seeds to do a lot better than commercial seeds we buy,” she says. But they didn’t. Apparently, the grasses evolved to handle the high metal content of the serpentine rocks,

so they tolerate well the serpentine soil but do not grow rapidly regardless of soil type.

As Casper’s team continues looking for plants to hold the soil in place, another group worries about whether buried asbestos can migrate through the soil. Geophysicist Douglas J. Jerolmack is studying the transport of asbestos and other fibers through water and soil. He had to start almost from scratch because little was known



Asbestos fibers (top) and glass rods (center) with similar aspect ratios and surface charges form similar aggregates. Both of them differ from the aggregates formed by glass spheres (bottom).

about the diffusion and aggregation behavior of asbestos and other rod-shaped colloids.

“When you look at research on the behavior of different species of asbestos, there was a lot of fundamental work on materials characterization and aggregation all through the 1970s,” Jerolmack says. “After asbestos got declared hazardous, fundamental research on asbestos just stopped.” Many modern-day materials characterization techniques haven’t been applied to asbestos, he says.

So his team started by looking at the diffusion of chrysotile asbestos fibers in water. Chrysotile is the most common type of asbestos in commercial use. The researchers found that fiber diffusion is size-dependent and agrees with predictions about how rod-shaped particles diffuse randomly (*Environ. Sci. Technol.* 2015, DOI: 10.1021/acs.est.5b03839).

Then they looked at how asbestos fibers cluster together. They compared the aggregation behavior of chrysotile asbestos fibers to that of glass spheres and glass rods—model objects. The glass rods had the same mass, size, aspect ratio, and surface charge as the asbestos fibers. “We found that the glass rods behaved identically to the asbestos fibers, and both of them were fundamentally distinct in their growth and aggregate structure from anything that had been reported before,” Jerolmack says.

They both behaved differently from the glass spheres, leading Jerolmack to believe that shape plays a significant role in aggregation behavior. He also thinks that the results may be applicable to other rod-shaped materials, such as carbon nanotubes, which are also an inhalation concern.

Jerolmack’s ultimate goal is to be able to do field studies in Ambler.

“There are so many open questions that I didn’t feel the wise thing to do first was a field campaign,” he says. “We need to be educated in the way we go about sampling in the environment. We could start taking samples willy-nilly, but it’s hard to isolate low concentrations of asbestos fibers in soil and water. Based on what we’ve learned, we now have an idea of how solution chemistry may influence the aggregates.” His team is using that information to design a field sampling campaign to see whether any of the capped asbestos in Ambler has migrated.

The Ambler community is worried about whether the asbestos can migrate through groundwater to nearby Wissahickon Creek.

“We don’t have any reason to believe right now that there’s been significant migration of the asbestos fibers through groundwater,” Jerolmack says. There have been some reports of asbestos fibers in the water, but because there are naturally occurring outcrops in the area, it’s not clear whether those fibers come from the Superfund site or natural sources, he adds.

The main reason the SRP center’s scientists and the surrounding community are concerned about asbestos’s containment and migration is its potential health effects. As a result, the center has focused four of its six projects on studying these.

One of the health-related projects is taking a historical look at the incidence of asbestos-related diseases in Ambler. Frances

K. Barg, Emmett, and coworkers are mining census data from 1930, a period of peak asbestos production in Ambler, to determine who among the people who lived in the area later developed an asbestos-related disease.

"We know who was there and where they were living. Did they work with asbestos? Did they live in a family with someone who did?" Emmett says. "We're looking to see what happened to those people. What did they die of?"

The historical approach Emmett, Barg, and the team is using is necessary because "less than 1% of the mesotheliomas from asbestos occur in the first 15 years following exposure," Emmett says. "The rate increases until about 45 years after exposure and then it flattens out."

The availability of census records, which are released after 72 years, is a key piece of the study. "We know exactly the names, family name, spouses, time of birth, whether they worked in the factory," Emmett says.

One of the goals is to determine the importance of community exposure compared with occupational exposure. Does living in a community with asbestos lead to an increase in asbestos-related disease even for people who don't work with asbestos? If so, what factors contribute to that increase? Emmett and his team have been able to track down death records for about 2,000 people, just over half of the cohort, so far.

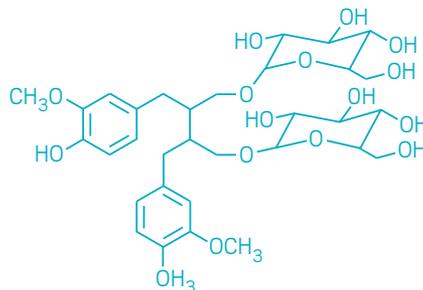
As the ethnographic study highlights, the long latency period for asbestos-related diseases is a challenge for studying such conditions. Joseph R. Testa, a geneticist at Fox Chase Cancer Center, is leading a project at the Penn center for developing animal models that can make it easier to study mesothelioma and potential prevention measures.

Testa's mesothelioma work predates the Penn center. By studying families with multiple cases of mesothelioma, he has discovered genetic mutations that can contribute to the development of the disease. He's identified mutations or deletions of the *BAP1*, *CDKN2A*, and *NF-2* tumor suppressor genes as being important for mesothelioma development.

Now he's using those mutations to genetically engineer mouse models of the disease. One type of mouse has a *BAP1* mutation. The other has both *CDKN2A* and *NF-2* mutations.

Testa uses the mice with two mutations to test potential protective agents because those mice develop mesothelioma quickly after asbestos exposure. "If they don't have a mutation, it takes about a year for the mesothelioma to become symptomatic," Testa says.

One limitation of the mouse models is that the researchers deliver the asbestos by



Researchers at Penn are studying a biphenolic from flaxseed, secoisolariciresinol diglucoside, as a potential chemopreventive for mesothelioma.

injection into the peritoneal space of the abdomen instead of by inhalation, which is the usual exposure route for humans. Nonetheless, with the mouse models, they see that crocidolite, a type of asbestos that's characterized by its needle like structure, is very carcinogenic. Chrysotile, though not as bad as crocidolite, is also carcinogenic in the mice.

Another Penn researcher, Melpo Christofidou-Solomidou, is using the mouse models to study asbestos fiber toxicity, which is strongly connected to inflammation. She's also evaluating antioxidants as a way to combat inflammatory processes in the lungs and other agents that might prevent lung cancers. She is especially interested in finding botanicals with protective properties. Botanicals could be nontoxic and attack multiple disease-related molecular pathways simultaneously, she says.

At the moment, she's got her sights set on the most bioactive component of the lignan component of flaxseed, a biphenolic called secoisolariciresinol diglucoside (SDG). In cell studies, SDG acts as a free-radical scavenger and decreases the release of inflammatory agents. It also activates *Nrf-2*, a gene that regulates the transcription of antioxidant enzymes.

Christofidou-Solomidou envisions using SDG as a prophylactic dietary supplement for people who know they have been or may be exposed to asbestos. But she acknowledges that such hopes are still premature. "A lot more studies need to happen. We have to go from mice to primates to man," she says. "There's a long regulatory pathway."

Diagnostic tools such as biomarkers are needed to help identify people who could benefit from intervention. Ian A. Blair, who is the director of the Penn SRP center, and coworkers are using high-resolution mass spectrometry to identify biomarkers of asbestos-related disease. They have analyzed blood serum samples from asbestos-exposed shipyard workers to identify

potential lipid and protein biomarkers of mesothelioma. They are focusing most closely on a protein called high-mobility group box-1, or HMGB-1, which is involved in inflammation. Other researchers have shown that the acetylated form of this protein is predictive of mesothelioma.

"We're developing a way to look at all the different acetylation states of HMGB-1," Blair says. The protein has 43 lysine residues as possible acetylation sites. Blair and his team want to be able to look at all the possible combinations of acetylation to see which ones are important.

They hope to eventually combine multiple biomarkers into a single assay. "Hopefully, along the way we'll discover a biomarker that's specific to asbestos exposure but not mesothelioma," Blair says. Such a marker could give people advance notice of whether they're at risk for these diseases that take so long to manifest themselves.

All this research is done with the needs of the community in mind, says Trevor M. Penning, deputy director of Penn's SRP center and director of the Center of Excellence in Environmental Toxicology.

"We pride ourselves on a model called community first communication. If we're doing community-engaged research, the community has a right to know about the results of our findings as soon as they've been vetted, rather than waiting for them to trickle down through peer review."

As far as Penning is concerned, the center's interdisciplinary training activities are as important as its research. "The individuals working on these projects come from different cultures and different perspectives on how to do their science," he says. "We put in place curricula and cross-training to allow these trainees to feel comfortable with the different components of working on Superfund hazardous waste."

And perhaps most important is the assistance the center can provide in policy decisions. "Often when we do bench-related science, we don't think about the impact of what we're doing in terms of public health policy and remediation strategies," Penning says. The research coming out of Penn's asbestos center, scientists there hope, could have near-term impact on the local governments that look after the Ambler sites.

But Penning sees the center's impact reaching the national level as well. "Congress needs to be informed that we have these problems that are going to impact public health," he says. "We're not allowed to lobby because we get federal dollars, but we can certainly provide persuasive information that might help in the decision-making process." ■

COMMENT

Teaching IUPAC recommendations

MICHAEL D. MOSHER, CHAIR, ACS COMMITTEE ON NOMENCLATURE, TERMINOLOGY & SYMBOLS

The Committee on Nomenclature, Terminology & Symbols (NTS) serves the American Chemical Society community through its review, recommendation, and action on matters related to the title of the committee. In the past, we have provided comments to the International Union of Pure & Applied Chemistry (IUPAC) and other organizations on issues of concern to chemists. Those comments reflect a desire to maintain a common core of units, nomenclature rules, definitions, and actions that can facilitate and ease communication among chemists across the world.

NTS encourages input and involvement from ACS members on fundamental issues such as these that impact our everyday work as chemists.

The standard temperature and pressure (STP) definition for gases as outlined in the "IUPAC Compendium of Chemical Terminology," 2nd Ed., also known as the "Gold Book," dictates the use of 273.15 K (0 °C) for standard temperature and 10⁵ pascals (1 bar) for standard pressure.

Prior to 1982, 1 atm (101,325 Pa) was commonly used to describe the standard pressure of a gas, and standard temperature values varied based upon the particular organization. For example, the National Institute of Standards & Technology (NIST) uses 293.15 K (20 °C) and 101.325 kPa (1 atm) to represent STP. The IUPAC recommendation in 1982 aligned STP more closely with the SI units developed by the International Bureau of Weights & Measures (BIPM). The BIPM proposed redefinition of the temperature unit, kelvin, does not change the numerical values of STP.

Although the use of 10⁵ Pa for the standard pressure for describing gases was recommended by IUPAC, its implementation has lagged in chemistry textbooks, particularly within general chemistry courses in the U.S. For example, many textbooks refer students to the use of atmospheres

in describing gases. The universal gas constant (R), to four significant digits, is then 0.08206 L·atm / mol·K. This causes a disconnection within a student's learning when they are asked to complete thermodynamic calculations using $R = 8.314 \text{ J / mol}\cdot\text{K}$.

Representing and performing calculations using the IUPAC recommended unit for pressure results in



Customs and preferences for reporting and communicating units should not be considered when educating our younger chemists.

$R = 8.314 \text{ L}\cdot\text{kPa} / \text{mol}\cdot\text{K}$. Thus, a more readily remembered value that is consistent with the

IUPAC recommendations is easily introduced. Students, then, only need to be concerned with the units of the universal gas constant based upon the type of calculation they are performing.

The use of the pascal as a unit for pressure in general chemistry curricula has limited impact on other topics in those courses. Because the density of a gas changes as the pressure changes, the molar volume of an ideal gas must be based on the IUPAC recommendations for STP. This results in a value of 22.71 L/mol (to four significant figures), rather than 22.41 L/mol with the NIST method. The difference, 1.3%, is reflective of the difference in the pressures (1 bar versus 1 atm) used to measure the molar volume.

Other pressure-related values, such as osmotic pressure, Π , and the gas equilibrium constant, K_p , are values that would have only limited adjustments based on the change to IUPAC units. Osmotic pressure would be reported in kilopascals or bar but would not fundamentally change as a result of the elimination of the unit atmosphere. The value of K_p would also not change because the terms of the mass action expression are taken relative to STP.

Other IUPAC recommendations are also overlooked when teaching general chemis-

try curricula in the U.S. Changes in thermodynamic units are typically introduced as a Greek delta, the thermodynamic unit, and the subscript for the process. For example, ΔH_{fus} is the symbolism currently used to represent the change in the enthalpy of fusion. That symbolism, under the recommendations of IUPAC, would be better written as $\Delta_{\text{fus}}H$. This representation is easy to read aloud. For example, $\Delta_{\text{vap}}S$ could be read

as "the change in the vaporization entropy."

Customs and preferences for reporting and communicating units should not be considered when educating our younger chemists. In fact, to many freshmen in college, even the use of the SI system appears foreign. Thus, why should we spend time to encourage the use of scientific language that includes units and symbols that are not commonly used among chemists across the world? Successful instances of change have occurred in the past. The conversion of energy terms from the calorie to the joule and the updating nomenclature of binary inorganic compounds containing transition metals proceeded quickly.

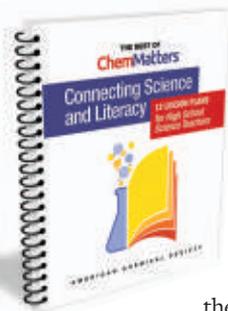
We, as chemists and educators of students of all ages, know that it seems counterproductive to teach a unit that is not commonly used and is not recommended by the scientific organization we entrust to provide uniformity in scientific communications. This is made even more counterproductive when we consider that many measurements are reported by instruments and software where the conversion into IUPAC recommendations is automatic.

NTS welcomes your input on any issue associated with nomenclature, terminology, or symbols. E-mail me at michael.mosher@unco.edu.

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

► Best of ChemMatters in the classroom

High school chemistry teachers now have access to a new set of teacher-tested lesson plans thanks to a book based on articles published in *ChemMatters*, ACS's magazine for teaching scientific literacy in the high school classroom. Topics covered in *ChemMatters* articles include Hollywood's special effects, the chemicals that give food its flavor, and sports supplements.



The new book, "The Best of *ChemMatters*: Connecting Science and Literacy," was developed by the ACS Education Division and consists of 12 lesson plans. For example, in the "Many Colors of Blood" lesson, students first read

the original *ChemMatters* article and then compare and contrast respiratory pigments found in the blood of various animals. The lesson can be downloaded at goo.gl/CPx1To (under "Sample Lesson Plan"), where the book is available for purchase.

The book can serve as a springboard for teachers to help students understand chemistry concepts and improve their scientific literacy, critical thinking, and reading comprehension skills.—LINDA WANG

► ACS International Center hosts discussion on creating a global workforce

On Sept. 29, the ACS International Center hosted a conversation by Rebecca Keiser, head of the Office of International Science



Rebecca Keiser gives a talk hosted by the ACS International Center.

ACS in Cuba

The Ernest Eliel Workshop—U.S. & Cuba Collaboration in Chemistry Education & Neglected Disease Drug Discovery took place at the University of Havana on Oct. 17–21. The workshop was a follow-up to then ACS President Diane Grob Schmidt's 2015 presidential visit to Cuba, discussions with the Cuban Chemical Society, and a symposium on U.S.-Cuba collaboration at the 2015 ACS national meeting in Boston. The workshop aimed to foster collaborations between Cuba and the U.S. and build on Indiana University-Purdue University Indianapolis (IUPUI)'s Distributed Drug Discovery (D3) program linking science education to neglected disease drug discovery. Activities comprised lectures by U.S. and Cuban scientists and students, hands-on laboratory experiments led by U.S. students, and collaborative research discussions. The workshop was funded by a \$3,000 ACS Global Innovation Grant awarded to the ACS Indiana Section. The funding was supplemented by an additional \$3,000 grant from IUPUI, as well as funding from Santa Clara University and Colorado College, which also participated in the workshop. Pictured here are attendees at the University of Havana.—LINDA WANG



& Engineering at NSF, on international science and the future of the global workforce. Her talk, "International Collaboration at the National Science Foundation: Expanding the Frontiers of Research & Creating a Globally Engaged Workforce," is available on the ACS International Center website at global.acs.org.

The ACS International Center is an online portal hosted by ACS to encourage global collaboration in the science, technology, engineering, and mathematics (STEM) fields and provide access to resources and opportunities to help prepare chemistry practitioners to be successful in the global workforce. The portal currently features postings of more than 600 research opportunities around the world.—CHRISTOPHER LAPRADE, ACS international activities manager

► Philadelphia technical presentations online

Technical recordings from the fall 2016 ACS national meeting in Philadelphia are now available to ACS members on the ACS Presentations on Demand website, presentations.acs.org. Users can search by title, meeting, topic, or speaker. Presentations on Demand Shorts, which are three- to five-minute condensed video versions of full lectures, are also available for download.—LINDA WANG

► Philadelphia committee reports now available

The official reports of ACS committees from the fall 2016 ACS national meeting, held in Philadelphia on Aug. 21–25, are now available online at goo.gl/xTNRC5. The major actions taken by the ACS Board and Council during the Philadelphia meeting were previously reported in *C&EN* (Aug. 29, page 5).—LINDA WANG

► ACS recognizes Genentech's support of ACS Scholars Program and Project SEED

The ACS Development Office held an event on Sept. 26 at Genentech in South San Francisco to recognize the company's role as a partner-level supporter of the ACS Scholars Program and Project SEED, which are two of ACS's educational programs to support chemistry students from underrepresented minority groups.

During the event, current and former ACS Scholars spoke of the impact the program has had on their lives, and Carolyn Bertozzi of Stanford University gave a talk titled "New Avenues for Cancer Immune Therapy Targeting the Glycocalyx."—LINDA WANG

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INORGANIC CHEMISTRY - KANSAS STATE UNIVERSITY

The Department of Chemistry (www.ksu.edu/chem) invites applications for a tenure-track position in Synthetic Inorganic Chemistry at the rank of Assistant Professor to begin in August 2017. A Ph.D. in chemistry and postdoctoral experience are required. The successful candidate will be expected to establish a creative and vibrant research program that attracts extramural funding and capable co-workers; s/he will also be expected to excel in teaching to a diverse population at the graduate and undergraduate levels. Applicants should submit their application as one **(1) complete pdf file** that includes a letter of interest, a curriculum vitae, descriptions of proposed research, a statement of teaching philosophy, and names and email contact information of three references at this website <http://careers.k-state.edu/cw/en-us/job/497904/assistant-professor>. Informal inquiries about the position can be made to the Chair of the Search Committee, University Distinguished Professor **Christer Aakeröy** (aakeroy@ksu.edu), Department of Chemistry, 213 CBC Building, Kansas State University, Manhattan KS 66506. Screening of applications will begin on January 16, 2017, and will continue until the position is filled.

Kansas State University is an Equal Opportunity Employer and actively seeks diversity among its employees. In accordance with Board of Regents policy, a background check will be required for the successful candidate. <http://chemistryjobs.acs.org/jobs/8592240>.

OREGON STATE UNIVERSITY, Department of Chemistry is seeking applicants for a 12-month, full-time, Research Associate (Post Doc). Salary is commensurate with education and experience. Required qualifications include PhD in Nuclear Chemistry or Nuclear Physics and experience in fission studies. Applicants should have a minimum of three years research experience, including research leading to the doctoral thesis. To review posting and apply, go to <http://oregonstate.edu/jobs>. Apply to posting # P00791UF. Closing date is December 31, 2016. OSU is an AA/EOE/Vets/Disabled. <http://chemistryjobs.acs.org/jobs/8612092>.

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Additional information is available from **Dr. Elsa Reichmanis**, chair of the search committee (ereichmanis@chbe.gatech.edu). Nominations should be directed to the chair of the search committee. Applications, including a cover letter, curriculum vitae, statement of research interests and plans, and names and contact information for three references, should be sent via email to chairsearch@chbe.gatech.edu.

Review of applications begins December 1, 2016, and will continue until the position is filled.

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The Department of Chemical Engineering at **University of Rochester** invites applications for tenure-track positions at all levels scheduled to begin in the Fall of 2017. Applicants are expected to have earned a Ph.D. degree in chemical engineering. Candidates should offer a plan to develop an internationally recognized research program that builds upon existing university/departmental strengths or contributes to recent initiatives in sustainable process engineering, applied data sciences and high energy density physics. The position is open to candidates specializing in any area of chemical engineering including, but not limited to, catalysis, chemical/biological separations, and biotechnology.

Information about the Chemical Engineering Department can be found at <http://www.che.rochester.edu>.

Applicants should show promise of excellence in teaching chemical engineering courses at both undergraduate and graduate levels. Interested applicants should complete an online application at <https://www.rochester.edu/faculty-recruiting>. Application materials include a CV, three recent publications, research and teaching statements and a list of at least three potential references. Applications received before December 15, 2016, will receive immediate attention; however applications will be received thereafter until the position is filled. Women and minorities are encouraged to apply. University of Rochester is an equal opportunity employer.

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Chemical & Engineering News (ISSN 0009-2347) is published weekly except for the last week in December by the American Chemical Society at 1155—16th St., N.W., Washington, DC 20036. Periodicals postage is paid at Washington, DC, and additional mailing offices.

POSTMASTER: Send address changes to: Chemical & Engineering News, Member & Subscriber Services, P.O. Box 3337, Columbus, OH 43210.

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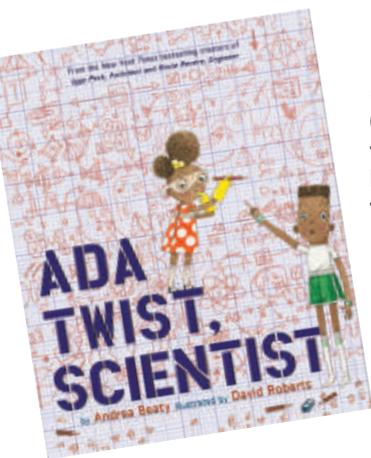
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Bethany Halford wrote this week’s column. Please send comments and suggestions to newsreports@acs.org.



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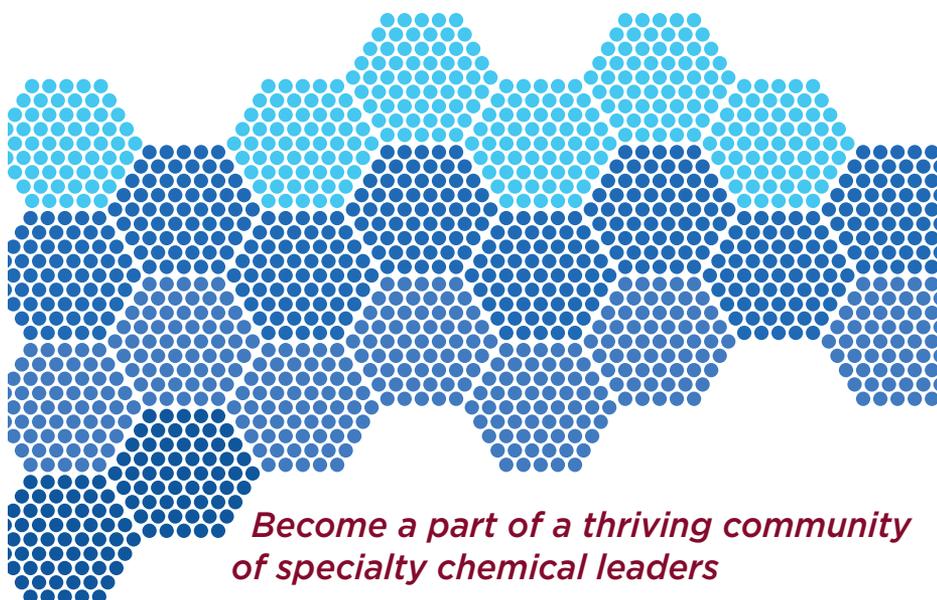
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