Update

STATE OF THE UNION ADDRESS IDENTIFIES IMPORTANCE OF MANUFACTURING AND ENERGY TO U.S. ECONOMY

President Obama identified several topics of interest to chemical engineers and the chemical industry, including manufacturing and energy, in his State of the Union address on Jan. 24. Industry reactions to Obama's speech varied. Several industry groups applauded Obama's emphasis on U.S. manufacturing but raised concerns that U.S. regulations could thwart such an initiative. Others focused on Obama's call for domestic energy development.

"We will not go back to an economy weakened by outsourcing, bad debt, and phony financial profits. Tonight, I want to speak about how we move forward, and lay out a blueprint for an economy that's built to last — an economy built on American manufacturing, American energy, skills for American workers, and a renewal of American values," Obama said.

In his hour-long speech, Obama introduced several initiatives as part of his "blueprint for an economy that's built to last." These include: keeping manufacturing in the U.S., expanding domestic energy production, and encouraging innovation, among others.

Obama spoke about the importance of bringing manufacturing back to the U.S. and how tax code changes will support this initiative. He called for a minimum tax for multinational companies that would go toward lowering taxes for companies that create jobs in the U.S. He also recommended giving high-tech companies an even bigger tax cut. "If you're a high-tech manufacturer, we should double the tax deduction you get for making your products here."

Creating new jobs will also come from innovation, Obama said. "After all, innovation is what America has always been about. Most new jobs are created in start-ups and small businesses," he said. In support of innovation, Obama encouraged Congress to continue investing in basic research. "Don't gut these investments in our budget … Support the same kind of research and innovation that led to the computer chip and the Internet," he said.

Innovative technologies have opened up millions of acres of land for oil and gas exploration, Obama noted, emphasizing the positive impact innovation has had on American-made energy. He cautioned, however, that with just 2% of the world's oil reserves, the U.S. could not pin its hopes on oil alone. "This country needs an all-out, all-of-the-above strategy that develops every available source of American energy," he said.

On natural gas, Obama boasted that the U.S. now has enough reserves to last America nearly 100 years, and shale rock has become an important source. He remarked that public research dollars are responsible for the technology used to extract natural gas from shale rock — touting the role of government support in energy development.

The Society of Chemical Manufacturers and Affiliates (SOCMA) is "pleased … that the president mentioned the importance of manufacturing," the organization said in a statement. "The association shares his passion for renewing America's robust manufacturing capability, but numerous concerns remain on how we arrive there," SOCMA said. "The chemical industry is staring down numerous regulations threatening its ability to compete … The EPA's Boiler MACT rule and its proposal to weaken our industry's competitiveness in developing new chemicals by forcing them to reveal confidential business information are prime examples."

The National Association of Manufacturers (NAM) is also concerned about the impact of regulations on U.S. manufacturing. According to NAM, it is 20% more expensive to manufacture in the U.S. than in the largest trading partners of the U.S. This cost gap "is not the work of our competitors but rather is self-inflicted by Washington," NAM said. "The Obama Administration must take action to put an end to the rampant overregulation and overreach by the National Labor Relations Board and the Environmental Protection Agency," it said.

A national energy strategy "must encourage robust energy development, diversify energy supplies, and give energy efficiency its due," the Ameri-

▲ President Barack Obama delivered the State of the Union address in the House Chamber at the U.S. Capitol on Jan. 24, 2012. Image courtesy of Pete Souza, the White House.

can Chemistry Council (ACC) said in response to the speech. "Fortunately, a golden opportunity is right under our feet … Natural gas from shale is a prime example of the 'homegrown energy' the President wants America to use. It's a game changer for the chemistry industry and other manufacturers, who can use more affordable and stable supplies to expand exports and create jobs," ACC said.

The reactions of scientific societies also varied. The American Association for the Advancement of Science (AAAS) noted the leanness of Obama's focus on science and technology. Compared with past years, AAAS said, "this year's State of the Union address did not place as much focus on energy innovation, technology and research." The American Chemical Society (ACS) agreed with Obama that, "our nation's economic recovery is directly tied to reinvigorating manufacturing and creating jobs across multiple sectors leading to broad-based prosperity."

AIChE has not traditionally commented on the State of the Union address or other speeches, but has focused on providing technical information on specific technical and regulatory matters that impact chemical engineers through activities such as congressional briefings and white papers.

MATERIALS

Scorpions Inspire Tough Surfaces

The bionic shield that protects scorpions from the violent sandstorms that sweep across their desert home forms the basis of a new strategy for making tougher surfaces.

One of the major causes of damage to process equipment is erosion by solid particles — the loss of material caused by dirt, grit, and other hard particles striking the surface. Methods do exist to protect equipment from particle erosion. Filters can be used to capture particles before they strike the surface, but these must be cleaned and replaced frequently. High-performance alloys and other surface-treatment technologies have been developed, and while these do significantly improve erosion resistance, they also greatly increase the cost of manufacture.

To devise better protection methods, Zhiwu Han, a professor of bionic engineering at Jilin Univ., and Wen Li, a professor at Jilin, and their colleagues have turned to the yellow fattail scorpion for inspiration.

"Some creatures living in sandy deserts, such as lizards, scorpions, and snakes, inevitably suffer erosion when hit by blowing sand at a high speed," Han says. "However, these species can live on sand and do very well under highly erosive conditions. This has provided a clue to the development of bionic methods for reducing erosion," he adds.

The body of the scorpion consists of three regions: the prosoma (*i.e.*, head), the mesosoma (*i.e.*, abdomen), and the metasoma (*i.e.*, tail). The researchers have identified the dorsal surface of the mesosoma as the part of the scorpion that is most subjected to sand and susceptible to erosion. This surface is covered by chitinous cuticle, which is hard and tough, and protects the scorpion if it is hit by sand or attacked by predators.

The researchers created models of the bumps and grooves on the cuticle surface of the scorpion's dorsal side by scanning the arachnid (which was first anesthetized) with a 3D laser and then fitting the data to curves by the least-squares polynomial curve-fitting method. The team then developed computer simulations to study how sand-laden air moves around the bumps and grooves of the scorpion's back. Based on their findings, they created actual samples with different surface morphologies and tested them experimentally in a wind tunnel.

▲ The scorpion has evolved a sophisticated shield to protect itself from damage caused by desert sandstorms.

They found that a series of grooves on the surface at a 30-degree angle to the flowing air provided the best protection against particle erosion.

"The special flow pattern in the groove has significant influence on the erosion resistance of the grooved sample," Li says. The rotating flow of air that occurs in the grooves has a cushioning effect, slowing down particles and reducing their impact energy. In addition, the rotating flow allows some particles to leave the surface along with the airflow and avoid impact.

The groove dimensions also play a role in erosion resistance, the researchers say. The distance (D) between grooves had the largest impact, followed by groove height (H), and then width (W); the optimal combination of these dimensions was: D = 2 mm, W = 5 mm, and H = 4 mm.

The research team says that its findings can be used to design better erosion-resistant surfaces for rocket motor tail nozzles, helicopter rotors and gas turbine blades, and other industrial equipment.

NANOTECHNOLOGY

Nanorods Line Up for Assembly

A simple method to control the self-assembly of nanorods could help overcome a major obstacle to using these tiny rods in electronic and optical devices.

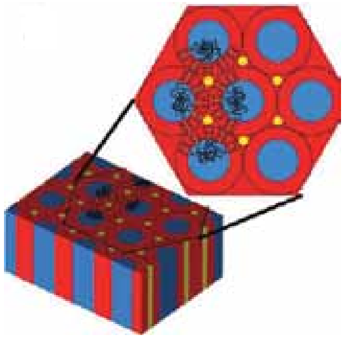
Nanoparticles of different shapes, sizes, and compositions exhibit unique

physical properties not demonstrated by their bulk counterparts. These extraordinary physical properties — optical, electrical, and mechanical — depend on the arrangement of the nanomaterials as well as on the properties of the individual particles. While methods have been developed to assemble and align some nanoparticles, including nanospheres, relatively little progress has been made for anisotropic materials such as nanorods.

Developed by researchers from the U.S. Dept. of Energy's (DOE) Lawrence Berkeley National Laboratory (LBNL), the new process relies on a block copolymer to guide the assembly of the nanorods.

"By varying the morphology of the block copolymers and the chemical nature of the nanorods, we can provide the controlled self-assembly in nanorods and nanorod-based nanocomposites that is critical for their use in the fabrication of optical and electronic devices," says lead researcher Ting Xu, an assistant professor of material science and engineering and of chemistry at the Univ. of California at Berkeley.

Block copolymers are known to microphase separate (*i.e.*, the blocks undergo a phase separation, but because they are covalently bonded to each other, they cannot demix macroscopically like oil and water) and form periodic microdomains, a few to tens of nanometers in size. These microdomains "provide an ideal structural framework for the co-assembly of nanorods," Xu says.



▲ The microphase separation of the block copolymer (blue) forms microdomains (red), which can be used to guide the assembly of nanorods. Image courtesy of LBNL.

▲ The tomography reconstruction shown in this transmission electron micrograph of cadmium sulfide nanorods that self-assembled within block copolymers reveals their ordered macroscopic alignment. Image courtesy of LBNL Center for Electron Microscopy.

The researchers mixed cadmium-based nanorods with a block copolymer — polystyrene-block-poly(4-vinylpyridine) — and a small molecule — 3-pentadecylphenol (PDP). The morphology of the copolymer, and thus the alignment of the nanorods, can be altered by using different small molecules. The small molecule controls the conformation of the polymer chains, which in turn controls the assembly of the nanorods.

The team made cadmium sulfide (CdS) and cadmium selenide (CdSe) nanorods with four different morphologies, including two that are highly sought-after: nanoscopic networks of nanorods, and nanorod arrays parallel to microdomains of the block copolymer, Xu says.

Xu and her colleagues view their method as a platform for building complex structures and hierarchiaical patterns of nanorod-based composites.

Nanosphere Structure Boosts Light Absorption

The optical equivalent of a whispering gallery — the phenomenon that transports a faint murmur from one end of a specially designed room to another without losing a syllable — could give solar cells a boost.

Engineers at Stanford Univ. have made a whispering gallery of sorts out of tiny spheres of nanocrystalline silicon, which is used to make thin-film solar cells. Instead of manipulating sound, however, these nanospheres trap and transport light.

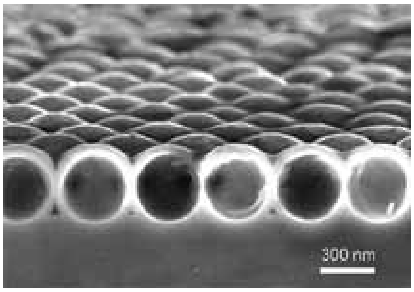
The team was able to create a layer of nanospheres just 100 nm thick that achieved performance similar to that of a micron-thick planar film of nanocrystalline silicon.

"Nanocrystalline silicon is a great photovoltaic material," says Shanhui Fan, a professor of electrical engineering at Stanford. "It has a high electrical efficiency and is durable in the harsh sun," he says.

A drawback of nanocrystalline silicon has been its poor light absorption, which necessitates the use of thick layers of the material for solar applications. Manufacturing thick layers of nanocrystalline silicon is challenging, and it can take up to five hours to produce a film as thin as 2 μm.

To make the hollow spheres, which they call nanoshells, the researchers started with a suspension of silica nanospheres, which they coated with nanocrystalline silicon using low-pressure chemical vapor deposition. Then they removed the silica spheres using hydrofluoric acid, which does not affect the silicon.

Each of the hollow spheres works like a specially designed dome — similar to the one near the famous Oyster Bar restaurant in New York City's Grand Central Station that causes sound to cling to the walls and travel along its circumference. Light is absorbed by the



▲ The thin spherical structure of the nanocrystalline silicon shown in this scanning electron microscope image improves light absorption by trapping the light inside the material, creating what are known as optical whispering galleries. Image courtesy of Yan Yao, Stanford Univ.

spheres, and instead of passing through them circulates around and around the inner perimeter. This is important because it gives the silicon material more time to absorb the light's energy.

"The light gets trapped inside the nanoshells," says Yi Cui, an associate professor of materials science engineering at Stanford. "It circulates round and round rather than passing through, and this is very desirable for solar applications."

The nanoshell structure not only uses substantially less material but also reduces manufacturing time.

It can take a few hours to deposit a micron-thick flat film of solid nanocrystalline silicon. But creating nanoshells that achieve similar light absorption takes just minutes, says post-doctoral researcher Yan Yao.

The team showed the versatility of the nanoshell structure by preparing several samples — single layers, multiple layers, and one on a flexible substrate.

"This is a new approach to broadband light absorption," Yao says. "It not only could lead to better solar cells, but it might be applied in other areas where efficient light absorption is important, such as solar fuels and photodetectors," he says.

CATALYSIS

Zeolite Catalyst Makes Diesel from Naphtha

Researchers have created a zeolite that holds promise for the direct conversion of naphtha into diesel — an increasingly important process for which there is currently no commercially available catalyst.

In addition to its potential usefulness in diesel production, the new zeolite also boasts an extremely complex atomic structure that could only be determined through a combination of x-ray crystallography and transmission-electron microscopy — advancing the field of zeolite structure determination to a new level.

The conversion of naphtha (*i.e.*, the main feedstock for producing gasoline) into diesel fuel has attracted a great deal of interest because of the increased demand for diesel, together with the overproduction of naphtha. The aromatics in heavy naphtha and the olefins in light naphtha can be converted, via alkylation, into diesel. However, this process is challenging because it requires selective solid-acid

catalysts that do not cause polyalkylation and extensive olefin oligomerization, and at the same time do not deactivate as a result of coke formation. No such catalyst is commercially available.

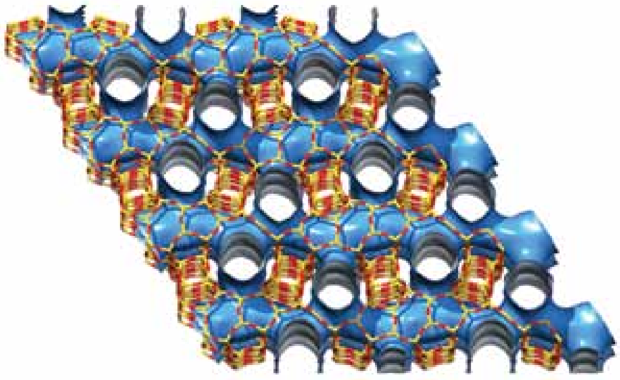
The new zeolite, called ITQ-39, is an aluminosilicate with 3D intersecting 10- and 12-ring channels. Just like other zeolites, it acts as a molecular sieve, using the size and shape of its pores to allow certain species to diffuse through the catalyst and react with the zeolite surface before exiting. This particular zeolite contains 12-ring channels with an effective diameter of 6.5–7.9 Å, which are interconnected by three 10-ring channels with an effective diameter of 4.5–6.0 Å.

"The 12-ring channels allow the aromatics to diffuse in and the monoalkylaromatics to diffuse out, while the 10-ring channels preferentially allow the C_5 to C_7 olefins to diffuse through," says Xiaodong Zou, a professor of materials and environmental chemistry at Stockholm Univ.

Much effort has gone into synthesizing such a zeolite, in the hopes of combining the catalytic behavior of two of the most successful and widely used zeolite catalysts: beta zeolite (with 3D intersecting 12-ring channels) and ZSM-5 zeolite (with 3D intersecting 10-ring channels). While zeolites sporting an internal structure of 10- and 12-ring channels have been made, most of them contain large 12-ring channels that "act more like windows" than channels, which significantly impairs their selectivity, says Avelino Corma, Director of the Instituto de Tecnología Química at the Universidad Politécnica de Valencia.

The new zeolite, called ITQ-39, contains "real" 10- and 12-ring channels that interconnect at discrete distances. The result: highly controlled flow of reactants and products.

"The large diesel molecules (*i.e.*, the reaction products) can exclusively diffuse through the 12-ring channels, while



▲ The structure of ITQ-39 (yellow and red) contains straight pairwise 12-ring channels that are interconnected by three 10-ring channels. The pairwise 12-ring channels are unique and have not been observed in any other zeolites. Image courtesy of Junliang Sun and Tom Willhammar.

the small molecules of naphtha (the reactants) can access the active zeolite sites through the 10- and 12-ring channels. The selective diffusional pathways reduce the secondary reactions and therefore the catalyst deactivation due to coke formation," Corma says.

The researchers compared the catalytic ability of ITQ-39 to that of beta zeolite and MCM-22 for the conversion of naphtha into diesel by alkylation. They achieved much higher conversions, better yields, and longer lifetimes with ITQ-39 than with the other two catalysts. (Beta and MCM-22 zeolites are used commercially for benzene alkylation, and patent literature claims their use for naphtha alkylation.)

The team took a novel approach to uncover ITQ-39's atomic structure.

"Zeolite structures are often complicated, and in the case of ITQ-39 disordered, which makes it hard to study the structure of such zeolites," Zou says. The structure of ITQ-39 was particularly difficult to determine "because this zeolite is an intergrowth of domains of three different structures, and the domain sizes are as small as a few nanometers," Zou says.

To overcome these challenges, Zou and her team developed several methods: 3D rotation electron-diffraction tomography, crystallographic image processing, and through-focus structure projection reconstruction. High-resolution transmission electron microscopy (HRTEM) images were taken of the crystals in different orientations, and these were combined to create 3D atomic structures.

"Due to the multi-level complexity of the zeolite structure, the researchers have had to extend the techniques for structure solution beyond what has been the limit in the past," says Raul Lobo, a professor of chemical and biomolecular engineering at the Univ. of Delaware, who was not involved in this research. "Consequently, the methods could be used in the future to solve both complex and simpler structures with less difficulty than has been the case," Lobo says. "It was a very elegant approach that must have required many many hours of a microscopist at the top of his or her game."

"The structure is neat as well, because it is an unexpected combination of building units of other zeolites that are known, yet assembled in a new, unique way," Lobo adds.

Update continues on next page

COMPUTING

Mini-Molecule Simulates Cellulose Pyrolysis in a Snap

Studying the high-temperature conversion of cellulose to biofuel has been a big headache for engineers, as the huge molecule undergoes tens of thousands to as many as a million reactions. Now, chemical engineers at the Univ. of Massachusetts at Amherst have discovered a tiny snippet of the molecule that behaves exactly like the full molecule, and they have used this cellulose stand-in to simulate the long-debated chemical pathways of cellulose pyrolysis.

The engineers plan to use the results of the simulation to build a complete kinetic model of cellulose pyrolysis, which could be used by biofuel producers to design and optimize their reactors.

Very little molecular information is available on the conversion of wood to biofuel via pyrolysis. The collection of such information has been hindered by the complexity of the cellulose molecule and the large number of reactions involved in the process.

Paul Dauenhauer, an assistant professor of chemical engineering at the Univ. of Massachusetts at Amherst, and his team estimated that it would take 10,000 years to simulate the high-temperature conversion of cellulose to biofuel using a first-principles computer model. First-principles simulations are time consuming because of the large number of calculations involved in modeling the formation of multiple products in a large number of parallel reactions.

"If you give every atom in the simulation the properties of its electrons and then you tell it to behave like it would in real life, you not only have to calculate how the atoms interact with each other, but then you have to calculate how that makes them change," says Dauenhauer. These calculations are repeated over and over as the reactions proceed through time, he says.

The engineers calculated how small a molecule would need to be to allow them to perform the simulation in a much shorter time. They identified about 100 molecules that fit in that size range, which they tested experimentally to determine which one behaved like the real cellulose molecule.

In order to evaluate the cellulose molecules, the engineers developed

a new thin-film pyrolysis technique, which offers several benefits over existing experimental methods (*e.g.*, powder and particle pyrolysis). Thin-film pyrolysis enables faster diffusion of volatile products through the intermediate liquid (2–4 orders of magnitude faster than in powder or particle pyrolysis) and extremely rapid temperature increases. They used this experimental method to screen the smaller molecules, and they found that the behavior of α-cyclodextrin, a small carbohydrate, is identical to that of cellulose.

The α-cyclodextrin "chemically behaves identical to cellulose — when it reacts, it vibrates and breaks apart in the same way that cellulose does. We can therefore simulate this molecule and see how it breaks apart, and that's the same way it will happen in the molecule we can't calculate," Dauenhauer says.

All of the information about the mini-cellulose molecule was plugged into the Car-Parrinello molecular dynamics model. Instead of taking thousands of years, this simulation was done in a month.

The simulation revealed the chemical pathways to the major products formed during pyrolysis of cellulose, including furans and glycoaldehyde.

"By using the mini-cellulose molecule cyclodextrin, we found that cellulose reacts to make furans in a very simple mechanism," Dauenhauer says. "We were looking at all the mechanisms that people proposed, and it wasn't even one that people have thought of," he adds.

With the chemical pathways in hand, the team plans to predict the rates of these pathways and use these to build a kinetic model of the conversion process. Once the kinetic model is defined, "we hope to be able to provide that model to any biofuel company that wants to predict how their reactor is working and how they can improve it," Dauenhauer says.

ENERGY

Process Upgrades Diesel Byproducts

A new catalytic process holds promise for converting byproducts of diesel manufacturing into higher-value chemicals in just one step.

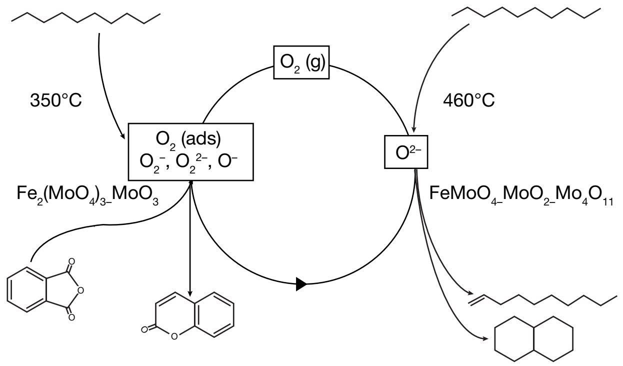
The increasing demand for diesel fuel will inevitably cause an increase in the production of diesel byproducts, including intermediate-length straight-chain alkanes (C_7–C_{12}),

which have little practical value.

"While the increased production of sulfur-free diesel has been a positive move, the glut of low-value byproducts will become a problem," says Stan Golunski, a professor of catalysis at Cardiff Univ. and Deputy Director of the Cardiff Catalysis Institute. "We hope our new process will lead to less waste and the creation of more useful chemicals for a range of industries," Golunski says.

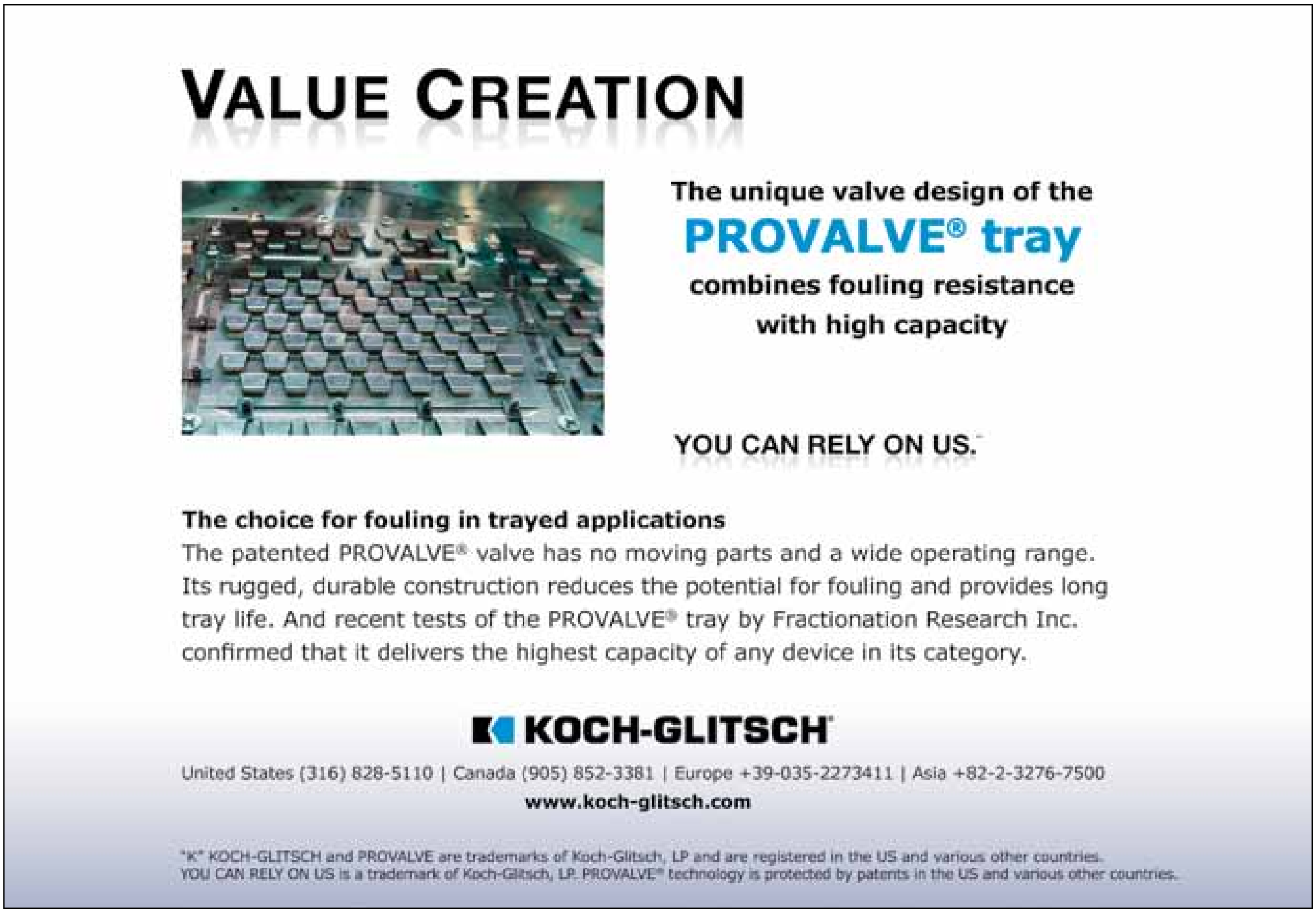
The one-step process transforms C_7–C_{12} linear alkanes into oxygenated aromatics via an iron-molybdate catalyst. While the catalyst itself is not new, this is the first time it has been used to upgrade C_7–C_{12} linear alkanes. In addition, the researchers found that the reaction is sustainable only while the mixed-metal-oxide catalyst is in its most oxygenated state — revealing new insights into the role of adsorbed oxygen species.

"This discovery breaks new ground, as it implies the involvement of oxygen that has not yet made the full transition from its molecular form to its ionic form," Golunski says. "This overturns a widely held view that this type of oxygen was too reactive to form anything other than carbon monoxide and carbon dioxide in reactions with hydrocarbons," he adds.



▲ The composition of the iron molybdate catalyst is temperature-dependent. At low temperatures (350°C), the catalyst delivers electrophilic adsorbed (ads) oxygen species, and at high temperatures (> 350°C), the catalyst delivers fully ionized lattice oxide ions. Image courtesy of Cardiff Catalysis Institute.

The synthetic conversion of C_7–C_{12} linear alkanes is fraught with challenges. These intermediate-length alkanes tend to either crack into shorter molecules, or dehydrogenate before forming useful products, depending on the presence of oxygen.



To address these challenges, the research team chose a metal molybdate catalyst. The team hypothesized that the catalyst's ability to activate and store oxygen as a selective species and its low surface acidity would be important for the partial oxidation of C_7–C_{12} alkanes.

To test their hypothesis, the researchers reacted gas-phase decane over an iron-molybdate catalyst in two temperature regimes. At higher temperatures (> 350°C) the reaction produced decene, which is used in the production of detergents, and water. At lower temperatures (250°C–350°C), the decane transforms into oxygenated aromatic molecules (*e.g.*, phthalic anhydride, which is used in the dye industry, and coumarin, which is used in the production of anti-coagulant drugs).

"The two regimes correlate with the different states of the catalyst, delivering either electrophilic adsorbed oxygen species at low temperatures or fully ionized lattice oxide ions at higher temperatures," Golunski says.

CHEM ECONOMICS

Energy Savings through Chemistry

The chemical industry produces many products that are responsible for conserving energy in a range of applications, most notably household operations, such as lighting and insulation, but also light vehicles, appliances, and packaging.

These products reduce the consumption of energy in the U.S. by 8.0–10.9 quadrillion Btu/yr, or 8.1%–11.1% of the total energy consumed in the U.S., according to an analysis recently conducted by the American Chemistry Council (ACC). For the study, ACC used data from a report prepared in 2009 by management consultancy McKinsey & Co. (*CEP*, Aug. 2009, pp. 10–11), converted the estimates of global greenhouse gas emission reductions into energy savings, and then estimated the share of those savings that is attributable to the U.S. chemistry industry. The analysis does not include the contribution of catalysts, which reduce the amount of crude oil required to produce fuel and make possible the processing of bioproducts.

To put these values into perspective, 8.0–10.9 quadrillion Btu is the amount of energy used to heat, cool, light, and power 41–56 million households — about one-third to one-half of all U.S. households. Alternatively, the energy savings could be used to power 98–135 million vehicles for a year, or 40%–55% of the cars on the road today. Chemistry makes all of this possible.

Within household operations, insulation and weatherization have been identified as the largest contributors to energy savings from chemical products. For example, the U.S. Environmental Protection Agency (EPA) estimates that homeowners can typically save up to 20% of heating and cooling costs by air-sealing their homes and adding insulation to attics, floors over crawl spaces, and accessible basement rim joists. Lighting is another major use of electricity, and newer compact fluorescent lamps (CFLs), for example, use 75% less energy than incandescent bulbs. CFLs contain noble gases (usually argon) and are coated with phosphor materials, which are products of chemistry.

The typical light vehicle today, with an average weight of 4,039 lb in 2010, contains 378 lb of plastic, or 9.4% by weight (*CEP*, Feb. 2012, p. 14). The favorable performance properties of plastics and composites are manifold, but weight savings is primary among these. For instance, composites are typically up to 40% lighter than steel parts of equal strength, and the weight reductions realized by their use translate directly into improved fuel efficiency. Improvements in synthetic rubber and reinforcing fibers have improved tire rolling (*i.e.*, lower friction and resistance) and thus energy efficiency. And, new and improved oil additives have led to greater engine efficiency. These are just a few of the many ways in which energy savings arise from chemistry in light vehicles.

Plastic housings and other components have helped to improve the energy efficiency of appliances. Today's washing machines, for example, largely use lightweight polypropylene tubs rather than heavier, stainless or enamel-coated steel tubs. The lighter tubs can be rotated with smaller motors and less energy than their heavier equivalents. In addition, insulation in refrigerators and freezers reduces energy losses.

In packaging, plastics have replaced heavier glass in many container applications. Because a plastic container weighs less than a glass container of the equivalent size, it requires less energy to transport glass bottles and jars from the producer to the consumer. Plastics have made similar inroads in other packaging applications.

These are merely the "tip of the iceberg" when it comes to energy savings from chemistry. Thousands upon thousands of energy-savings applications exist.

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AIChE JOURNAL Highlight

Chemical Engineers are Needed to "Green" the Building Industry

Unlike almost every other artifact produced by modern industrial society — such as automobiles, aircraft, and electronic devices — the design, construction, and operation of buildings is still highly fragmented and comparatively unsophisticated. Materials of construction, coatings, cladding, as well as electrical, mechanical, and other components can be selected independently with little, or no, thought given to their interactions and the effects of their coupling on the building's performance. As a result, many buildings are highly inefficient energy consumers.

New buildings are being designed to meet a higher level of quality, such as that set by the Leadership in Energy and Environmental Design (LEED) rating system, but even these buildings underperform, says Pennsylvania State Univ. chemical engineering professor Henry Foley. "The bigger problem that we face, however, is in the approximately five million commercial buildings in the U.S. that occupy a total of 71,658 million ft^2 of space and that are highly deficient in terms of their energy efficiency," Foley says. "If nothing is done, these buildings will continue to over consume and waste energy for decades to come," he warns.

In the March *AIChE Journal* Perspective article, "Challenges and Opportunities in Engineered Retrofits of Buildings for Improved Energy Efficiency and Habitability," Foley discusses the technical challenges associated with effectively retrofitting buildings and points out that chemical engineers have the training, insight, and disciplinary culture to tackle these challenges.

The primary goal of engineered retrofitting is to increase the energy efficiency of the commercial building sector by as much as 50% in 10–15 years, and to do so with better economics than are represented by doing nothing. This goal will not be met with small improvements to the current methods used by the industry, Foley says. Rather, a real solution will require breakthroughs and innovations based on completely new and deeper thinking about the problem.

"Engineered retrofitting of commercial buildings must be taken on by professionals who are used to dealing with complexity, as well as to designing and controlling systems of systems, using model-based design principles, and operating within tightly coupled economic constraints," Foley says. Chemical engineers fit this bill of requirements and are familiar with the unit operations of importance to energy consumption in buildings — heating, ventilation, and air conditioning.

▲ The Empire State Building has undergone an extensive retrofit to increase its efficiency and earn a rating of LEED Gold — symbolizing the new level of performance that can be achieved for older commercial buildings.

One way chemical engineers can contribute to building retrofits is in the use of virtual design. Process simulators that have been developed over the last 30 years have significantly streamlined the design process, especially for plant retrofitting. The building industry, on the other hand, uses relatively rudimentary design tools. This is not to say that efforts have not been made to create useful simulation tools. Building information management (BIM) tools, for example, are available for construction management.

However, Foley believes, BIM and other tools still leave much to be desired compared to the model-based design tools used by process engineers in the chemical industry. There simply seems to be no equivalent in the building industry to the computer-aided simulation and design tools used by chemical engineers.

"An immediate need is for highly integrated building simulation tools that approach the levels of sophistication that chemical engineers have come to expect with process simulators. Without such modeling tools, it also becomes very difficult to do rigorous control of the building once it is constructed," Foley says.

In addition to better design tools, engineered retrofitting will also require economic analyses, better control systems and operation, and an integrated approach to the business model for building retrofits, Foley notes.