WORLD CHEMICAL OUTLOOK

The pipeline holds uncertainty, but industry remains upbeat  
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Cover story

WORLD CHEMICAL OUTLOOK

Rosy forecasts for 2016 didn’t pan out, but the industry is optimistic about 2017.

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German firm is selected for its dedication to making its own business better.

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Quote of the week

“Microfibers are the biggest plastic pollution issue you haven’t heard of yet.”

—Angela Howe, legal director, Surfrider Foundation

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Communicating science

This is only the second issue of the year, and while we are all still catching up after the holidays, I’d like to highlight a couple of stories—both on the topic of science communications—that I came across in the first days of 2017.

The first one is a story published by Un-Dark, the digital publication of the Knight Science Journalism Fellowship Program. The article tells the story of octogenarian Donald McCartor, who managed to have a scientific paper published in the science section of the New York Times at the end of December. Newspapers aren’t in the business of publishing research papers, so this is highly unusual. So how did he do it? McCartor, who has no current academic affiliation, had originally submitted the paper in 2014 to Physical Review Letters, an American Physical Society journal, but it had been rejected without review. As you are well aware, this is a very common practice in publishing, known as triage or prescreening. Frustrated by the refusal and motivated by the desire to “share his ideas about quantum mechanics and free will,” McCartor got around the problem by publishing the non-peer-reviewed paper as an advertisement and paying the NYT for a double page spread.

But, if the author was willing to pay for its publication, why not publish it in one of the many predatory open access journals? It is unlikely the paper would have made it through in a bona fide open access journal, but their predatory equivalents have very relaxed rules for peer review. Here is where McCartor shows savviness: Had he done that, the paper probably would have gotten lost in the internet ether and wouldn’t have had the impact that he has achieved by publishing it in the NYT.

From the NYT’s perspective, because the paper is flagged as an advertisement, they do not judge the merits of its content and will publish anything that falls within their accepted standards, which rule out nudity, hate speech, and the like.

McCartor has achieved his goal of getting his views heard by taking his paper out of the arena where these fights are generally fought: the peer-reviewed literature. There are some ethical issues there in my view but, in any case, the approach he’s taken is unlikely to catch on because the final bill from the NYT came to $4,400. Still, given the publicity that doing this has afforded the author, one could argue that it is money well spent.

The other science communication story that caught my eye was a research paper published in the peer-reviewed journal Public Understanding of Science under the title “When science becomes too easy: Science popularization inclines laypeople to underrate their dependence on experts.” The researchers involved in the study caution that making science accessible for the lay public “may lead to the risk of audiences relying overly strongly on their own epistemic capabilities when making judgments about scientific claims.”

The researchers found that popularized articles led laypeople to agree more with the scientific conclusions described in the articles than scientific articles addressed to expert audiences. Interestingly, popularized articles were not deemed to be more credible but more comprehensible, which in turn influenced the ease of information being processed and thus gave the reader greater confidence to make a judgment. Conversely, popularized articles led laypeople to believe that the issues discussed were less complex and less controversial than did the scientific articles, leading individuals to rely on their own judgment despite lacking the depth of knowledge to make appropriate assessments.

The solutions recommended by the authors are unsurprising: including warnings that issues are complex and controversial (I’m not a fan of this) and improving science education. But there is a trend emerging here that is worrisome, and it is the idea that “popularization” of science is equivalent to trivializing, which is not the same thing. What are your views?
With the support of my amazing mentor, I was able to step out of my comfort zone, which was a closed niche; wherever my twin sister was, and gain self-confidence. My time in the lab assured me of my capabilities and instilled within me a sense of accomplishment that will forever motivate me to take risks, work hard, and never give up. Furthermore, the experience Project SEED bestowed upon me encouraged me to "reach for the stars."

- M. Casarez

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Density functional theory (DFT) is a widely used computational method for carrying out quantum calculations in chemistry, materials science, and biology research. Despite its enormous popularity and ongoing modifications and updates, DFT seems to be getting worse at predicting key electronic properties, according to a study (Science 2017, DOI: 10.1126/science.aah5975).

The finding suggests that users of DFT programs should carefully evaluate and benchmark results of their computations. And it may encourage DFT specialists and developers to redouble their efforts to improve the method’s capabilities.

For decades, researchers have depended on quantum methods to calculate electronic structures, bond lengths, and molecular geometries and energies. The values of those properties and others can be obtained with high accuracy from wave-function-based quantum methods. But applying those methods to all but the simplest chemical systems is complex, arduous, and expensive.

DFT simplifies the calculations. It sidesteps the use of wave functions to account for the motions of electrons. Instead, DFT determines electronic properties from the three-dimensional densities of the systems’ electron clouds. That simplification has helped put quantum calculations in the hands of large numbers of researchers, not just hard-core theoreticians.

But as Michael G. Medvedev and Ivan S. Bushmarinov of the Russian Academy of Sciences and coworkers report, although DFT continues to provide ever more accurate energy values, thanks to ongoing method development and refinements, it is getting worse at predicting electron densities.

The team carried out DFT calculations on 14 types of atoms and ions using 128 different functionals—mathematical descriptions of electron density—developed since 1970. They compared those results with ones obtained from high-level ab-initio wave function quantum methods, which are known to be highly accurate. They find that until about 2000, DFT-calculated energies and electron density values improved hand-in-hand. Since then, however, the energies have continued to improve, but the densities have become less accurate.

For some applications in chemistry and biology, the energies and geometries of molecules are the most important pieces of information, says Sharon Hammes-Schiffer, a chemistry professor and specialist in computational methods at the University of Illinois, Urbana-Champaign.

“If the electron density does not affect these properties, then perhaps the inaccurate electron density is irrelevant,” she adds. It may have little effect on chemical bonding.

The key issue in Hammes-Schiffer’s view is that some modern functionals “may be giving the correct energies for the wrong reason.” She argues that this subject merits further investigation because “most scientists would prefer to obtain the correct answer for the correct reason.”—MITCH JACOBY

Highlights

Phosphorus takes a star turn
Catalytic hydrogenation’s mechanism clarified
The molecular effects of gastric bypass surgery
Structure of HIV’s DNA tool solved
Smog grows as industry pros pers in China
New drug approvals plummet in 2016
DOE funds cleantech, but will it last?
Some pet flea collars carry risks for humans, EPA says

THEORETICAL CHEMISTRY

Density functional theory heads the wrong way

Theoretical method may be getting the right answer for the wrong reasons

Density functional theory (DFT) is a widely used computational method for carrying out quantum calculations in chemistry, materials science, and biology research. Despite its enormous popularity and ongoing modifications and updates, DFT seems to be getting worse at predicting key electronic properties, according to a study (Science 2017, DOI: 10.1126/science.aah5975).

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Spread

User-friendly DFT methods, including ones based on the local density approximation (LDA) and variants of the generalized gradient approximation (GGA), gave increasingly more accurate electron density values until about 2000. Since then, the errors have been growing.
SYNTHESIS

Phosphorus garners an organic starring role

Chemists prepare the phosphorus analog of cyanuric acid for the first time

Over time, chemists have synthesized an incredible array of molecules that combine carbon, hydrogen, nitrogen, and oxygen. Second row periodic table elements such as phosphorus and sulfur have made important guest appearances in compounds, but they tend not to form heavy analogs of common CHNO organic molecules. A research team based at ETH Zurich has reported a rare exception by preparing the phosphorus analog of cyanuric acid.

A six-membered heterocyclic ring, cyanuric acid, C₃N₃(OH)₃, and its derivatives are often used as polymer cross-linking agents and to make industrial chemicals such as herbicides and dyes. Riccardo Suter, Zoltan Benkő, and Hansjörg Grützmacher, who led the discovery team, believe the phosphorus analog, the triphosphabenzenecyanuric acid, C₃P₃(OH)₃, could play a similar role to make phosphorus-containing plastics and could serve as a valuable ligand for metal catalysts (Angew. Chem. Int. Ed. 2016, DOI: 10.1002/anie.201610146).

The researchers thought they might be able to make the phosphorus analog of cyanuric acid by first generating an analog of isocyanic acid (HNCO) and trimerizing it. But their efforts to make HPCO failed. After some trial-and-error, they figured out that by using Na(OCP) in conjunction with an organoborane they could generate a boryl-substituted phosphoalkyne. Trimerization of this molecule yielded the needed C₃P₃ ring on a multigram scale. Subsequent treatment of this borylated intermediate with tert-butyl alcohol led to the target C₃P₃(OH)₃.

Grützmacher and coworkers have made a significant breakthrough,” says Jose M. Goicoechea of the University of Oxford, whose group first synthesized a phosphorus analog of urea, H₂PC(O)NH₂, in 2013. “Their notable finding promises to give rise to a lot of fascinating follow-up chemistry.”

Grützmacher says there is no immediate plan to commercially develop the phosphorus analog. For now, his group is focusing on using the aromatic C₃P₃(OH)₃ and its borylated and silylated derivatives as π-accepting ligands to prepare transition-metal complexes. —STEVE RITTER

STRUCTURAL BIOLOGY

Probing different types of Alzheimer’s

Differences in fibril structure may correlate with different forms of the disease

A hallmark of Alzheimer’s disease is the accumulation of amyloid-β fibrils in the brain. It’s still an open question whether structural differences in these fibrils correlate with different subtypes of the disease.

To help answer that question, Robert Tycko and coworkers at the National Institutes of Health have used brain tissue from patients with one of three forms of Alzheimer’s disease to seed the formation of fibrils in the lab. These fibrils were made from 40-residue and 42-residue amyloid-β peptides, common to the disease. Nuclear magnetic resonance spectroscopy signatures of the fibrils suggest that there may indeed be a correlation between fibril structure and disease manifestation (Nature 2017, DOI: 10.1038/nature20814).

The NMR spectra revealed that for all subtypes there’s one predominant fibril structure for the Aβ-40 peptide and two for the Aβ-42 peptide. For the Aβ-40 peptide “in most cases the predominant structure seems to account for about 80% of the fibrils we derive from brain tissue,” Tycko says. Samples from one subtype, marked by rapid disease progression, show signs of greater structural heterogeneity than the others. That heterogeneity may be a contributing factor in that form of Alzheimer’s.

“It is incredibly difficult to get structural information about amyloid fibers, even for simple in vitro proteins,” says Martin T. Zanni, a chemistry professor at the University of Wisconsin, Madison, who studies amyloid formation. “It looks like Tycko has discovered the most important (or at least more predominant) polymorph—the one we should all be studying.”

“We don’t know what the 3-D structures look like and how different they are from structures that have been determined,” Tycko says. “We’re now trying to figure out what those structures really are.” —CELIA ARNAUD
CA L T A L Y S I S

Study confirms ‘hydrogen spillover’

In catalytic hydrogenation, dissociated hydrogens reduce substrates on two types of surfaces, but with drastically different efficiencies

In some industrial processes, flowing hydrogen molecules over solid surfaces containing catalytic metals reduces organic molecules by hydrogenation. On the basis of a mechanism proposed in the 1960s, chemists think such reactions may proceed through the movement of hydrogen atoms in a process called “hydrogen spillover.” But researchers haven’t been able to confirm this mechanism because models of the reaction are difficult to create and analyze.

With a new, realistic model system, researchers have shown definitively that hydrogen spillover occurs on two key types of catalytic surfaces, called reducible and nonreducible supports, but to a drastically different extent. The information could help chemists design better catalysts as well as improve hydrogenation processes and hydrogen storage for fuel cells. The approach could also help scientists determine whether hydrogen spillover occurs more generally in important research and industrial reactions.

In hydrogen spillover, catalytic platinum nanoparticles on a solid support dissociate H₂ into H atoms. The atoms migrate, or spill over, onto the support, where they can reduce a nearby substrate such as iron oxide. Chemists previously have shown that the process occurs readily on reducible surfaces such as titanium oxide but have struggled to observe it on nonreducible supports such as aluminum oxide.

Yasin Ekinci of the Paul Scherrer Institute, Jeroen A. van Bokhoven of Paul Scherrer Institute and ETH Zurich, and coworkers used electron beam lithography to precisely deposit platinum and mixed iron oxide nanoparticles separated by various distances on TiO₂ and Al₂O₃ supports. They then used X-ray absorption spectromicroscopy and density functional theory to analyze the extent to which H atoms reduced iron oxide.

Spillover is about ten orders of magnitude more efficient on TiO₂ than on Al₂O₃; the researchers found (Nature 2017, DOI: 10.1038/nature20782). And on the nonreducible support, spillover is restricted to extremely short platinum-to-iron-oxide distances because of a competing hydrogen desorption process. The findings suggest that the potential of spillover-based hydrogenation is severely limited on nonreducible supports.

The enhanced understanding that the study provides could help improve the performance, lifetime, and costs of spillover-based hydrogenation systems, comments materials physicist A. Alec Talin of Sandia National Laboratories.—STU BORMAN


Possible molecular mechanism behind gastric bypass success identified

Researchers pinpoint lipid involved in dietary changes after surgery in rats

Gastric bypass surgery is one of the most successful weight-loss interventions for treating obesity. Now, by performing the surgery on rats, scientists at Leipzig University have identified a molecular pathway between the gut and the brain that may explain the surgery’s underlying success.

Gastric bypass surgery reroutes the intestines and creates a much smaller stomach pouch, making patients feel full faster. When Wiebke K. Fenske and colleagues performed the surgery on rats, not only did the rodents lose weight, they also preferred low-fat foods to high-fat foods.

At the same time, Fenske’s team saw that the surgery increased synthesis of oleoylthanolamide (OEA) in the intestines, a change they believe is responsible for the weight loss and behavior shift. OEA is a lipid that binds the α-type peroxisome proliferator-activated receptor (PPAR-α), which helps absorb, store, and use fat. When the researchers chemically inhibited PPAR-α in rats that had undergone surgery, their preference switched from a low-fat diet to a high-fat one (Cell Metab. 2017, DOI: 10.1016/j.cmet.2016.12.006).

The team also showed that the OEA pathway connects the gut to the brain via the vagus nerve, and that severing that nerve or blocking downstream dopamine receptors in the brain caused the rats to return to their high-fat-prefering ways.

Hans-Rudolf Berthoud of Louisiana State University says that although the research demonstrates lots of interesting changes in the rats’ physiology, “The question is, which changes are important?” Many pathways are being studied as the basis for obesity beyond OEA, he notes.

Daniele Piomelli of the University of California, Irvine, says if the study is “confirmed in humans, it would provide a mechanistic basis for the therapeutic effects of bariatric surgery. It does not need to be the only basis, of course, but could be an important one.”—RYAN CROSS
SPECTROSCOPY

**Actinide covalency measured by EPR**

Mounting evidence suggests that actinide bonds have notable covalent character, making their chemistry more akin to transition metals than lanthanides. That covalency can be directly measured using pulsed electron paramagnetic resonance spectroscopy, yielding some surprising results, reports a team from the University of Manchester (Nat. Chem. 2016, DOI: 10.1038/nchem.2692). So-called superhyperfine coupling of a metal’s unpaired electrons with ligand nuclei that have non-zero spin can be used to assess covalency, but signals couldn’t be resolved by older EPR techniques. Using newer pulsed methods, Floriana Tuna, Eric J. L. McInnes, David P. Mills, and coworkers studied thorium(III) and uranium(III) organometallic complexes with ligands derived from the cyclopentadienyl anion (Cp). Computational analysis of the Th and U complexes suggested that they had very similar, weakly covalent bonds. But the EPR measurements indicate that the complexes differ, with much more covalency in U-Cp bonds than in Th-Cp bonds. Unexpectedly, the Th complex more closely resembles the analogous lanthanide ytterbium complex from the opposite end of the periodic table. “Such results highlight the need for new experimental data on systematic families of well-defined complexes,” the authors say.—JYLLIAN KEMSLEY

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NANOMATERIALS

**Superstretchy semiconducting polymers**

Silicon has enabled science journalists to cover topics that were once written about only by science fiction authors: implantable sensors, wearable smart gadgets, and even electronic skin. But silicon is naturally more rigid than is desirable for devices that ought to bend and stretch like living tissue. Some scientists have thus turned to semiconducting polymers to create such devices, but these materials have struggled to achieve flexibility without compromising electrical performance. An international research team has now created thin polymer films that can stretch up to twice their initial length while still allowing electrical charge to flow at rates comparable to silicon (Science 2017, DOI: 10.1126/science.aah4496). Led by Stanford University’s Zhenan Bao and Jong Won Chung of Samsung Advanced Institute of Technology, the team showed that wearable circuits made with the films can withstand bending, twisting, and even light stabbing. This ductile durability comes from confinement. When mixed with an elastic styrene copolymer, some conjugated polymers separate and confine themselves, forming nanoscopic, fibrous aggregates. This nanofracture impedes the semiconducting polymer’s inclination to crystallize and facilitates the movement of electrical charges, resulting in an uncompromising stretchy semiconductor, the team reports.—MATT DAVENPORT

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DRUG DEVELOPMENT

**Blood clot prevention with lower bleeding risk**

People with a high risk of suffering from a heart attack or stroke often take drugs that prevent formation of clots in their blood vessels. These drugs have a narrow so-called therapeutic window: Dosages that are high enough to effectively limit harmful clotting can also increase a person’s risk of life-threatening bleeding. A team of researchers at Bristol-Meyers Squibb and the University of Montreal reports a new strategy that could widen that window (Sci. Transl. Med. 2017, DOI: 10.1126/scitranslmed.aaf294). The enzyme thrombin plays a key role in activating platelet cells to start the clotting process. One of its functions is to turn on protease-activated receptors (PARs) by cutting off a bit of the N-terminus of the proteins. The drug vorapaxar works by turning off one member of that family, PAR1. The BMS-led team decided to investigate the potential of targeting the less studied PAR4. The researchers screened 1.1 million small molecule compounds to find one that blocked the receptor. Chemists optimized the resulting imidazothiadiazole compound to produce BMS986120. This compound was more effective in reducing clotting in cynomolgus monkeys and had a lower bleeding risk than did the approved drug clopidogrel. BMS has started a phase II clinical trial with a related molecule, BMS986141.—MICHAEL TORRICE
When chemists need a superstrong acid, they often reach for triflic acid, CF₃SO₂H; triflimide, (CF₃SO₂)₂N; or perhaps tris(triflyl)methane, (CF₃SO₂)₃CH. These acids and the salts made from them are sought after as electrolytes in fuel cells, stabilizers of reactive species, and as catalysts. In seeking to diversify the strong organic acid family, researchers led by Denis Höfler and Benjamin List of the Max Planck Institute for Kohlenforschung have designed a new C–H acid: 1,1,3,3-tetratriflylpropene (Angew. Chem. Int. Ed. 2016, DOI: 10.1002/anie.201609923). Creating a new organic superacid typically starts with designing the corresponding anion, strategically locating electron-withdrawing substituents adjacent to a target C–H bond in such a way as to delocalize the negative charge to reduce its basicity. The trifyl group is often used because it’s one of the most electron-withdrawing groups known, and including more triflyl groups typically increases the acidity of C–H bonds. The researchers were looking to create a new acid with more than three electron-withdrawing groups and to keep the molecule symmetrical for distributing the negative charge. That led them to try installing four triflyl groups on propene, which they did in a two-step method starting from commercially available bis(triflyl)methane. The team found that tetratriflylpropene has the highest catalytic activity among other trifyl compounds tested for challenging Mukaiyama aldol reactions, Friedel–Crafts acylations, and other reactions.—STEVE RITTER

**REAGENTS**

🔹 **Tetratriflylpropene: A new organic superacid**

How HIV inserts DNA into hosts

When HIV infects a host cell, the pathogen converts its RNA code to DNA and then docks the genetic material in a host’s genome. The first glimpse of the HIV machinery that performs this insertion comes courtesy of a team of researchers led by Dmitry Lyumkis at the Salk Institute for Biological Studies.

More than 25 years after the discovery of HIV, the mechanisms by which the virus integrates its genetic material into the host genome are still not fully understood. This is because the viral assembly machinery, known as the intasome, is constantly being refined by host cells to prevent the viral genetic material from integrating into the host’s genome. As a result, the intasome is constantly evolving, making it difficult to study.

The team of researchers led by Dmitry Lyumkis at the Salk Institute for Biological Studies have now developed a new system that allows them to study the intasome in detail. They used cryo-electron microscopy to image HIV’s intasome at a resolution of 3.5 to 4.5Å. The group found that several amino acid residues in and near the machinery’s active site are positioned differently than what was previously known.

**HIV machinery known as the intasome (two views shown here) integrates viral DNA (dark gray) into host DNA (light gray).**

(Science 2017, DOI: 10.1126/science.aah7002). Called the intasome, HIV’s insertion machinery is targeted and blocked by drugs such as raltegravir and elvitegravir. To develop these drugs and to study HIV’s intasome, scientists have relied on biochemical techniques, computer modeling, and X-ray crystallography coursework describing individual domains within the insertion machinery and the structures of intasomes from related viruses, such as PFV, the prototype foamy virus. Lyumkis’s team used cryo-electron microscopy to image HIV’s intasome with a resolution of 3.5 to 4.5Å. The group found that several amino acid residues in and near the machinery’s active site are positioned differently in HIV compared to PFV. The new work “provides important guidance for rationally improving clinically relevant inhibitors,” notes the team. In another study published in Science, researchers led by Peter Cherepanov at London’s Francis Crick Institute report the cryo-electron structure of an intasome from a maedi-visna lentivirus, which could provide a platform for screening HIV inhibitors, “the team notes.”

**Biocatalytic cofactor recycled efficiently**

Oxidoreductase enzymes are used extensively as biocatalysts for industrial and academic reactions, including pharmaceutical synthesis. But they almost exclusively require expensive cofactors such as NADP⁺, the oxidized form of the biological cofactor nicotinamide adenine dinucleotide phosphate. The reagent currently costs about $22,000 per mole. Enzymes that can recycle it from its reduced form, NADPH, have drawbacks that have limited their use, such as low activity, unwanted by-product generation, and short lifetimes. Guided by nature, which uses an NADP⁺-producing glutathione reductase system to maintain a reducing environment within cells, researchers have now developed a similar system for regenerating NADP⁺ from NADPH. Rudolf K. Alleman of Cardiff University and coworkers devised the system, which uses an organic-disulfide oxidizing agent and bacterial glutaredoxin and glutathione reductase to regenerate NADP⁺ (ACS Catal. 2016, DOI: 10.1021/acscatal.6b03661). The primary recurrent cost is for the inexpensive organic disulfides, so the process could reduce the price of NADP⁺ to about $0.05 per mole, a more than five-order-of-magnitude improvement. The system, which “is superior to all existing methods” for regenerating NADP⁺, “offers many advantages for commercial and academic users,” the researchers say.—STU BORMAN
As Chinese industry booms, residents choke

Manufacturing rebound in China could be short-lived if authorities crack down on pollution

Bucking a general slowdown in economic growth, China posted its best manufacturing performance in four years last month. However, worsening air pollution in many Chinese cities could cause authorities to clamp down on the chemical plants and other factories that are contributing to this strong performance.

Pedestrians wearing masks in Beijing earlier this month.

“Manufacturing companies in China reported the strongest upturn in operating conditions since January 2013 at the end of 2016,” reports Caixin Insight Group, a financial data provider. Caixin publishes a monthly Purchasing Managers Index that, like its U.S. equivalent, provides a reliable assessment of the health of the manufacturing sector.

“Production expanded at the fastest pace in nearly six years, supported by a solid increase in total new work,” Caixin said. Caixin was unable to decide if the Chinese economy, slowing for the past three years, is accelerating again. Whereas the economy grew at annual rates exceeding 10% for most of the past 20 years, the Asian Development Bank estimates that China expanded at 6.6% in 2016, a rate lower than India’s.

The manufacturing resurgence could be threatened by dangerously high levels of air pollution in northern China. The U.S. Embassy in Beijing, which is equipped to measure outdoor air quality, reports that its Air Quality Index repeatedly exceeded 400 last week, a level it considers “hazardous.” Northern China has been shrouded in dangerous smog for most of this winter.

China has reacted to its toxic air by increasing controls on manufacturers or ordering them to suspend operations. On Dec. 30, the Beijing Environmental Bureau said it was inspecting manufacturers in the vast city for possible violations of emissions regulations. In November, China had ordered the temporary suspension of production in the northern part of the country. Among those affected were some major Chinese drug manufacturers, including CSPC Pharmaceutical.

Some foreign chemical producers see China's struggle to improve its air quality as a source of business opportunity. Firms including Lanxess, Henkel, and BASF are working with car manufacturers in China to develop lightweight parts that help lower fuel consumption. Last year, BASF disclosed that it created an emissions catalyst for the Chinese car manufacturer Geely. —JEAN-FRANÇOIS TREMBLAY

New drug approvals plummet in 2016

Pharmaceutical industry doomsayers have been licking their chops for months watching the roster of drug approvals for 2016 limp to a weak total of 22, following a record of 45 approvals in 2015. The roughly 50% drop comes after five years of generally increasing Food & Drug Administration approvals.

Seeing the low numbers coming, industry watchers have been waxing leery regarding a possible industry downturn. Questions about whether drug companies will be able to adequately fund investment in R&D were sharpened by this year’s disappointing approval tally.

Industry analysts, however, say the downturn is normal. “You always have to expect some cyclicity both in the submissions and the number of drugs approved,” says Jon Lange, head of Ernst & Young’s life sciences R&D division.

Lange acknowledges that the drop, in part, reflects the increasing difficulty that drugmakers experience in hitting the mark in tough areas such as Alzheimer’s disease and oncology. On the other hand, a number of drugs that were expected to be approved last year were given fast-track approval, which boosted the count for 2015.

John LaMattina, a senior partner at PureTech Ventures and former head of R&D at Pfizer, agrees that the downturn is largely normal.

“After two outstanding years of approvals, especially considering how much more difficult it is to get drugs approved now than 20 years ago, it is not surprising that only 22 drugs were approved in 2016,” he says. “However, if this level of productivity continues for the rest of this decade, one would have to worry about the health of the biopharmaceutical industry.” —RICK MULLIN

SNAPSHOT

Start-up electric car company Faraday Futures unveiled its new, preproduction FF91 model at last week’s Consumer Electronics Show. The luxury vehicle has a range of 608 km—compared with the Tesla 3’s range of 346 km—thanks to a lithium-ion battery engineered for greater energy density. It accelerates from 0 to 100 km per hour in 2.4 seconds.
PHARMACEUTICALS

Drug manufacturing woes grow

Issues raised in FDA inspections delay approvals

Several companies are trying to overcome manufacturing roadblocks that stopped their new drugs from being approved by FDA in 2016. In responses to their applications, FDA cited problems found during preapproval plant inspections. Most problems were in Western facilities and centered on formulation, rather than active ingredient production.

Only two companies—AstraZeneca and Opko Health—responded to the problems in time to refile in 2016. And Opko got an approval after its manufacturing partner, Catalent, fixed problems at its St. Petersburg, Fla., extended-release capsule plant. Ocular Therapeutics expects to refile this quarter, while Roche’s review is delayed until late March.

Meanwhile, Sanofi and Regeneron Pharmaceuticals face a major setback for the potential blockbuster drug sarilumab, a monoclonal antibody targeting the interleukin-6 receptor. If approved, it will compete in the rheumatoid arthritis field against Abbvie’s Humira, the industry’s top-selling drug.

During an October earnings call, Sanofi CEO Olivier Brandicourt said the company was working quickly to address deficiencies at a fill-and-finish facility in Le Trait, France. He said the issues should be resolved before the expected March review date for an even bigger potential blockbuster,

Glitches

Manufacturing problems delayed new drug applications in 2016

<table>
<thead>
<tr>
<th>COMPANY</th>
<th>DRUG</th>
<th>DISCLOSED</th>
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<tbody>
<tr>
<td>AstraZeneca</td>
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<tr>
<td>Opko Health</td>
<td>Rayaldee</td>
<td>March</td>
</tr>
<tr>
<td>Soon to be refiled</td>
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<td>Ocular Therapeutics</td>
<td>Dextenza</td>
<td>July</td>
</tr>
<tr>
<td>Roche</td>
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<tr>
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<td>Cempra</td>
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<td>Portola</td>
<td>Andexa</td>
<td>August</td>
</tr>
<tr>
<td>Sanofi/Regeneron</td>
<td>Sarilumab</td>
<td>October</td>
</tr>
<tr>
<td>Valeant</td>
<td>Latanoprostene</td>
<td>July</td>
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</table>

Sources: Companies

Drug manufacturing woes grow

In the waning days of 2016, the bioenergy technologies office of the U.S. Department of Energy announced six awards totaling just under $13 million to companies planning pilot- and demonstration-scale biorefinery projects.

DOE said it anticipates awarding an additional phase of funding in 2018 to help firms construct and operate the facilities. However, President-elect Trump has stated that he does not support subsidies for new energy projects. In a 2012 Twitter comment, he criticized a DOE loan that was given to the solar firm Solyndra, which went bankrupt.

Under the current DOE program, LanzaTech will receive $4 million to expand the use of a demonstration facility in Soperton, Ga., that makes jet fuel and diesel from ethanol. The company uses microbes to make ethanol from industrial waste gases and converts it to fuel using a process it developed with Pacific Northwest National Laboratory.

The new funds will allow LanzaTech to plan an expansion from 15,000 L per year of fuels output to more than 11 million L. In addition, the company will convert ethanol made from gasified biomass in a process developed by the company Aemetis.

Biobased jet fuel is also being targeted by Avapco, which will get $3.7 million for a Thomaston, Ga., biorefinery that uses woody biomass. The firm will also produce cellulosic diesel and other products with biobased chemicals developer Genomatica.

Global Algae Innovations, meanwhile, was awarded $1.2 million to make improvements to its algae production processes. The company is planning a pilot-scale algae biofuel facility in Hawaii that will use high-productivity cultivation and energy-efficient harvesting technologies.

BIOFUELS

DOE funds cleantech, but will it last?

LanzaTech, Global Algae Innovations among awardees for small-scale, biobased projects

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Even after President Trump takes office, DOE is not likely to cancel the second phase of the grant program for successful awardees, says Victor Oh, an analyst at Lux Research, “But during Donald Trump’s four-year term, I can’t imagine a lot of new support for the types of early-stage technologies that had been getting funding under the Obama Administration,” Oh predicts. —MELODY BOMGARDNER
**Mergers & Acquisitions**

**Air Products, Huntsman complete sales**

Air Products & Chemicals has completed the $3.8 billion sale of its performance materials division to Evonik Industries (see page 18). The business, which had sales of about $1.1 billion in 2015, makes epoxy curing agents, polyurethane additives, and specialty surfactants. The sale completes Air Products’ effort to exit chemicals and focus on industrial gases. It spun off its electronics materials business as Versum Materials last October. Separately, Huntsman Corp. has completed the sale of its European surfactants business to Innospec for $253 million. Huntsman says it remains committed to the surfactants business in the U.S. and Australia.—ALEX TULLO

**Persistent Pollutants**

**DuPont settles mercury suit**

DuPont has agreed to pay $50 million to clean up mercury released into Virginia’s South River between 1929 and 1950. The deal, with the state of Virginia and the U.S. Departments of Justice and the Interior, is subject to a federal judge’s final approval. DuPont used the mercury at a facility in Waynesboro, Va., where it manufactured acetate yarn and flake. Other legacy environmental problems continue to plague DuPont. Last month the town of Carneys Point, N.J., filed a $1 billion suit seeking the cleanup of the firm’s former Chambers Works manufacturing site.—MARC REISCH

**Catalysis**

**Covestro funds catalyst R&D center**

Covestro and Germany’s RWTH Aachen University have extended a catalyst research collaboration. Covestro will contribute $13 million over the next seven years to the university’s CAT Catalytic Center, a unit jointly operated by the partners. In operation since 2007, the center has 35 employees. It previously developed a zinc-based catalyst used in a new Covestro plant in Dormagen, Germany, that makes polyols from carbon dioxide.—ALEX SCOTT

**Agriculture**

**Sumitomo, Purdue target plant analysis**

Sumitomo Chemical will join up with Jian Jin, an assistant professor of agricultural and biological engineering at Purdue University, to develop technology for analyzing the shapes of plant roots and leaves via imaging. The information will be used to suggest which fertilizers or crop protection chemicals should be applied. Sumitomo and Purdue researchers have worked together on other projects including new platforms for chemical substance analysis.—MELODY BOMGARDNER

**Mergers & Acquisitions**

**Air Liquide exits diving equipment**

Air Liquide has sold Aqua Lung, a diving equipment maker founded by French deep-sea explorer Jacques Cousteau and Air Liquide engineer Émile Gagnan, to Montagu Private Equity. The 70-year-old firm has annual sales of more than $200 million and 1,000 employees. Air Liquide says it wants to focus on integrating the industrial gases firm Airgas, which it recently purchased for more than $10 billion.—MARC REISCH

**Start-Ups**

**Synthego raises funds from big names**

Synthego, a four-year-old genome engineering tools firm, has raised $41 million in a Series B funding round. Investors include the technology venture firms 8VC and AME Cloud Ventures, backed by Yahoo founder Jerry Yang. Jennifer Doudna, a UC Berkeley professor and CRISPR/Cas9 pioneer, also invested. Synthego provides synthetic RNA sequences critical for employing CRISPR technology. The company was founded by former SpaceX engineers Paul and Michael Dabrowski.—ANN THAYER

**Pharmaceutical Chemicals**

**Lonza to make drug active for Aurinia**

Lonza has signed an agreement to manufacture voclosporin for use by the biotech firm Aurinia in a Phase III clinical trial of the drug as a lupus nephritis treatment. Lonza
BIOTECHNOLOGY

A flurry of deals signed by J&J

Johnson & Johnson started the new year by announcing 15 collaborations across its drug, medical device, and consumer health care businesses. For example, the company will develop a CB1-targeting antibody, namacizumab, for nonalcoholic steatohepatitis with Bird Rock Bio. It will explore ketamine analog technology for depression with Amorsa Therapeutics. And it will work on small molecules to potentially address cataracts with Murugappan Muthukumar, a professor of polymer science and engineering at UMass Amherst.—MICHAEL MCCOY

DRUG SAFETY

Chinese firm hampers FDA inspection

FDA has banned from the U.S. drugs made by Baoying County Fukang Medical Appliance after the company hampered the agency’s work. During an inspection in June, FDA officials observed that the company does not properly maintain the cleanliness of its finished product warehouse or provide sanitary facilities to its staff. And a company manager refused to explain how it conducts microbiological testing of products it ships to the U.S., claiming that the procedure is a trade secret. FDA did not disclose what Fukang makes. On websites where its products are sold, the company is described as a supplier of medical consumables such as cotton balls and tongue depressors.—JEAN-FRANÇOIS TREMBLAY

AGRICULTURE

Lilly, Bayer help animal health deal

Eli Lilly & Co. has spent $885 million to buy three animal vaccine product lines in the U.S. from Boehringer Ingelheim, along with a manufacturing and R&D site. Meanwhile, Bayer is acquiring two parasite control products. The U.S. Federal Trade Commission required Boehringer to divest the businesses to complete a $13.5 billion swap of its consumer health business for Sanofi’s animal health subsidiary Merial on Jan. 1. Last year, France’s Ceva Santé Animale bought nine Merial products to address European regulatory concerns.—ANN THAYER

START-UPS

Life science fund gets interdisciplinary

Digitalis, an investment firm that targets life sciences companies working to combine statistics and computing with traditional chemistry and biology, has launched a $100 million investment fund. The firm is also looking to cofound companies that can solve major health care challenges. “We saw a clear need for a health-focused fund that was not bound strictly in life sciences nor information technology, but rather brought different fields together in new ways,” says founder Geoffrey W. Smith. To date, Digitalis has invested in three firms active in computational microbiome research, T-cell sequencing, and health monitoring.—RICK MULLIN

Business Roundup

—Altana has acquired Solvay’s formulated resins business, a maker of epoxy and urethane products with annual sales of about $20 million. The deal includes production and research facilities in Olean, N.Y.

—Linde will soon break ground on a $40 million air separation unit in Adel, Ga. The plant, which will supply atmospheric gases to hospitals and industrial customers, will open in 2019.

—Albemarle has received Chilean government approval to expand the capacity of its lithium salts plant in Antofagasta, Chile, to more than 80,000 metric tons per year. Separately, the company has completed its purchase of the lithium business of China’s Jiangli New Materials for $145 million.

—DuPont Industrial Biosciences has received a grant from the Bill & Melinda Gates Foundation to research new production systems for antibodies and other protein-based medicines. DuPont seeks to use its industrial protein manufacturing skills to lower the cost of biologic drugs.

—Formosa Mitsui Advanced Chemicals, a joint venture of Formosa Plastics and Mitsui Chemicals, will add 2,000 metric tons per year of capacity for lithium-ion battery electrolyte solutions at its plant in Ningbo, China. The move will more than double the plant’s size.

—Monsanto has licensed CRISPR/Cpf1 genome-editing technology for agriculture from the Broad Institute of MIT & Harvard. The company says the technology is a simpler and more precise tool than the older CRISPR/Cas9 system.

—MilliporeSigma has acquired BioControl Systems, a Bellevue, Wash.-based maker of food safety test kits with annual sales of $24 million and 100 employees. MilliporeSigma already supplies microbial quality control products to pharmaceutical customers.

—Asclepis has raised $100 million in series B funding from investors including Goldman Sachs and Tasley Pharmaceutical. Asclepis aims to be the first Chinese firm to launch a new drug in China that treats chronic hepatitis C.
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PHARMACEUTICALS

▶ Texas sues FDA over execution drug

Texas last week filed a lawsuit seeking to force FDA to decide whether the state may legally import thiopental sodium, a drug crucial to administering lethal injections. In July 2015, U.S. Customs agents, at FDA’s request, seized 1,000 vials of thiopental sodium at a Houston airport “for further analysis,” according to the court filing. The barbiturate has not been approved by FDA for injection into humans. But the Texas Department of Criminal Justice argues that importation is lawful for the purposes of carrying out death sentences. “FDA has an obligation to fulfill its responsibilities faithfully and in a timely manner,” says Texas Attorney General Ken Paxton. “My office will not allow FDA to sit on its hands and thereby impair Texas’ responsibility to carry out its law enforcement duties.” FDA says it does not comment on pending or ongoing litigation. Texas and other states have struggled for years to obtain lethal injection drugs as U.S. manufacturers have stopped producing them, and suppliers in Europe have prohibited their export due to opposition to the death penalty.—GLEN HESS, special to C&EN

CHEMICAL REGULATION

▶ EU queues up substances for possible restrictions

The European Union has taken the first step toward constraining the use of four substances—bisphenol A (BPA), a perfluorinated acid, and two alkylphenols. BPA, which is estrogenic, is widely used in thermal receipt paper, linings of food cans, and some plastics. Perfluorodecanoic acid has been used as a plasticizer, lubricant, surfactant, wetting agent, and a corrosion inhibitor, according to the European Chemicals Agency (ECHA). It persists in the environment, bioaccumulates, and is toxic for reproduction, ECHA says. One alkylphenol is 4-heptylphenol, which is used in lubricants in both its branched and linear forms. The other is 4-tert-amylphenol, used as an industrial processing aid and sold for research applications. Both have endocrine disrupting properties, ECHA says. All four chemicals are being placed on the EU’s list of substances of very high concern. Chemicals on this list become candidates for strict control under the EU’s Registration, Evaluation, Authorisation & Restriction of Chemicals program. Such controls bar the use of a chemical in the EU unless companies obtain special permission, called authorization, from ECHA.—CHERYL HOGUE

PESTICIDES

EPA finds risks with flea collar chemical

Tetrachlorvinphos (TCVP), an organophosphate insecticide used to control fleas and ticks on pets and livestock, may pose a health risk to people in their homes and to workers who apply it, EPA says. These conclusions are in a final human health assessment the agency released on Jan. 4. The agency has contacted pesticide makers to discuss ways to reduce exposure to the chemical. EPA plans to propose a rule requiring such reductions later this year. In the meantime, the agency is advising consumers to keep children away from TCVP pet collars, spray, and powder products, and to wash hands thoroughly with soap and water after handling TCVP products. The agency conducted the assessment in response to a 2009 petition from the Natural Resources Defense Council to ban pet products containing TCVP. The environmental group claims that the pesticide poses unacceptable risks to children’s developing brains and nervous systems. EPA initially denied the group’s petition, saying in 2014 that TCVP pet products pose no risk to human health. NRDC appealed the decision, and as part of that litigation the agency agreed to revise the human health risk assessment.—BRITT ERICKSON
The great lint migration

Researchers and apparel makers are hot on the trail of synthetic microfibers in the environment

MELODY M. BOMGARDNER, C&EN WEST COAST

For many people who enjoy exploring the outdoors, a jacket made of polyester fleece is a wardrobe staple. The fluffy material is warm, lightweight, long-wearing, and often made from recycled soda bottles.

But researchers are increasingly worried that fibers from fleece and other synthetic garments are making journeys of their own to soils, rivers, and oceans where they can damage wildlife and even end up in the human food supply.

Scientists have dubbed these escapees “microfibers” because they are commonly only tens of microns wide and millimeters long. They are a tiny, often invisible, subset of the larger class of microplastics, which include plastic beads that enhance the scrubbing action of some personal care products. Another source of microplastics is small particles that come from larger, degraded plastic items.

Microplastics are a pollution problem because they can be mistaken for food by marine life both big and small. They can interrupt normal feeding and digestion processes and leach chemicals such as colorants and other additives. In addition, plastic bits can attract and carry around persistent pollutants such as pesticides and flame retardants that adsorb on their surfaces.

Indeed, the environmental case against microplastics was strong enough to spur U.S. legislators to prohibit the use of microbeads in personal care products.

It would be much more difficult to outlaw what is essentially lint. Microfibers may seem like innocuous stuff to the average consumer, but researchers and sustainability experts in the apparel industry are concerned that the fibers—which may be made of polyester, polypropylene, or acrylic and can include chemicals designed to repel stains or water—carry environmental risks similar to microbeads.

“Microfibers are the biggest plastic pollution issue you haven’t heard of yet,” says Angela Howe, legal director for the advocacy group Surfrider Foundation.

Researchers and apparel industry representatives say they are just beginning to get a handle on the various routes the fibers take to the environment and the problems they pose. One way such fibers are entering streams and oceans is from washing machines, researchers say. Once in the water they can be consumed by fish and become enmeshed in their intestinal tracts, innovating at the Outdoor Industry Association, a trade group.

Last year, a team of master’s degree students at the University of California, Santa Barbara’s Bren School of Environmental Science & Management investigated the amount of fiber that is released into wastewater when consumers wash polyester garments. In the study, sponsored by the apparel firm Patagonia, the team laundered five new and aged jackets and sweaters and used filters to trap fibers from rinse water.

They found that each garment released up to 2 g of microfibers in a single wash, equivalent to more than 0.3% of the item’s mass. The team found that top-loading washing machines caused the release of about seven times more fibers than front-loading machines. In addition, me-
environment—for example, when wastewater sludge is used in agriculture as a fertilizer,” says Elizabeth O. Ruff, one of the Bren researchers. “From there, the fibers can run off into the water system.”

To date, however, researchers have not quantified the total amount of synthetic fiber going to soils, rivers, or oceans or shown what proportion comes from people washing clothes.

Researchers point out that fibers can also escape into the air and be carried into the atmosphere and deposited in rain. And clothing is just one industry that uses synthetic fibers, Jensen points out. “We don’t have a grasp on what other industries might be contributing—say industrial materials or carpets.”

One early study looked for the presence of micrometer-sized plastic debris in an estuary in the southern U.K. Researchers found particles of polyvinyl chloride and nylon—which are not as commonly used in fabrics—in addition to polyester (Environ. Sci. Technol., 2010 DOI: 10.1021/est903784c).

There is a similar lack of data about where synthetic fibers end up, though they are generally found in the same places as other microplastics: oceans, lakes, rivers, and river sediments. One study found more than 100 microfiber particles per kg of river sediment along Germany’s Rhine and Main rivers. (Environ. Sci. Technol. 2015, DOI: 10.1021/acs.est.5b00492).

Most marine research on microplastics has not tracked microfibers because they are difficult to capture and analyze, according to Chelsea Rochman, a professor of ecology and evolutionary biology at the University of Toronto.

“We weren’t noticing fibers in the ocean and environments where we used plankton nets—lots of microfibers go through those 330 micron holes,” Rochman says. “Even when microfibers are sampled, they can be difficult to analyze because of their size. Reliable characterization is required to distinguish the synthetic fibers from cellulose or other natural materials. And lab techniques can be plagued by contamination by fibers floating around indoors.”

Scientists are now using newer methods to capture and analyze microfibers. Instead of nets, Rochman takes water samples with plastic bottles and uses micro FTIR and Raman spectroscopy to analyze even the tiniest fibers.

“The techniques are becoming more like forensics science as we look for smaller and smaller fibers,” Rochman says. “When we look for them, microfibers are the most common type of microplastics we see in animals and sediments.”

Rochman says there is no doubt we are consuming microfibers—especially when we eat certain type of fish—particularly those that are eaten whole like sardines or oysters.

“The big question is: Does it matter?” she asks. “We can make estimates of how much microplastics we eat in a year but we don’t know if there is cause for concern for human health.”

But brands such as Patagonia—which is known for its fleece jackets—aren’t waiting for all the evidence to come in. Elissa Loughman, Patagonia’s senior manager of product responsibility, lists several tactics that may mitigate fiber pollution: changing fabric and clothing production methods, finding ways to capture and dispose of fibers in washing machines, and updating processes at wastewater treatment plants.

“We just don’t have a super effective and tangible solution at this time,” Loughman says, “but we are working on what we can tell consumers to do.”

For example, an advocacy group called the Rozalia Project has developed a prototype microfiber catcher. The hollow plastic sphere, a bit larger than a softball, is designed with a large surface area that grabs fibers from rinse water.

Rozalia executive director Rachael Z. Miller says many industry groups are working to investigate and solve microfiber pollution, but consumers will also have to do their part.

“Right now, not a lot of people know this is happening, but we believe it will be the next big issue in ocean plastics pollution,” Miller says. “It’s not like other marine debris problems that are easy for consumers to write off because they are not actively dumping. What I find is that people are interested to hear about it and want to be part of the solution.”

Plastic food

Synthetic fibers were the most common man-made material found in fish from a California market.

<table>
<thead>
<tr>
<th>COMMON NAME</th>
<th>NUMBER OF FISH COLLECTED</th>
<th>NUMBER OF FISH WITH MAN-MADE DEBRIS</th>
<th>NUMBER OF DEBRIS PIECES, RANGE</th>
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<td>3</td>
<td>0–1</td>
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<td>0</td>
<td>0</td>
<td>na</td>
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<tr>
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<td>1</td>
<td>0–1</td>
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<td>Striped bass</td>
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<td>0–3</td>
<td>fiber, film, foam</td>
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<td>Chinook salmon</td>
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<td>Pacific sanddab</td>
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<td>3</td>
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<td>fiber, film</td>
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<td>1</td>
<td>0–1</td>
<td>film</td>
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<tr>
<td>Copper rockfish</td>
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<tr>
<td>Vermilion rockfish</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>na</td>
</tr>
</tbody>
</table>

Note: Fish was purchased from a market in Half Moon Bay, south of San Francisco. na = not applicable.

Source: Scientific Reports, 2015, DOI: 10.1038/srep14340
WHEN Evonik Industries’ specialty chemical rivals found out about a couple of the German firm’s recent initiatives, they probably admired, or were even envious of, how closely the company tracks the latest trends.

One is Evonik’s Tattoo Care concept. Skin, stressed in the process of tattooing, needs proper conditioning, the company noted in a press release last month. Evonik recommended customers create skin care products containing ingredients such as its SK-Influx V, a synergistic lipid concentrate touted as restoring the skin’s protective barrier. The market opportunity is large, the company says, because “every fifth American,” and about as many Europeans, has at least one tattoo.

Another initiative also appears to be aimed at the millennial. “Most of the shampoos and conditioners on the market for men are made for head hair and are not automatically suitable for beards,” the company disclosed in September. It advised formulating body washes with its Tego Sulfsuccinate DO 75, an anionic surfactant that solubilizes oils.

One wouldn’t think Evonik could be so hip. The company’s roots stretch to the 19th century as the precious metal processing firm Deutsche Gold- und Silber-Scheideanstalt, or Degussa. It was known as Degussa until 2007, when a corporate realignment at its parent company, the German coal miner RAG, recast it as Evonik. The company didn’t become independent until its 2013 public offering. In 2015, it shed the last vestige of its conglomerate structure through the sale of its real estate holdings.

Now that it can focus on specialty chemicals without distraction, Evonik is wasting no time. It recently made a couple of slick acquisitions, initiated countless capital spending projects, and set ambitious research goals. No other specialty chemical company seems to be pursuing self-improvement with such alacrity and at such a grand scale. That makes Evonik C&EN’s company of the year for 2016.

Evonik’s $3.8 billion purchase of Air Products & Chemicals’ performance materials division ranks as one of the largest chemical deals of 2016. Evonik paid an ample price for an enterprise with about $1.1 billion in annual sales and $240 million in pretax profits. But much like buying an expensive suit, it’s getting a tailored cut. Chief Executive Officer Klaus Engel boasted to analysts in May that the purchase “provides an excellent and complementary fit with Evonik on all levels.”

CEOs normally say such things when they make acquisitions. In Evonik’s case, it might actually be true: All three of the businesses in the Air Products divi-
The largest of them is curing agents for epoxy resins. Evonik already supplies the epoxy industry with isophorone diamine cross-linkers. The next largest business is polyurethane additives such as amine catalysts. It will fit well with Evonik’s large polyurethane foam stabilizer business. The third is specialty additives, mostly wetting agents for coatings. Evonik already has a broad line of additives for waterborne paints.

Evonik also made a tidy purchase with its $630 million acquisition of J.M. Huber’s silica business. Unlike Evonik’s existing silica unit, which is focused on industrial markets such as tires, the Huber unit emphasizes consumer products such as silicas that thicken and lend abrasion to toothpaste.

Silica is also one of the major targets of Silica is also one of the major targets of Evonik’s aggressive capital investment program. Just days after it unveiled the Huber purchase, Evonik disclosed plans to spend $120 million to build a precipitated silica plant in São Paulo, Brazil.

Evonik also has been playing offense in amino acids. The firm broke ground in October on a 150,000-metric-ton-per-year dl-methionine complex in Singapore. The plant will double production of the animal feed additive when it comes on-stream in 2019. The company also started production of Aquavi Met-Met in Belgium. This is a dipeptide of methionine that enhances the uptake of the amino acid in farmed shrimp and dissolves slowly in water, reducing waste.

Recently, Evonik acquired a biotechnological route to l-methionine from France’s Metabolic Explorer. Methionine is currently made from a chemical route that begins with acrolein, methyl mercaptan, and hydrogen cyanide. Evonik already uses biobased routes to make l-lysine, l-threonine and l-tryptophan. This year, it added an l-valine product line.

The company’s projects in other businesses are many. For example, it is expanding output of poly-lactic-glycolic acid, a biodegradable polymer used in drug delivery and medical devices, in Darmstadt, Germany, and Birmingham, Ala. The company is increasing capacity of the biodiesel catalyst sodium methylate in Mobile, Ala., and spending about $50 million to expand gas separation modules in Schörfling, Austria.

Evonik has high-tech aspirations as well. It aims to increase sales by more than $1 billion from new initiatives in areas such as nutrition and smart materials by 2025.

But Evonik’s actual R&D spending levels are modest. In 2015, it shelled out $482 million on R&D, or about 3.2% of sales, slightly below the average for large chemical companies that year. However, the company has been trying to improve. R&D spending has grown on average 6% annually since 2010.

Some of that money is going into its collaboration with HP to develop nylon 12 resins suitable for HP’s new three-dimensional printing business. Last year, it commercialized biosurfactants, molecules such as sophorolipids and rhamnolipids that exist in nature. Evonik has begun fermenting them at a facility in Slovakia.

The past year might have been a big one for planning for the future, but it wasn’t a stellar one financially. For the first nine months, Evonik’s sales slipped 7.6% and operating income fell 14.8%. Its stock price has been moving sideways.

When it reported earnings in October, the company reached for the excuses that have been the rounds in the chemical industry. Developed economies are posting sluggish growth, the Chinese economy has cooled, and key countries in Latin America, such as Brazil, are in recession.

But as plants get built, new businesses grow, synergy is cultivated with acquisitions, and the latest consumer trends are uncovered, Evonik’s sales and profit numbers may respond in turn.
DETERMINING the structures of enzymes and other biomolecules with X-ray crystallography has deepened biologists’ understanding of the inner workings of cells and led to the design of many important drugs. Increasingly, researchers are using computer modeling to attain a more realistic picture of the movement of these biomolecules in their natural environment. Rommie E. Amaro, a professor of chemistry and biochemistry at the University of California, San Diego (UCSD), uses computational techniques to predict how enzymes regularly shift their configurations, revealing potential vulnerable areas for drug targeting. C&EN talked with Amaro about how she’s using dynamic models of enzymes to develop a new class of cancer drugs, work that is being commercialized by Actavalon, a San Diego start-up Amaro cofounded.

How did you get into working on computational drug design?
I fell in love with physical chemistry as a chemical engineering undergraduate at the University of Illinois, Urbana-Champaign (UIUC). I ended up doing a biophysics research project with Zan Luthey-Schulten predicting the structure of a protein involved in histidine biosynthesis, and I just loved it. I could not wait for Saturday, and not because of tailgating but because I could go to the lab. I didn’t have to worry about classes, and I could just do research. I was there for hours. That was when I knew something was wrong with me (laughs)!

From there I went to work for Kraft Foods for a couple of years doing very traditional chemical engineering and product development for Philadelphia Cream Cheese, which was a ton of fun. But I missed something—I went back to graduate school to find out what it was. And I fell back in love with computational chemistry, and with molecular dynamics simulations. The work of Klaus Schulten at UIUC was tremendously influential, and later, as a postdoc with Andy McCammon at UCSD, I learned about pharmacology and drug design.

What can computational techniques give you that X-ray crystallography alone cannot?
These days, X-ray crystallography is constantly driving to higher and higher resolution. In rational drug discovery, usually people start with a crystal structure, which is a high-resolution image of the relative locations of the atoms in the drug receptor, then try to screen and discover small molecules that bind with very high affinity and stay for a long time. That’s the standard protocol—to rely on static images of proteins. Of course, we know that, as important as X-ray crystallography data are, it’s like taking a Polaroid snapshot of a dynamic, moving machine.

If a drug receptor is flopping around, then the technique can’t resolve the relative positions of the amino acid residues. So researchers do all these tricks to try to immobilize these proteins. It’s different than the protein’s actual environment in vivo.

Where my lab has been trying to push the envelope is in trying to use molecular dynamics simulations to predict how these proteins or drug targets move over time. We then select out structures from what we call the trajectory of the drug target and use those alternative structures in drug discovery.

How are these simulations enabling you to make new cancer drugs?
It turns out that in more than 50% of human cancers, the gene for a protein called p53 has one single mutation that basically renders it inactive. This protein binds to DNA to activate gene expression that triggers cell death when cells are damaged, causing them to die instead of grow.
into tumors. When p53 is inactive, it can’t prevent tumor growth. We try to develop small molecules that would reactivate p53 because this would be a broad-spectrum cancer therapy.

More than 100 static images of p53 are available in the Protein Data Bank, and they all have fairly similar structural features. We might start with one of these and do an analysis on it. We place the protein in what we call a bath of water—all these simulated water molecules—and ions to mimic the solution environment. Then we might see a movement of a side chain, or we might see an entirely new pocket open up—a pocket that wasn’t evident in the crystal structure but reveals itself in these predictive simulations. Often times, those pockets are actually druggable. We find these pockets and then we try to design small molecules that bind to them.

In p53, a pocket basically revealed itself after we simulated just a few tens of nanoseconds of the enzyme dynamics (PLOS Comput. Biol. 2011, DOI: 10.1371/journal.pcbi.1002238). Then we used this pocket to design and discover reactivation compounds. The p53 protein turned out to be a nice example of the power computation can play in drug discovery.

How are computing advances changing your work?

One thing that’s exciting about our field right now is the meteoric rise in the ability of commodity graphical processing units, or GPUs, to carry out molecular dynamics simulations. GPUs have become very high performance because they’re used to render realistic graphics in real time for video games. It turns out that those same processors are highly amenable to the kinds of scientific calculations that we use for drug discovery.

This has been a game changer. Coming back to p53, when we originally did that work we ran the simulations on supercomputers, and it took a couple of months to generate the dynamics data. Today we can do those exact same simulations in probably three hours on a single GPU.

Are there still things that have to be done on supercomputers?

As the system size scales, we still need to go to supercomputers. We have simulations now that contain multiple hundreds of millions of atoms. Those have to run on some of the biggest computers in the world.

More recently, we’ve been interested in continuing to develop models that are more accurate and more realistic. We have built a model of p53 on a supercomputer that’s gone from 50,000 atoms to 1.5 million (Oncogene 2016, DOI: 10.1038/onc.2016.321), and we’re looking at time scales of the enzyme dynamics that are not just tens of nanoseconds but more on the order of microseconds. We can ask totally different questions now that we have these much larger, more realistic simulations of p53. For example, how does p53 bind to DNA, and how does the sequence within the DNA itself change the binding dynamics?

You can’t run that newer work on a GPU—or you could, but it would be super slow. I think five years from now, with improvements to GPUs, maybe we will be routinely simulating 2 million atoms on a single GPU chip. And 10 years from now, we’ll be simulating whole cells with more than 1 billion atoms on future supercomputers now being designed.

Katherine Bourzac is a freelance writer. This interview first appeared in ACS Central Science: cenm.ag/amaro. It has been edited for length and clarity.

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In the recent past, BASF’s performance in Asia has been nothing to get excited about. From 2012 to 2015, the German chemical giant’s sales in the region stagnated in euros, the currency by which BASF measures its performance. But for 2017 and beyond, things are looking up, says Sanjeev Gandhi, the company’s board member responsible for Asia and the Pacific.

With new plants coming on-line and consumers demanding better products, firm’s regional head is optimistic

JEAN-FRANÇOIS TREMBLAY, C&EN HONG KONG

In the recent past, BASF’s performance in Asia has been nothing to get excited about. From 2012 to 2015, the German chemical giant’s sales in the region stagnated in euros, the currency by which BASF measures its performance. But for 2017 and beyond, things are looking up, says Sanjeev Gandhi, the company’s board member responsible for Asia and the Pacific.

“In the past four, five years, we had a massive increase in investment in Asia and the Pacific,” he tells C&EN from the company’s office in Hong Kong’s Central district. “We are now starting to bring those capacities on-stream.”

Even though growth in China, Asia’s largest chemical market, has been slowing for the past four years, BASF continued to invest in new facilities and new R&D centers, as well as in strengthening its sales infrastructure. BASF’s efforts will pay off in the coming years, Gandhi predicts, regardless of whether the Chinese economy returns to its past rate of rapid growth.

“With our current asset base, our new capacities, our sales infrastructure, and our investment in R&D, we are in a pole position to be one of the leaders in terms of market growth,” Gandhi says. “We plan to grow in Asia at a rate slightly higher than average chemical market growth.”

But how much the Asian chemical market will grow in the near future is uncertain because Asia could be affected by external factors such as the U.K. leaving the European Union or trade policies adopted by the new U.S. Administration. The Asian Development Bank expects Asia, minus Japan, to experience average growth of 5.7% in 2017. The largest economy, China, will grow 6.4%, the bank expects.

In 2017, BASF will welcome the start-up of a $500 million aroma chemical plant in Malaysia, a polyisobutylene plant in Malaysia, automotive coating and process catalyst plants in Shanghai, and a mobile emissions catalyst plant in Thailand. Within a year or two, BASF will also be increasing production at its polyurethane complex in Chongqing, China. The facility has been operating below capacity because of delays in the supply of raw materials, such as chlorine, from local operators.

BASF already sells all those materials in Asia, in some cases by sourcing from its plants in Europe and the U.S. But being closer to customers in Asia will boost competitiveness and, therefore, sales, Gandhi anticipates. “Sourcing from abroad is ineffective and slow,” he says. “It adds lead times that our customers don’t appreciate.”

To sell more chemicals and materials in Asia, BASF can rely on a sales force of several thousand people, says Gandhi, who himself sold commodity chemicals in India for BASF in the 1990s. “We have a presence in 16 countries in Asia, where customers or business partners, within a very short period of time, can expect to meet our people face to face,” he says.

To support its sales organization, BASF is setting up new R&D and technical centers that can assist customers in customizing raw materials for their new products. For instance, this spring the firm will inaugurate a new research campus in Mumbai that will employ around 300 scientists. The center will be smaller than the company’s main regional research facility in Shanghai but still big enough to support several of BASF’s businesses in southern Asia.

BASF’s investment in new facilities is happening at a time when Asian economic growth is slowing, especially in China. But Gandhi remains upbeat.

Much of the slowdown in China, he says, can be attributed to an economic "rebal-
ancing” engineered by the government to promote the growth of service industries and de-emphasize the importance of exports. This transition led initially to lower demand for some of BASF’s materials, but demand has since recovered on a stronger foundation, he says.

Meanwhile, China’s car and construction industries, two areas in which BASF is very active, continue to grow. Construction is a particularly important driver of business for BASF, Gandhi notes. “When people buy a new apartment, or an office, then they buy furnishing, they buy ‘white goods,’ and so on, and there’s a lot of BASF chemistry in those items.”

The enduring vigor of the construction market in China is surprising given that tens of thousands of apartments sit vacant across the country, often clustered together in so-called ghost cities. Despite this overbuilding, a property crash in China is far from imminent, according to David Jiang, president of the chemical market survey firm Sinodata Consulting.

“The level of construction activity cannot continue forever when we have already built enough apartments for the next five to 10 years,” Jiang says. “But the government continues to support the real estate industry because it can raise revenues by selling land to developers.” As a result, Jiang says, the construction industry will remain buoyant in China in the near term.

While certain sectors of the Chinese economy remain healthy, in India, demand is vigorous across the board, Gandhi says. “As in China, people in India want better products, better cars, better houses, better food,” he says. India’s economy has been growing faster than China’s for the past two years, but, for BASF, the market is less important than China’s. “We are quite happy with the business,” Gandhi explains, “but the market size in India is not even close to what it is in China.”

BASF also has a well-developed presence in Asia’s second-largest economy, Japan. One of the main goals there is to keep pace in a country that is particularly innovative in chemicals and materials. A key focus is battery materials, an industry for which Japan is the recognized leader. BASF has two battery materials plants in Japan as well as an R&D center.

BASF’s sales force has also targeted Japan’s unique and hard-to-penetrate market for crop protection products. “Japan produces high-value specialty crops that are consumed locally or exported,” Gandhi says. “It’s a closed market, so once you’re in, you’re in.”

With regional sales of more than $13 billion annually, BASF is the only Western company among the 10 largest chemical players in Asia, Gandhi notes. Given its continued investment in the region, BASF has a steadily expanding footprint that could make it one of the top five players in Asia in the years ahead.

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A local player

BASF says it’s the only Western firm among the top 10 chemical suppliers in Asia.

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<tr>
<th>RANK</th>
<th>COMPANY</th>
<th>2015 SALES ($BILLIONS)</th>
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<tbody>
<tr>
<td>1</td>
<td>Sinopec</td>
<td>45.9</td>
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<td>Formosa Plastics</td>
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<td>3</td>
<td>ChemChina</td>
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<td>4</td>
<td>Mitsubishi Chemical</td>
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<td>5</td>
<td>LG Chem</td>
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<td>6</td>
<td>Sumitomo Chemical</td>
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<td>9</td>
<td>Reliance Industries</td>
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<td>10</td>
<td>Mitsui Chemicals</td>
<td>11.7</td>
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Note: Data based on sales in Asia for BASF and total sales for all other firms.

Source: BASF

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A local player

BASF says it’s the only Western firm among the top 10 chemical suppliers in Asia.
EDUCATION

NOBCChE cultivates young scientists

Annual conference nurtures growth of black chemists and chemical engineers

JEFF HUBER, special to C&EN

As soon as Murrell Godfrey heard mention of Cameroon, a lightbulb turned on in his head.
The director of the forensic chemistry program at the University of Mississippi was talking with Kelly Njine Mouapi, a graduate student at the University of Louisville, at a social event during November’s annual meeting of the National Organization for the Professional Advancement of Black Chemists & Chemical Engineers (NOBCChE, pronounced no-buh-shay). When Mouapi said she was from Cameroon, Godfrey immediately remembered meeting another Cameroonian earlier during the conference. He then scanned the room, found the person he was thinking of, and walked Mouapi over for an introduction.

Elizabeth Ndonta, a postdoc at the University of California, Berkeley, was happy to be approached. And she became even happier when she learned about all the commonalities she shares with Mouapi. As the two discovered, not only are they both female scientists who grew up in Cameroon, but they’re also both biochemists focused on the study of proteins. And with Mouapi exploring postdoc opportunities at places such as Scripps Research Institute California, where Ndonta’s lab was previously located, Ndonta had contacts and firsthand experience to pass along.

Later, reflecting upon the similarities she and Ndonta possess, Mouapi couldn’t believe her luck. “She’s in biochemistry. She’s a black woman scientist. It’s just amazing,” Mouapi enthused. “It’s too much of a coincidence, and I’m happy about it—really happy about it.”

The coincidence might have flabbergasted Mouapi, but Godfrey, chair of NOBCChE’s southeast regional section, appeared less surprised by the encounter. As a NOBCChE veteran who attended his first conference in the late ’90s and has returned to the annual meeting every year since, Godfrey can personally attest to the feeling of camaraderie and community that pervades the conference. At NOBCChE, he explained, “we’re about family and bringing people together from all walks of life.”

The 2016 conference, held in Raleigh, N.C., was no exception, bringing together hundreds of minority chemists and chemical engineers. It was an opportunity to reconnect with old friends, meet new ones, and participate in an array of activities including a career fair, research symposia, and professional development sessions that fell under the conference theme of “Paradigm Shift: Cultivating STEM Leadership to Solve Grand Challenges.”

This commitment to developing leaders in science, technology, engineering, and mathematics was established right from the start of the conference during the opening luncheon, which is named after Winifred Burks-Houck, NOBCChE’s first female president. Presenting the lunch’s honorary lecture, Tashni-Ann Dubroy, president of Shaw University, described the long and winding road that led her to eventually become the second-youngest person to serve as Shaw’s president—a journey that included growing up in Jamaica, stints in industry and academia, and the founding of the hair care company Tea & Honey Blends and the Brilliant & Beautiful Foundation for mentoring women in science.

“Who is going to follow this young girl who came from Jamaica, who had a big dream, and who’s been able to experience so many things in life at such a young age?” Dubroy asked as she looked at the crowd of conference attendees before her. “The answer is that it’s you. We’ve got to cultivate you.”

To foster this spirit of encouragement, the conference hosted several educational workshops, including one focused on entrepreneurship led by Nicholas H. Oberlies, a chemistry professor at the University of North Carolina, Greensboro, and his business partner Cedric Pearce, chief executive officer of the natural products firm Mycosynthetix. Oberlies and Pearce talked about how their respective backgrounds in academia and industry helped them find companies that work to translate basic science discoveries into commercial projects.

“Don’t be afraid of entrepreneurship,” Oberlies told the workshop’s audience of undergraduate and graduate students. “I guarantee you that if you know how to solve a structure from an NMR spectrum, or look at a mass spectrum, or you know what IR stands for,” he said, “you can figure out the business stuff. But it takes a little bit of a different mind-set and a little bit of guts.”

That message resonated with Jalisa N. Holmes, a Ph.D. candidate in chemistry at Georgia State University, who attended the
workshop. “Hearing these guys, knowing that they came from other positions before starting their own businesses, lets me know that it’s possible” to launch my own start-up, she said.

Such empowerment being instilled into NOBCChE attendees is exactly why Karelle Aiken, a chemistry professor at Georgia Southern University, made it a point to bring students with her to the conference. Since helping to organize a NOBCChE student chapter at her school in 2008, Aiken has encouraged many to attend the conference and present their research. She said she does this because the opportunity augments the support that students are already receiving from Aiken and her colleagues.

When students are at school, Aiken said, “they don’t take us seriously when we say, ‘You’re doing a good job.’ ” But all that changes when representatives from academia and industry approach students presenting research at NOBCChE and recognize their hard work. “It means so much more to them,” Aiken explained.

Just as impactful, Aiken continued, is the effect that walking into a conference full of minority scientists can have on students’ resolve and determination to complete their studies and earn their degrees. For instance, Aiken remembers the first time she ever brought a group of students to NOBCChE. “They had never been in a room where the majority of the scientists looked like them,” she said. “It took them from ‘I’m really trying to do this’ to ‘Oh, I belong in STEM.’ ”

Kwaku Kyei-Baffour, a Ph.D. candidate in organic chemistry at Purdue University, said he could relate to discovering that sense of belonging at NOBCChE. Born and raised in Ghana, Kyei-Baffour noted that “there are not so many Africans or black Americans in the program” at Purdue. But after attending NOBCChE for the first time this past November, he was pleasantly surprised to meet other chemists from Ghana.

“I thought I was more alone in this country being a Ghanaian here doing chemistry,” he said, but “I’ve met so many Ghanaians” at NOBCChE.

Those encounters clearly left a positive impression on Kyei-Baffour because, later, when asked whether he plans on coming back to NOBCChE again in the future, the young organic chemist didn’t hesitate in his response. “Definitely,” he said.
Business people are by nature optimists, and that was true a year ago when companies and economists forecast a buoyant 2016 for the global chemical economy. In the end, however, business didn’t live up to expectations. U.S. chemical production rose a sluggish 1.6%, and European output didn’t grow at all. Overall economic growth slowed in China and India. Perhaps chastened, the Europeans have lowered their outlook for 2017. But in the U.S. and Asia, industry executives are once again calling for a good year ahead. Given the political uncertainty roiling much of the world, those executives would be wise to have a “plan B” at hand.
PETROCHEMICALS

Despite new capacity, 2017 will likely be a strong year

Normally, a year in which a lot of new chemical capacity opens is a period of diminished prices and thin profit margins. But the slow of new ethylene plants destined to come on stream in 2017 doesn’t necessarily mean it will be a bad year for petrochemical makers.

The biggest names in petrochemicals—Dow Chemical, ExxonMobil, and Chevron Phillips—each have world-scale ethylene cracker complexes slated to start up on the U.S. Gulf Coast in 2017. Other firms, such as Mexichem, Indorama, and LyondellBasell Industries, are completing smaller crackers and large ethylene expansions.

Observers say this new capacity is sorely needed. LyondellBasell CEO Bob Patel told analysts in November that he doesn’t expect a repeat of the late 2000s, when a fleet of new crackers in the Middle East flooded the world with new production. From 2007 to 2011, when there was a recession, global capacity addition exceeded growth in demand by about eight crackers worth of output.

But over the past five years, demand has outstripped new supply by about three ethylene crackers worth. “Even with eight cracker equivalents forecast to come online in the U.S. by 2021, the forecast is relatively balanced over the next five years,” Patel said.

“The globe has no spare capacity like it did when the big Middle East wave came,” points out Steve Lewandowski, vice president of olefins at the consulting firm IHS Markit.

Lewandowski says the market for ethylene will only get tighter for most of 2017. He doesn’t expect the big new crackers to start up midyear as scheduled. Given the complexity of turning on massive multi-billion-dollar units, he says, the fourth quarter is a more realistic expectation. And it could be well into 2018 before these plants ramp up and operate full out.

Moreover, Lewandowski points out that most firms, including Chevron Phillips and ExxonMobil, aim to get their polyethylene plants running before they inaugurate new ethylene crackers. To do so, they will need to tap the limited quantities of ethylene available in the merchant market. “We definitely won’t have enough ethylene in the U.S. to fill out all the derivatives,” he says.

The new year is beginning with higher oil prices. In November, OPEC and Russia agreed to a deal that would cut global oil production by about 1%. Prices jumped from about $45 per barrel to more than $52 in the subsequent weeks.

In Lewandowski’s view, that kind of modest movement in oil prices is not enough to undermine petrochemical consumption. “If we jumped to $120 I would say something different, but a move $10 up, I don’t think it’s a killer for global demand,” he says.—ALEX TULLO

UNITED STATES

A new year begins, marked by optimism

After six years of sluggish growth, output from the U.S. chemical industry will expand by 3.6% in 2017, according to a projection by the American Chemistry Council, the country’s largest chemical trade group.

The figure implies that much will change from 2016, when ACC estimates output grew by a mere 1.6%. An earlier prediction by the group called for more robust growth of 3.1% in 2016.

Overall U.S. economic growth will remain modest, ACC says, but the chemical industry will be a source of strength because cheap shale gas provides a strong competitive advantage, and the industry serves fast-growing global markets. Economist predictions for global growth this year range from 3.1 to 3.4%, compared with about 2.8% in 2016.

The shale gas boom continues to attract investment and chemical jobs to the U.S. Gulf Coast, says ACC chief economist T. Kevin Swift. In addition, “chemical companies in the U.S. continue to innovate, focusing on improving efficiencies as well as on new, leading-edge product development,” he says.

ACC’s figures assume that factors dragging down the chemical economy will moderate or improve in 2017. A glut in supply chain inventories has evened out, for one. Swift also predicts that automotive builds and single-family home construction will be robust. And he says business investment will increase, reversing a strong postrecession trend.

What’s more, Swift alludes to a new, business-friendly climate under the incoming Trump Administration, saying “tax and regulatory reform will go far to rejuvenate U.S. economic dynamism and performance.” Although Trump has promised to erect trade barriers, Swift says total trade will pick up slightly in 2017.

Recent surveys show ACC is not alone in its optimism. According to the Conference Board, consumer confidence in November returned to prerecession levels, due in part to positive views of the labor market. And a survey of home-builder confidence by the National Association of Home Builders resulted in its highest reading since 2005.

But government figures show single-family home starts sank 4.1% in November. Also that month, new vehicle sales—which have been a big area of spending—shrank 2.0%, as measured by J.D. Power and LMC Automotive. Fiscal moves by the new administration will influence buying, the survey partners say. “The economy and industry could be facing a boom or bust depending on which policies are focused on and implemented.”—MELODY BOMGARDNER
Agriculture

Changing landscape ahead for crop solutions

According to the U.S. Department of Agriculture, farmers won’t see much relief from low commodity prices this year, and spending on inputs—seeds, fertilizer, and crop protection chemicals—will continue to be modest. What will increase are investments in technologies that help growers do more with less.

Big agriculture corporations such as soon-to-merge Bayer and Monsanto, as well as start-ups and smaller agriculture firms, are working on multiple ways to help plants thrive with less water, chemicals, and fertilizer while fending off heat, diseases, and other stresses.

Some advances—such as precision imaging and data-based decision-support tools—will be tested on farms this year. Others, such as CRISPR/Cas9 and other gene editing techniques, will move forward in the lab and be commercialized in future years.

As big ag firms consolidate, they will merge once-competitive product development projects, says Scott Duncan, head of the North American agriculture practice at the consulting firm Bain. “So a meaningful amount of R&D and capital will get redirected into other places such as precision agriculture or big data solutions.” He points out that venture capitalists, private equity investors, and established tech firms are also investing in such technologies, which have come to be known as agtech.

In many cases, agtech innovations look nothing like traditional chemicals and seeds. For example, Bayer has formed a research collaboration with FaunaPhotonics to develop a light detection and ranging—or LIDAR—to track the whereabouts and movements of pest insects. LIDAR can even distinguish among insect species by detecting insect body sizes and wing beat frequencies. LIDAR is similar to radar but uses lasers to map objects in space. And farmers will detect insect damage in real time—along with crop conditions such as nutrient levels and disease—from space satellites or with drones. Start-up Gamaya recently raised $2.1 million to commercialize hyperspectral cameras small and light enough to be carried by drones. Co-founder Igor Ivanov, a veteran of big data business applications, says the firm is deploying drones on huge industrial-scale corn, soybean, and sugarcane operations in Brazil.

“Brazilian agriculture is very export-focused, very dynamic,” Ivanov explains. “Growers are keen to use technology to improve production efficiency.”

Meanwhile, smaller firms that develop specialty crops or regionally specific varieties will get new opportunities to improve traits and seeds through gene editing. “The minimum efficient scale to do really radical gene work is coming down and will continue to come down,” Duncan predicts. —MELODY BOMGARDNER

Europe

Sustainability to offer growth opportunities in anemic market

Economists are at sixes and sevens as to whether the European Union will experience higher economic growth and a consequent hike in chemical demand in 2017. Some say the U.K.’s decision to leave the EU could destabilize the region, dampening economic growth. Sustainability, though, is set to drive chemical demand.

CEFIC, Europe’s leading chemical industry trade group, expects a 0.5% uptick in chemical production across the EU in 2017 after no growth in 2016. Petrochemical makers will continue to profit from low oil prices, while demand for polymers from the auto industry is expected to soften. Specialty and consumer chemicals will be supported by moderate demand growth from business and consumers, CEFIC says.

The German chemical industry association VCI predicts German production will not grow in 2017. “The chemical business in 2017 is expected to remain without significant momentum, especially with the political uncertainty and economic risks in foreign markets around the globe,” says Kurt Bock, president of VCI and CEO of BASF.

One of the uncertainties is the U.K.’s pending exit from the European Union. Offsetting the so-called Brexit to a degree, VCI expects digitalization—such as using digital mapping systems to apply agrochemicals—and sustainability to help drive growth in Germany.

Another plus, according to Jefferies stock analyst Laurence Alexander, is that favorable European Central Bank policies in the year ahead will keep borrowing costs low and maintain a weak euro currency. The corporate “poster child” for 2017 could be the Dutch firm DSM, Alexander says, thanks to relatively noncyclical end markets such as nutrition and a favorable foreign exchange footprint.

Paul Hodges, chair of the U.K. consulting firm International eChem, agrees with VCI that sustainability is becoming more important for the EU’s chemical industry. He notes that the circular economy—in which products are designed from the outset to be reused and recycled—is becoming a major initiative in Europe.

“Sustainability is replacing globalization as a key driver for the economy,” Hodges recently told attendees of an ACS webinar. This new normal could drive demand for reusable or biodegradable materials in applications including clean water and sanitation, digital health care, and intelligent food packaging, he said.

But the effect of economic stimulus policies—predominantly the printing of more money—in EU countries in recent years could also be coming home to roost, according to Hodges. The likelihood now is a drawn-out downturn in prosperity in Europe, he said. —ALEX SCOTT
PHARMACEUTICALS

Immuno-oncology therapies set to take center stage

At about $90 billion in sales and more than 10% of the 2016 pharmaceutical market, oncology has become the world’s largest drug sector. Expected to grow two to three times faster than the overall market, cancer treatments should retain the top spot for at least another five years, according to the market research firm EvaluatePharma.

Driving this growth are new therapies, such as checkpoint inhibitors, that stimulate the immune system to fight many different cancers. In 2017, sales of checkpoint inhibitors alone should grow 40–50% to approach $6 billion, according to a market analysis by Decision Resources.

Among the current big sellers are Bristol-Myers Squibb’s Yervoy, which was launched in 2011 and blocks CTLA4. In 2014, BMS’s Opdivo and Merck & Co.’s Keytruda became the first anti-PD-1 drugs. And in May 2016, Roche got approval for Tecentriq, the first PD-L1 inhibitor. These firms, along with AstraZeneca, Pfizer, Merck KGaA, and a host of small companies, have many more immunotherapies in development.

In fact, 2017 should be a defining year for immuno-oncology therapies, particularly for lung cancer, Deutsche Bank stock analyst Gregg Gilbert told clients in a recent report. Lung cancer is the world’s most common cause of cancer deaths. And sales of drugs for non-small cell lung cancers (NSCLC), which make up about 85% of lung cancers, are heading toward $60 billion per year by 2020, he estimates.

This year, clinical trials results are expected not only for single therapies but also for combinations of PD-1 and PD-L1 inhibitors with chemotherapies and CTLA4 agents. These results, Gilbert points out, could start segmenting the market among therapies and provide clarity on which patients may benefit.

Despite this potential, there’s a lot to be learned about using these new drugs. The outcomes of recent clinical trials of Opdivo and Keytruda suggest that the benefits may depend on patients’ levels of PD-L1 expression. Merck, which targeted patients with high expression levels, won an early approval for Keytruda as a first-line NSCLC treatment, while BMS, which didn’t, got disappointing results with Opdivo.

Although immunotherapies, including as-yet-unapproved chimeric antigen receptor T-cell (CART) therapies, could transform cancer care, they do present risks. Recent reports reveal dangerous side effects for the checkpoint inhibitors, such as uncontrolled immune reactions that can lead to organ attack.

And a Phase II trial of Juno Therapeutics’ anti-CD19 CART therapy was halted twice after patients died. Still, encouraging early efficacy data has been reported in hematologic cancers and, as Juno pauses, other firms are advancing. Analysts anticipate that Kite Pharma or Novartis could launch the first anti-CD19 CART therapy in 2017.—ANN THAYER

ASIA

China is slowing down, but regional growth is solid

Key sectors of the Chinese economy are going strong. India is booming, and chronically weak Japan is not in a recession. It’s unclear how Brexit or the new U.S. administration will impact Asia, but the outlook for 2017 is positive for chemical companies operating in the region.

Managers are talking about expansion. “Our key focus for 2017 will be to increase local manufacturing in Asia,” says Mike Horton, the China-based president of Asia-Pacific operations for the paint, coatings, and specialty materials producer PPG Industries.

PPG’s desire to expand its manufacturing footprint in Asia stems from an optimistic view of sales growth in the region. Although the Indian economy is growing faster in percentage terms, China will be where most economic expansion takes place in absolute terms. Horton says it is China where PPG will look first to build new plants or acquire existing ones to accommodate demand growth, particularly from the automotive sector and, surprisingly, construction.

Despite the Chinese media attention that tens of thousands of surplus apartments have attracted, they are more the exception than the rule in the country, Horton claims. Demand absorbs new supply in many cities, he says. And outside the housing sector, he adds, the government is investing in the construction of new airports and train stations.

Finally, consumer demand for new cars remains strong, with the China Association of Automobile Manufacturers reporting 14% growth during the first 10 months of 2016. Demand should remain robust in 2017. Horton says, although the possible phase-out of a government subsidy for the purchase of small cars might affect sales temporarily.

At BASF, Sanjeev Gandhi, the board member responsible for Asia and the Pacific, is also upbeat about 2017. Notably, he expects an improvement in profit margins for materials used in the manufacturing of polyurethanes. BASF produces these raw materials at massive plants in Shanghai and Chongqing, China.

The slowdown in China is not a significant concern, Gandhi argues. One of the reasons it happened, he says, is that the economy has been through a restructuring to lessen dependence on export-oriented manufacturers. This rebalancing, he says, was one of the most positive and significant changes to happen in Asia in 2016.

Meanwhile, Japan, Asia’s second-largest economy, will not be dragging down the region. In its latest outlook report, the Manila-based Asian Development Bank notes that Japan should manage to grow by almost 1% in 2017. Overall, the bank expects the economies of Asia to be stable in 2017. Excluding Japan, it says, Asia will grow by 5.7%.—JEAN-FRANÇOIS TREMBLAY
RENEWABLES

Paris Agreement, consumers to drive demand for biobased chemicals

In 2017, the 114 countries that signed and ratified the Paris climate change agreement will start rolling out strategies for meeting their commitments. Together they account for almost 80% of global emissions of greenhouse gases. This year, those policies will dovetail with consumer preferences—and increasingly stringent product policies at major retailers—to tilt supply chains in favor of bio-derived ingredients.

Although the U.S. ratified the Paris Agreement, it is unclear whether the new Trump Administration will implement the policies needed to reduce emissions. Similarly, Trump’s appointees may be less inclined than the Obama administration to back new renewable technologies through loans and grants.

As always, companies will sell into markets that offer incentives. In biofuels, low-carbon fuel standards in California, Oregon, and Washington will attract shipments of cellulosic ethanol from the Midwest.

Northern European nations are investing in facilities that make fuel from wood. China and other Asian countries are raising biofuel targets, but so far rely on first-generation biofuels.

Firms working to commercialize biobased chemicals will continue to find the rest of the world more welcoming than the U.S.—especially while oil prices are low. Many of the largest producers of biobased materials are located in Brazil, Canada, France, Italy, and Indonesia.

In April, biobased specialty chemical firm Elevance Renewable Sciences, which has its main plant in Indonesia, sold a site in Natchez, Miss., where it had planned to start chemical production. BioAmber, now in Canada, plans to start bio-succinic acid production in China. And Amyris is working with the government of Queensland, Australia, to make biobased farnesene and other products for the Asian market.

But all is not lost for biobased companies in the U.S. Synthetic biology firms such as Zymergen and Ginkgo Bioworks that develop microbes for biobased chemical makers attracted hundreds of millions of dollars from venture capitalists last year. “Growth of these platforms should lead to even bigger numbers for the segment in 2017,” Lux Research predicts.

Meanwhile, Green Biologics, which makes biobased n-butanol and acetone using modified microbes, has begun shipping from its plant in Little Falls, Minn. There are commodity markets for those chemicals, but the firm is focusing on applications—such as cosmetics and specialty coatings—where biobased inputs are highly sought or offer better performance.

“Necessity and the market drove us here,” explains Tim Staub, head of business development for Green Biologics. “We work through one application at a time, differentiate where we can, and avoid those where we can’t.”—MELODY BOMGARDNER

CANADA

New spending may knock country out of a rut

Once again, the Canadian chemical industry was true to its slow and steady form in 2016. However, 2017 should prove to be an exciting year for Canadian chemical makers. Plans for multi-billion-dollar expansions may receive final go-ahead, while mergers and acquisitions are set to create bigger Canadian companies.

Sales for the sector declined by 2% in 2016 to $17.3 billion, according to the Chemistry Industry Association of Canada (CIAC), the country’s industry trade group, largely due to lower selling prices. Volumes increased by nearly 4%. This year, CIAC sees sales increasing 1% as prices strengthen, but volumes are expected to decline by 2%.

Capital spending in Canada fell nearly 8% in 2016, to $815 million, according to David Podruzný, CIAC’s vice president of business and economics, as companies wrapped up expansion projects.

Now, another wave of expansions may soon be coming to Canada. Last month, the Alberta government approved hefty incentives for two proposed petrochemical projects. “If they go ahead as projected, we should see capital spending ramping up,” Podruzný says.

About $225 million in government royalty credits are earmarked for a joint venture between Petrochemical Industry Co. of Kuwait and Pembina Pipeline Corp. It plans to build a $3 billion complex to convert propane into propylene and then polypropylene.

Another $150 million in royalty credits is set aside for Inter Pipeline, which also wants to build a propane dehydrogenation plant in Alberta. That project was first unveiled a year ago by another firm, Williams Cos. North American Polypropylene (NAPP), an affiliate of the U.S. private equity firm Gaordia Capital, signed on to build a related polypropylene plant.

NAPP is now suing Williams and Inter Pipeline in a Texas court. NAPP alleges that Williams cut it out of the project when Williams sold its Canadian operations to Inter Pipeline.

The Canadian industry is also seeing sizable consolidation. Last month, Chemtrade Logistics agreed to purchase Canexus for $680 million. Chemtrade makes inorganic chemicals, including sulfuric acid and sodium nitrate. Canexus makes chlorine and sodium chloride.

Additionally, two of the nation’s largest fertilizer makers, Potash Corp. of Saskatchewan and Agrium, are merging to form a company with $21 billion in annual revenues.—ALEX TULLO
ELECTRONIC MATERIALS
Stars will align in semiconductors and displays

Usually, suppliers of electronic materials can’t catch a break. When business is booming in flat panel displays, the semiconductor industry is in the doldrums. Or vice-versa. This year, though, demand should be strong from both major markets.

“It’s almost too good to be true,” says Mitsunobu Koshiba, president of the electronic chemicals producer JSR. The company produces materials used by both display and chip makers.

The price of displays didn’t drop as much as expected in 2016, with the consequence that materials makers weren’t under heavy pressure to drop their prices. Materials suppliers had feared a disaster with the ramp up of new display plants in China that would flood the market, Koshiba recalls. In anticipation, Samsung closed production lines in South Korea that together accounted for 3% of world display supply, Koshiba says. “The market is well balanced now,” he says.

The robustness of the semiconductor market is also a surprise, Koshiba notes. At the beginning of 2016, semiconductor makers expected demand to weaken in the second half of the year, once manufacturers had shipped their Christmas season orders. Instead, “by June, the industry noticed that chip inventories were too low,” he says.

Demand has been strong for the workhorse chips, cut from 200 mm silicon wafers, that are often used in vehicle electronics, according to Mark Thirsk, a partner at the electronic materials research firm Linx Consulting. It has also been strong for cutting-edge chips featuring ultrathin circuit lines that are typically produced from 300 mm wafers. In between, demand for more standard chips made from 300 mm wafers is softer.

Multiple patterning, a manufacturing method that involves repeated lithographic exposure of silicon wafers, is also driving demand, Thirsk notes. Each exposure results in 10 to 15 additional manufacturing steps requiring deposition chemicals, etchants, cleaners, and other materials.

In 2017, the electronics industry eagerly anticipates the first commercial use of extreme ultraviolet lithography after several years of delay. But it’s not clear how profitable extreme ultraviolet lithography will be for materials suppliers, Thirsk says. JSR and other companies have invested so much in the necessary materials that it could be difficult for them to harvest much of a profit, even with premium pricing.

The electronic materials industry is full of surprises and rapid boom-bust cycles. Not all materials will do well in 2017. Color filters for displays, for instance, are badly oversupplied, Koshiba notes. But on the whole, suppliers should enjoy a rare period when most of their business shines.—JEAN-FRANÇOIS TREMBLAY

Both chip fabrication and display manufacturing should do well in 2017.

Contractors, such as France’s Axyntis, should see the negative countered with the positive for another good year.

OUTSOURCING
Pharmaceutical chemicals expected to glide through political, pipeline waves

The pharmaceutical chemicals sector has been in a rut for several years—a very nice rut in which most companies report double-digit growth serving an industry with an ever-growing appetite for contract manufacturing and related services. The year ahead promises more of the same, but with a few significant disturbances in the landscape.

“Call it the year of extreme volatility,” says Guy Villax, CEO of Hovione, a Portuguese contract manufacturer. He and others point to countervailing forces of political uncertainty in the U.S. and Europe on the one hand, and a validated strategy of serving the drug industry’s growing outsourcing needs on the other.

James Bruno, president of the consulting firm Chemical & Pharmaceutical Solutions, also senses uncertainty. “With this presidential election, I think everybody is adopting a wait-and-see attitude,” he says. President-elect Trump is promising a big corporate tax cut, Bruno points out, but interest rates have already risen and are likely to go up again.

And there are other signs of concern. Bruno points to a drop in U.S. drug approvals to 22 in 2016 from 45 in 2015. “People are wondering if this is a fluke because we set a record the year before, or are we back to there not being a really good pipeline?”

Consultant Roger LaForce sees the year ahead as one of consolidation in the wake of recent deals. Closing out 2016 was the purchase of a big Zach System plant in Italy by Fabbrica Italiana Sintetici, a move that will create one of the largest contract manufacturers globally, LaForce says. And everyone points to Lonza’s recent agreement to buy Capsugel as solidifying the contract development and manufacturing organization model of offering everything from drug active manufacturing to final dosage formulation. As drug companies drop in-house manufacturing, they are contracting on a strategic basis, Villax says, and require a broad range of services.

“People will be going more and more toward the one-stop shop,” agrees Ampac Fine Chemicals CEO Aslam Malik. In general, Malik sees acquisitions picking up. “People will start buying in 2017. And if you are the sell side, you will get a good price,” he adds, noting that Lonza is paying $55 billion for Capsugel.

For some, the positive and negative forces will likely balance out, making for continued clear sailing this year. “In the end, I’m not sure anything really changes,” says Shawn Cavanagh, chief operating officer of Cambrex. “The market overall has been and will continue to be good for contract manufacturers who have invested in capacity and capabilities.”—RICK MULLIN
SPECIALTY CHEMICALS

Sector is expected to regain momentum this year

Globally, specialty chemicals output is expected to regain momentum in 2017 after a slower-than-expected increase in 2016, according to the American Chemistry Council. The trade association anticipates a production rise of 3.3% in 2017 after a 2.6% increase last year.

ACC had expected a 3.9% production jump in 2016, but the downturn in oil and gas drilling, a global slowdown in manufacturing, and weakness in China held production back. Observers are now looking for a stronger year for specialties because of higher energy prices, renewed infrastructure spending, and a potential manufacturing uptick, particularly in the U.S. and Asia.

Paint, now a $135 billion-per-year global market, could see 3% output growth in 2017, says Phil Phillips, president of Chemark Consulting. Adhesives and sealants, a $45 billion market, will grow in tandem with paint, he adds.

In the U.S., the incoming Trump Administration is likely to trigger a rise in demand for highway markings and sealants as well as paint used on rail cars, Phillips says.

Pipeline construction projects under the new administration should spur demand for powder coatings used on pipe interiors to increase the flow of oil and gas to their destination, Phillips adds. Similarly, pipeline construction in China to speed fuels to market for a growing middle class will increase coatings demand, he says.

In addition, U.S. infrastructure spending will spur production of additives that aid concrete’s workability and improve its durability, says Ray Will, a director at the consulting firm IHS Markit. U.S. demand for the additives generally grows at about 3% a year, but he predicts a 5% increase this year.

If the Trump Administration renegotiates trade agreements, as it has threatened to do, U.S. exports of specialty chemicals could be compromised, Will warns. On the other hand, if the administration succeeds in expanding the U.S. manufacturing base, then specialty chemical makers will benefit from stronger local demand, he says.

Higher energy prices may be on the horizon if Saudi Arabia is able to get oil-producing nations to limit output. If that transpires, U.S. oil producers will increase their own output, Will predicts, pushing up demand for oilfield chemicals.

Specialty chemical production targeted at consumers will also rise. Kunal Mahajan, who tracks the $90 billion-per-year specialty cosmetic ingredients segment at the consulting firm Kline, says growth for the category is fastest in Asia where consumer buying power is on the rise. Demand for ingredients such as sunscreens, rheology modifiers, and preservatives will grow at about 7% in China and India this year, compared with 2% in the U.S. and other developed countries.—MARC REISCH

LATIN AMERICA

A struggling region looks for recovery

Stretching roughly 10,000 km from the Rio Grande to Tierra del Fuego, Latin America cannot be generalized. Economic performance in the region ranges from disaster (Venezuela) to stability (Mexico).

But it is fair to say that the the region’s economies have been slumping recently. The world’s economy grew by 11% since 2013, but collectively Latin America hasn’t seen any growth, according to the International Monetary Fund. And although the situation might not get worse, 2017 isn’t likely to be much of a year for recovery either.

The region’s largest economy, Brazil, is experiencing its “deepest recession in decades,” IMF says, noting that the problem is compounded by a corruption scandal and political crisis that led to the ouster of President Dilma Vana Rousseff in August of last year. IMF says the “recession may be nearing its end” and expects a smidgen of economic growth in 2017.

IMF expects that growth in Argentina will rebound as a new government, sworn into office in late 2015, improves management of the economy. There is no such hope in Venezuela, where the economy contracted a staggering 10% in 2016, leading to food scarcity and a breakdown in social order. Mexico, IMF says, will likely remain on its steady course.

Rina Quijada, senior director at IHS Markit’s Chemical Insight business in Latin America, says Brazil’s largest chemical maker, Braskem, is succeeding despite the slack home economy. Exports helped keep production at high levels even though plastic resin demand in Brazil declined by an estimated 5% in 2016.

In Mexico, the main event has been the start-up of a new ethylene and polyethylene joint venture between Braskem and the Mexican firm Idera. However, the state oil company Pemex, in order to supply the partnership with feedstock ethane, has had to throttle back its own production of ethylene and its derivatives.

“A common denominator in most of the countries is that the state-owned oil companies are financially distressed,” Quijada says.

An exception, she says, is Argentina’s YPF, which is starting to produce significant quantities of natural gas from shale. Dow Chemical, which has partnered with YPF in natural gas exploration, is interested in using the new gas source as a feedstock for its Argentinian operations and possibly for an expansion. Quijada thinks this could lead to a new chemical project early in the next decade.—ALEX TULLO
INSTRUMENTATION

Pharma and diagnostics offer continued growth

As sellers of a range of products across several industries, lab and analytical instrument suppliers can find their businesses rocked by all sorts of market dynamics. Sometimes the net result is positive; other times not. “While 2016 offered a strong combination of improving end markets, the 2017 outlook is less compelling,” Goldman Sachs stock analyst Isaac Ro told clients in a recent report.

Several factors are in play this year. U.S. academic funding has benefited from legislation, such as the 21st Century Cures Act, but any annual increases are not guaranteed under the new administration, Ro pointed out. Meanwhile, growth is modest in Japan, somewhat stronger in China, and slowing in Europe.

On the industrial side, lab spending should be helped by policy changes—such as the Paris Agreement on climate change and China’s latest five-year plan—and a slightly higher forecast for the global economy, Ro added. Biopharmaceutical production remains strong, but drug R&D spending is decelerating and could be disrupted by a pickup in mergers and acquisitions.

Instrumentation sales reached about $47 billion in 2016 and are anticipated to grow about 4% in 2017, according to Agilent Technologies. “Predicting end-market growth in today’s uncertain political and economic environment is challenging,” Agilent CEO Mike McMullen said when reporting fiscal year sales in November.

The slowest growing end markets are chemicals and energy, which makes up about 10% of instrument sales, and academia and government, which together are just under 20%. Both are expected to increase by 1–3% in 2017. Sales to the pharmaceutical sector, which is 25% of the market, should grow up to 6%.

Rounding out the market and seeing the fastest growth at up to 8% is clinical diagnostics. To tap into it, suppliers have been actively building their businesses. In early 2016, Thermo Fisher Scientific paid $1.3 billion to buy the genetic analysis firm Affymetrix. More recently, Danaher spent $4.8 billion on molecular diagnostics provider Cepheid.

At the same time, equipment makers are joining with pharmaceutical and other partners to combine diagnostics with drugs. In October, Thermo Fisher joined the Cancer Moonshot initiative. Then in December, the company launched an immunotherapy program with Washington University School of Medicine in St. Louis.

Meanwhile, Roche Diagnostics’ Ventana

MIDDLE EAST

Buoyant outlook seen, as downstream diversification continues

Chemical sales in the Middle East will remain buoyant in 2017 despite challenging global economic conditions, according to the region’s largest industry organization, the Gulf Petrochemicals & Chemicals Association.

Overall, the outlook is positive, according to Ahmad Al-Ohali, CEO of Sipchem, a Saudi Arabian petrochemicals firm. Al-Ohali is a director on the board of GPCA. “From 2007–2016, 139 petrochemical projects were introduced in the Gulf Cooperation Council valued at $215 billion. This is tremendous growth, and there are similar opportunities in the future,” he says.

But Middle East chemical makers are concerned about the rising competitiveness of the U.S. petrochemical industry with its low-cost natural gas from shale. “The future holds no certainties,” Ohali says.

Abdulaziz Judaimi, head of chemicals for Saudi Aramco, argues that the only way to ensure competitiveness and growth is to “continue developing more differentiated, higher-value products; continue creating strong brand identities; and continue upgrading to stay ahead of the curve.”

The Middle East is already adding high-value specialty chemical products. The industry’s diversification strategy took a major step forward in November when Sadara, a $20 billion chemical complex operated jointly by Dow Chemical and Saudi Aramco, officially opened in Jubail, Saudi Arabia. The Sadara complex will produce a swathe of polymers and specialty chemicals in plants set to start up every week for the next few months. It will mostly use naphtha as feedstock.

Sadara’s opening marks “a major change point” for the Middle East, says Paul Bjacek, head of chemicals research at the advisory firm Accenture. Sadara has economies of scale combined with highly efficient processes that will make it cost-competitive globally, he says.

In line with the region’s diversification strategy, Sadara is adjacent to an industrial park for downstream manufacturing activities, including plastic part production.

Another development that promises to shape the Middle East petrochemical landscape is the lifting in 2016 of international sanctions on Iran. The country has the potential to become a major petrochemical producer in the next few years. However, headwinds loom, Bjacek cautions. “It is more than five years away because there are plenty of investment opportunities first in North America,” he says.—ALEX SCOTT
Predicting science policy under the new Administration

DONNA NELSON, ACS PAST-PRESIDENT

With the new Trump Administration entering office, conventional political wisdom is changing, and it is still too early to know exactly what that means. Nevertheless, many scientists are asking what the implications for science will be as a result of the changes in Washington, D.C. What will ACS’s priorities be, and how will the society interact with the new Administration?

President-elect Trump has been appointing his cabinet, and he is reportedly seeking counsel, studying areas of concern, and evaluating various ideas in making his decisions. The President-elect has shown that he changes his mind about people, policies, and ideas, so initial or previous discussions about topics should not be considered final.

The above activities do little to clarify his positions or thoughts on science. On Dec. 1, 2016, ACS hosted the webinar, “Looking into the Crystal Ball: Government, Politics, and the Chemistry Enterprise.” Although we cannot know future science policy, available information enables some predictions.

Considering Trump’s recent statements

President-elect Trump’s answers to the 20 questions posed by ScienceDebate.org offer some insights, with the obvious caveat that he might change his mind. Patterns in his answers reveal that they can be roughly sorted into three categories, revealing his approach to the following 20 topics:

1. Let market forces prevail (innovation, research, energy, nuclear power, food, global challenges, space, and immigration).
2. Determine how to distribute limited resources (free internet, mental health, public health, water, vaccination, and opioids).
3. Discuss the issue with interested parties (climate change, biodiversity, and scientific integrity).

Importantly, these three controversial topics are planned for discussion, for which we should prepare.

Three of the topics—ocean health, education, and regulation—fall into multiple categories.

Scientists’ message to President-elect Trump

We must ensure that Trump, his appointees, other policy-makers, and the public recognize and appreciate the value that science brings to the world. Science, technology, and the people practicing them are responsible for virtually all of the recent benefits and improvements in our lives. This is the justification for increasing funding for scientific research and education, so we must ensure that everyone knows this to generate support for science.

For science to maintain its solid foundation, be universally and highly respected, and remain reliable for the future, scientists must continue to ensure the integrity of scientific facts, peer review, and basic research in the scientific method.

Prepare to assist policy-makers

President-elect Trump must finish the urgent task of filling his cabinet positions. However, he knows that science is critical to many areas he has designated as important, such as innovation, national security, and the economy, and it is certain that he will focus on science soon. In the meantime, we should be patient and prepare a list of science issues and goals, so that when the future President and his Administration request scientific guidance and information, we will be ready to assist them. The chemistry community can help by doing the following:

1. Prepare to discuss the broad range of global issues, such as climate change; energy; cyber security; biodiversity; science, technology, engineering, and math (STEM) education; advanced manufacturing; and opioid addiction.
2. Develop the agility to respond rapidly, clearly, directly, and respectfully when the Administration needs assistance.

Finally, as always, I would greatly appreciate your e-mailing me your thoughts, ideas, and concerns at dnelson@ou.edu.

Views expressed on this page are those of the author and not necessarily those of ACS.
2017 Cope and Cope Scholar award winners

Recipients are honored for contributions of major significance to chemistry

EDITED BY LINDA WANG

The following vignettes highlight the recipients of the Arthur C. Cope Award and the Arthur C. Cope Scholar Awards, administered by the American Chemical Society for 2017. Vignettes for the rest of the ACS national award recipients were published in the Jan. 2 issue of C&EN.

Recipients of the Cope Award and Cope Scholar Awards will be honored at a ceremony at the fall ACS national meeting in Washington, D.C., Aug. 20–24.

Arthur C. Cope Award:
Carolyn R. Bertozzi

Sponsor: Arthur C. Cope Fund
Citation: For pioneering the field of bioorthogonal chemistry, and for its innovative applications to the field of glycobiology.
Current position: Anne T. and Robert M. Bass Professor of Chemistry, Stanford University
Education: A.B., chemistry, Harvard University; Ph.D., chemistry, University of California, Berkeley

Bertozzi on the biggest research challenge she has had to overcome: “Straddling interfaces between scientific disciplines that prioritize different kinds of problems and value different modes of intervention. This can make it hard, for example, to convince grant review panels to fund a proposal, or journal editors to publish a paper. It takes significant patience and persistence, sometimes, but it’s worth the effort!”

What her colleagues say: “Bertozzi has pioneered a field called bioorthogonal chemistry, and has applied this novel chemistry to install artificial sugars on the surface of living cells. The approach allowed her to study the role sugars play in diseases like cancer and inflammation, and to target specific cells in a living body for imaging or drug delivery applications.”—Chaitan Kho sla, Stanford University

Arthur C. Cope Scholar Awards:

Alejandro L. Briseno

Citation: For his outstanding accomplishments on the design and synthesis of unconventional, chemically stable polycyclic aromatic hydrocarbons and their charge transport properties.
Current position: associate professor of polymer science and engineering, University of Massachusetts, Amherst
Education: B.S., biology, California State University, Los Angeles; Ph.D., organic materials chemistry, University of Washington, Seattle

Briseno on what gets his creative juices flowing: “Like most scientists, we become fascinated by the unexplainable. My creative juices begin to flow when we make leaps and bounds towards understanding the observations we were previously unable to comprehend. Oftentimes, the juices flow too hard and we lose sleep. We need to be careful when this happens because it is important to rest our minds and step away in order to return with a fresh perspective.”

What his colleagues say: “Briseno is internationally recognized for developing efficient synthetic routes to achieve chemically stable oligoacenes and oligothiophenes for application in organic electronics. His research is also renowned for studies centered on crystal growth mechanism and fundamental charge transport in organic crystals and polymer thin films.”—Antonio Facchetti, Northwestern University

Sherry R. Chemler

Citation: For the development of stereoselective copper-catalyzed alkene difunctionalization reactions and their applications in the synthesis of saturated oxygen and nitrogen heterocycles.
Current position: professor of chemistry, University at Buffalo, SUNY
Education: B.A., chemistry, Boston University; Ph.D., chemistry, Indiana University

Chemler on what she hopes to accomplish in the next decade: “I’d like to provide a practical solution to a problem of global significance, likely in the areas of sustainability and health care, while concurrently pushing the envelope of new reactivity in organometallic chemistry.”

What her colleagues say: “Chemler has been at the forefront of the discovery and development of a powerful new category of chemical transformations—transition metal catalyzed polar/radical cascades. She has chosen to work with Cu(II), a cheap and abundant transition metal, and alkenes, readily available organic substrates. Her primary synthesis targets are nitrogen and oxygen heterocycles, moieties of critical importance to the pharmaceutical industry. Her discoveries in this area offer original and effective solutions to truly important problems.”—John P. Richard, University at Buffalo, SUNY
Guangbin Dong

Citation: For his outstanding accomplishments on transition-metal catalyzed synthetic methods involving carbon-carbon and carbon-hydrogen bond activation.

Current position: professor of chemistry, University of Chicago

Education: B.S., chemistry, Peking University; Ph.D., chemistry, Stanford University

Dong on what gets his creative juices flowing: “It often starts with a good question being asked by either the students or myself. Some questions are purely driven by curiosity; others are driven by known unsolved problems. These questions provide inspiration for creating new approaches.”

What his colleagues say: “His creativity and insights establish him as one of the very best young organic chemists in his generation.”—Stephen F. Martin, University of Texas, Austin

P. Andrew Evans

Citation: For his development of innovative rhodium-catalyzed reactions and their applications to the synthesis of biologically relevant complex molecules.

Current position: professor and Alfred R. Bader Chair of Organic Chemistry, and Tier I Canada Research Chair in Organic & Organometallic Chemistry, Queen’s University

Education: B.Sc., applied chemistry, Newcastle Polytechnic; Ph.D., synthetic organic chemistry, University of Cambridge

Evans on what gets his creative juices flowing: “I have always been very competitive, which is why I like to work on challenging problems. I think I have done my most creative work when the initial plan has not worked out as anticipated.”

What his colleagues say: “Andy has become a leader among his peers, and his star is still clearly on the rise. Although he has already made an impact in methods development, heterocyclic synthesis, and natural products synthesis, I think that it does not compare to the influence he will bear on the field in the next few years as he continues to develop allylrhodium chemistry.”—Gary A. Molander, University of Pennsylvania

M.G. Finn

Citation: For the development of chemical ligation methods and platforms, applied to bioconjugation and materials chemistry.

Current position: professor and chair of chemistry and biochemistry, and professor of biology, Georgia Institute of Technology

Education: B.S., chemistry, California Institute of Technology; Ph.D., inorganic chemistry, Massachusetts Institute of Technology

Finn on what gets his creative juices flowing: “The students and postdocs that I work with, and the colleagues that I talk to. And a good problem to think about. Those are what send me to the literature, and then, every once in a while, to a good idea. The longer I’m around, the more things I find interesting, which is helpful.”

What his colleagues say: “The Cu-catalyzed and in situ click chemistry work from the Finn laboratory has inspired thousands of reported applications by academic and industrial laboratories in organic, medicinal, biochemical, and materials chemistry. Professor Finn also initiated the exploration of the organic chemistry of virus-based nanoparticles and their use as platforms for biologically active polyvalent structures, leading the way to what is now a very active area of research the world over.”—Mostafa A. El-Sayed, Georgia Institute of Technology

Paul J. Hergenrother

Citation: For innovative use and application of organic synthesis to solve critical problems at the frontiers of chemical biology and translational drug discovery.

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

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

Hergenrother on what gets his creative juices flowing: “I am most interested in understanding currently intractable problems in medicine and thinking about how we can use chemistry to solve them. We live in a special time, where genomic data now allow for an unprecedented look at the molecular features of disease, and it is up to chemists to find the right drug for the right patient.”

What his colleagues say: “Hergenrother is a leader in academic compound screening and development, and in thinking about the types of compounds that should be populating compound screening collections. Typical compound collections are largely composed of small molecules that are flat and hydrophobic. He uses readily available complex natural products as the starting point for the drug discovery process and converts them to compounds of equal complexity but high diversity.”—Stephen F. Martin, University of Texas, Austin

Thomas R. Hoye

Citation: For creative contributions across an impressively broad spectrum of organic chemistry, including the development of the hexadehydro-Diels-Alder (HDDA) reaction.

Current position: professor of chemistry, University of Minnesota, Twin Cities

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

Hoye on his biggest research challenge: “Maintaining an adequate balance between my levels of (i) commitment to research coworkers, and (ii) secured research funding, a challenge shared by many. This is exacerbated with each passing year and decade as our academic institutions, country-wide, take ever-increasing portions of research grant dollars into their central coffers via ever-escalating tuition (and overhead) rates. My first NIH R01 grant award, the direct costs of which have grown in lock-step with inflation, allowed me to support six graduate research assistants; my latest grant: three and a half.”

What his colleagues say: “The sheer breadth of his program alone marks Tom as a rare breed—all the more so when considered in light of the high caliber of his contributions. Tom is one of those few whose work just keeps getting better and better. This speaks further to his dedication and full commitment to his science.”—Amos B. Smith, University of Pennsylvania
Kathlyn A. Parker

Citation: For outstanding and creative contributions to the synthesis of structurally complex organic targets.

Current position: professor of chemistry, Stony Brook University, SUNY

Education: B.A., chemistry, Northwestern University; Ph.D., organic chemistry, Stanford University

Parker on her scientific role models and why: “I have several role models who were my mentors. Jim Marshall, my chemistry teacher in college—not only is he a superbly organized lecturer but he personally taught me how to work in the lab. W. S. Johnson, who taught high standards. Gilbert Stork, who has the ability to share his thought processes ... what a teaching skill that is! And Madeleine Joullie, who is a more recent friend. Madeleine never quits, and she never loses her good humor.”

What her colleagues say: "Kathy’s contributions to organic synthesis place her among the notable players in this field. Her recent publications are strong and have attracted significant attention. She is known internationally for her compact and creative syntheses of complex natural product targets. Her approach is to invent novel—and efficient—solutions to challenging problems in synthesis. Her work epitomizes excellence in organic chemistry and is most certainly deserving of recognition with a Cope Scholar Award.”—Nicole S. Sampson, Stony Brook University

Mikiko Sodeoka

Citation: For her seminal contributions to the fields of transition-metal chemistry, synthetic organic chemistry, organofluorine chemistry, and chemical biology through the development of innovative methodologies and tools.

Current position: chief scientist, RIKEN, Japan

Education: B.A., Ph.D., pharmaceutical science, Chiba University, Japan

Sodeoka on her scientific role models: “There are many scientists who influenced me, but if I have to choose, it is my former mentor, Professor Masakatsu Shibasaki. His enthusiasm to chemistry opened up my passion as a researcher, and I learned many important things from him. Professor Masako Nakagawa, a supervisor when I was a student, is also my role model. She was one of the rare female organic chemists in Japan at that time and showed me that women can be excellent chemists.”

What her colleagues say: “Dr. Sodeoka’s pioneering works and a series of publications opened a new avenue of research in transition-metal chemistry and catalysis, triggering extensive follow-up studies around the world. She has also expanded her superb synthetic skills and creative thinking to chemical biology and has been making seminal contributions.”—Iwao Ojima, Stony Brook University, SUNY

Christopher D. Vanderwal

Citation: For the development of efficient chemical syntheses of structurally complex and biologically significant natural products.

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

Education: B.Sc., biochemistry, M.Sc., chemistry, University of Ottawa; Ph.D., chemistry, Scripps Research Institute

Vanderwal on what he hopes to accomplish in the next decade: “I’d love to crack into something really important in biology without compromising my love of the creativity of natural product synthesis. In other words, I want to continue to spend time doing what I love best, but see (and show) its impacts.”

What his colleagues say: “Chris Vanderwal’s accomplishments to date, coupled with his remarkable creativity and exquisite taste in problem selection, establish him as one of the world’s leading synthetic organic chemists. The short chemical synthesis strategies introduced by Vanderwal are defining what is possible in chemical synthesis today.”—Larry E. Overman, University of California, Irvine

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Happy rats: Pink ears, widely angled.

Now, a group of researchers from the University of Bern has documented how to spot happiness in rats (PLOS One 2016, DOI: 10.1371/journal.pone.0166446). After all, gauging the happiness of research rats can be important for certain studies.

So how does one make rats happy? By “playful manual tickling administered by the experimenter,” the Bern researchers report. They used two different tickling procedures. In one, the experimenter used one hand to turn a rat on its back and tickle the rat’s neck, chest, and stomach areas using the same hand. The other procedure involved using two hands to hold a rat on its back and tickling the sides and nape of the neck.

Rats that appeared to like tickling—those that emitted positive vocalizations during tickling and that seemed to seek out the experimenter’s hand for more—were used to determine facial indicators of positive emotion. They had pinker ear color and ears angled more to the side and back.

At least, those are the indicators presented by 15 male rats of a specific type used by the Bern researchers. As with much clinical work, more studies with greater diversity of subjects are needed to determine whether pink, widely angled ears indicate happiness across all rats.

Jyllian Kemsley wrote this week’s column. Please send comments and suggestions to newscripts@acs.org.
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