Breaking the Ice (Formation)

New nanomaterials developed at Harvard Univ. prevent the formation of ice by repelling water droplets before they can freeze.

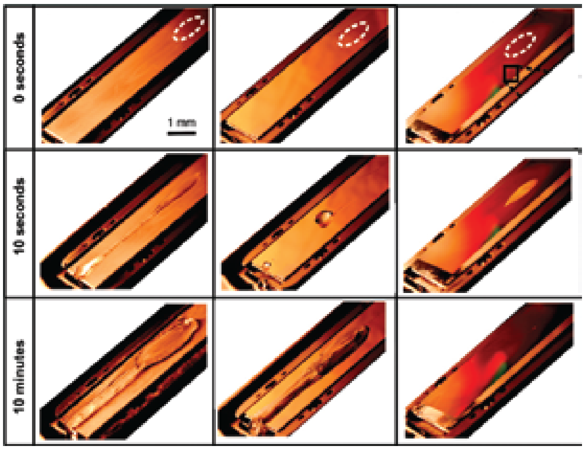
The materials could serve as the basis for new coatings to keep airplane wings, power lines, and even highways free of ice during the winter months. With their inherent ice-preventing capabilities, they are more efficient and environmentally friendly than traditional solutions, such as chemical sprays, salts, and direct heating. Furthermore, they do not corrode the structures to which they are applied, and they avoid the need for detection and activation that can sometimes cause current methods to fail.

While traditional solutions focus on fighting ice buildup, the Harvard team, led by materials science professor Joanna Aizenberg, concentrated on ice formation. "We wanted to take a completely different tack and design materials that inherently prevent ice formation by repelling the water droplets," she says.

Because ice formation is a dynamic process rather than a static event, the researchers began by studying how water droplets impact and freeze on supercooled surfaces. "Freezing starts with droplets colliding with a surface, but very little is known about what happens when droplets hit surfaces at low temperatures," Aizenberg explains.

The team initially found inspiration in nature — mosquitoes defog their eyes and water striders keep their legs dry with an array of bristles that repel droplets by reducing the surface area that each one touches. Learning from and mastering concepts from nature is a goal of the engineers. To study the dynamics of droplet freezing on such surfaces, they watched high-speed videos of supercooled droplets hitting surfaces modeled on the natural ones.

They observed that when a cold droplet comes in contact with a nanostructured surface, it initially spreads out in a thin layer, but then quickly returns to its spherical shape and bounces off before it has a chance to freeze. On smooth surfaces (absent nanostructure properties), however, the droplet remains spread out and can freeze. This knowledge allowed the team to model the dynamic behavior of impacting droplets at a high level of detail.

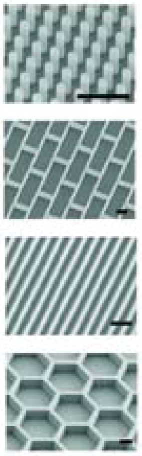


▲ Ice accumulates on hydrophilic flat aluminum (left) and hydrophobic smooth fluorinated silicon (center). White dashed circles indicated the position of water impact. Ice accumulation was not observed on the superhydrophobic microstructured fluorinated silicon (right) surfaces even after a significant period of time. Images courtesy of the laboratory of Joanna Aizenberg.

To create an ice-preventing design, the team tested a wide variety of structures that mimic those found in nature. "We fabricated surfaces with various geometries and feature sizes — bristles, blades, and interconnected patterns such as honeycombs and bricks — to test and understand parameters for optimization," explains graduate student Lidiya Mishchenko.

Testing a wide range of surfaces also enabled the team to optimize the new nanomaterial's pressure stability. The tests revealed that the interconnected patterns of honeycombs and bricks are highly stable and are able to withstand high-impact collisions such as those that airplanes experience in flight.

The superhydrophobic nanomaterial is effective at preventing ice nucleation at temperatures as low as –30°C. Below that, the structures still provide an advantage over conventional materials, because their reduced contact area prevents the droplets from fully wetting the surface. Thus, the ice that forms below these temperatures does not adhere well to the surface and is much easier to remove.



▶ Exemplary hydrophobic surfaces are fabricated with various geometries, including posts, bricks, blades, and honeycombs.

"We see this approach as a radical and much-needed shift in anti-ice technologies," says Aizenberg. "The concept of friction-free surfaces that deflect supercooled water droplets before ice nucleation can even occur is more than just a theory or the subject of proof-of-principle experiments. We have begun to test this promising technology in real-world settings to provide a comprehensive framework for optimizing these robust ice-free surfaces for a wide range of applications, each of which may have a specific set of performance requirements."

The researchers plan to develop a nanostructure-based coating that can be integrated directly into a variety of materials, and they hope that it will soon be commercialized.

ENERGY

Precious Catalyst Enhances Fuel Cell Vehicle Practicality

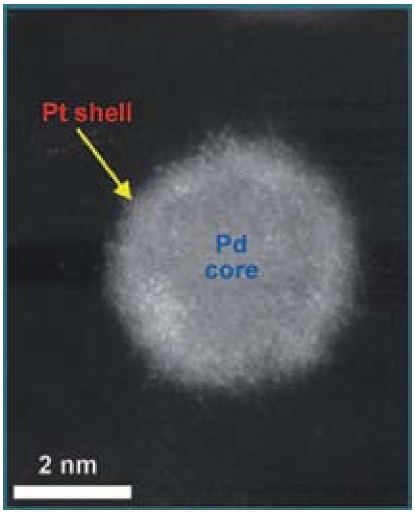
Researchers at the U.S. Dept. of Energy's (DOE) Brookhaven National Laboratory (BNL) have developed a new electrocatalyst that improves the reactivity and stability of fuel cells and may increase the practicality of fuel-cell-powered vehicles.

Stop-and-go traffic can be more than an annoyance to a driver — the oxidation and reduction cycling that is triggered by changes in voltage that occur during stop-and-go driving damages the precious platinum metal that catalyzes the reactions in automotive fuel cells. The platinum eventually dissolves, resulting in irreversible damage to the fuel cell.

Before large numbers of fuel-cell-powered vehicles can be developed, scientists will need to devise a way to protect the platinum, the most expensive component of fuel cells. They also need to reduce the amount of platinum needed to make catalytically active electrodes.

The BNL team tackled these problems by creating catalysts composed of a single layer of platinum over a palladium, or a palladium-gold alloy, nanoparticle core. "Our studies of the structure and activity of the catalyst — and comparisons with platinum-carbon catalysts currently in use — illustrate that the palladium core protects the fine layer of platinum surrounding the particles, enabling it to maintain reactivity for a much longer period of time," explains chemist Radoslav Adzic, who leads the research team at BNL's Chemistry Dept.

Palladium from the new catalyst's core is more reactive than the platinum in oxidation and reduction reactions. Tests simulating the voltage cycling of stop-and-go driving revealed that after 100,000 cycles (a sizeable fraction of the lifetime of a car), a significant amount of palladium had been oxidized, dissolved, and moved away from the cathode. The dissolved palladium ions were then reduced by hydrogen diffusing from the anode.



▲ Platinum monolayers act as shells for palladium nanoparticles at the core of a new electrocatalyst. The high-activity catalyst has an ultralow platinum content, but high platinum utilization. Photo courtesy of Brookhaven National Laboratory.

As the palladium core dissolved, the platinum monolayer shell contracted slightly. "This contraction of the platinum lattice makes the catalyst more active and the stability of the particles increases," Adzic notes. Along with stability, the reactivity of the catalyst remained high — it was reduced by only 37% after 100,000 cycles.

To improve catalytic activity, the team then added small amounts of gold to the palladium to create a palladium-gold core. This addition further enhanced stability and increased reactivity — the reactivity of the palladium-gold core dropped by only 30% after 200,000 cycles.

In comparison, traditional platinum-carbon catalysts lose almost 70% of their reactivity after fewer cycles. "This level of activity and stability indicates that this is a practical catalyst," says Adzic.

MATERIALS

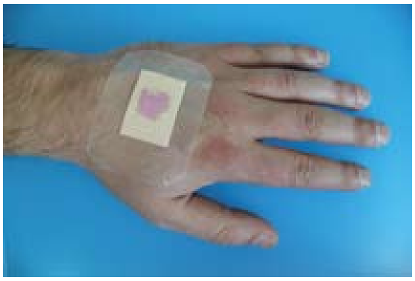
Making Sure Time Heals All Wounds

Scientists at the Fraunhofer Research Institution for Modular Solid State Technologies (EMFT) in Regensburg, Germany have developed materials for wound dressings and plasters that change color to indicate pathological changes in the skin, including the presence of an infection.

The body begins to repair wounds shortly after they happen. Smaller wounds tend to heal within a few days, but larger, gaping wounds take longer to heal. Even several days after an injury, the site is still prone to infection, but traditional dressings that protect the injury site need to be removed in order to check for changes. This can expose the wound to infection-causing bacteria, and can be painful for the patient.

The EMFT scientists developed a dressing that changes color from yellow to purple in the presence of a possible infection.

"We have developed an indicator dye that reacts to different pH values, and we have integrated it into a dressing and a plaster. Healthy skin and healed wounds usually have a pH below 5. If the pH increases, it is shifting from the acid to the alkaline range, which indicates complications in the healing of the wound. If the pH is between 6.5 and 8.5, an infection



▲ EMFT scientists developed a dressing that changes color from yellow to purple if the pH of the skin is between 6.5 and 8.5 — a range that frequently indicates infection. Photo courtesy of Fraunhofer EMFT.

is frequently present and the indicator color strip turns purple," explains EMFT scientist Sabine Trupp.

She notes that the team created a dye that reacts sensitively in the correct pH range, and clearly changes color. The dye is immobilized on the fibers of a dressing material to ensure that it is not transferred to the wound. Several synthesis steps are necessary to obtain this multifunctional dye whose structure is comparable to commercially available food dyes.

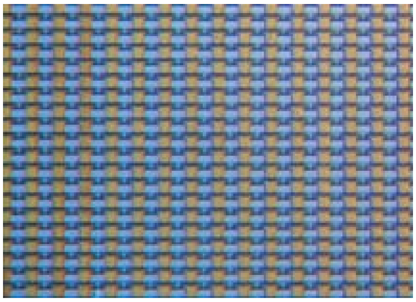
Initial tests of the prototype dressing have proved successful at indicating changes in pH. "Previous studies of the pH value in acute as well as in chronic wounds have shown that it plays a key role in wound healing," says Trupp.

The team's next step will be to use the dressing in a clinical study, and plans for this have already been made. The scientists also envision further improvements to the dressing. They plan to integrate optical sensor modules into the dressing to measure the pH value and display the results on an external unit. This would allow for the precise determination of the skin's pH and provide more information about how the wound is healing.

Template-Grown Graphene Ushers in a New Generation of Electronics

Researchers at the Georgia Institute of Technology have devised a new method for fabricating nanometer-scale graphene that may become the basis for a new type of high-performance electronic devices.

Graphene, a honeycomb lattice made of a single layer of carbon atoms, has excellent electronic properties. However, its use in electronic devices such as field-effect transistors is impractical at room temperature without the introduction of a bandgap (*i.e.,* an energy range in a solid from which electrons are excluded).



▲ Using a new templated-growth technique, Georgia Tech researchers have fabricated an array of 10,000 graphene transistors. The graphene's smooth edges help to avoid electron scattering. Photo courtesy of Walt de Heer.

The Georgia Tech team has developed a template that could direct the growth of graphene structures to form nanoribbons of specific widths without the use of destructive cutting techniques that introduce rough edges onto the structure. "If the edges are too rough, electrons passing through the ribbons scatter against the edges and reduce the desirable properties of graphene," explains physics professor Walt de Heer.

The method involves etching patterns into the silicon carbide surfaces on which epitaxial graphene (a monocrystalline film deposited on a monocrystalline substrate) is grown. These patterns form the templates that direct graphene growth. The resulting structures have smooth edges, so they avoid electron-scattering problems. "Using this approach, we can make very narrow ribbons of interconnected graphene without the rough edges," says de Heer.

When developing these structures, the team initially used traditional microelectronics techniques to etch contours into silicon carbide wafers. The etched wafer was heated to 1,500°C to melt and polish the rough edges created by the initial etching process. The team then drove silicon atoms off the surface of silicon carbide in an effort to grow graphene.

Because the heating time was short, the graphene grew only on the edges, rather than across the entire surface. "By using the silicon carbide to provide the template, we can grow graphene in exactly the sizes and shapes that we want," notes de Heer.

Depending on the width of the graphene nanoribbon, the material acts as either a semiconductor or a conductor. By controlling the depth of the template, the researchers can create both types of structures simultaneously, using the same process. "The same material can be either a conductor or a semiconductor depending on its shape," says de Heer.

This new approach could enable the production of advanced electronic devices whose leads and semiconducting ribbons are made from the same material. This can help to avoid electrical resistance that accumulates at junctions between different electrical materials.

The scientists also applied a dielectric material and metal gate to the nanoribbons to construct field-effect transistors, which was previously impractical. This achievement demonstrates graphene's viability as an electronic material, but de Heer considers it to be only the first of many steps that can be performed with the material.

Graphene may become the foundation for high-performance electronic devices that will capitalize on its unique properties in applications for which the higher cost is justified. De Heer notes that silicon will continue to be used in applications that do not require such high performance.

NANOTECHNOLOGY

Oxygen Enhances the Brightness of Nanotubes

Scientists at Rice Univ. have devised a method of applying ozone to nanotubes to make them shine brighter. This development could expand

opportunities for biological uses of nanotubes as well as the creation of new materials.

By adding tiny amounts of ozone to batches of structurally sorted single-walled carbon nanotubes and exposing them to light, physical chemist Bruce Weisman and his colleagues decorate nanotubes with oxygen atoms to systematically change their near-infrared (NIR) fluorescence. This enhances the intensity of the nanotubes' natural fluorescence and shifts the wavelength at which they fluoresce.

"We're not the first people to study the effects of ozone reacting with nanotubes," says Weisman. "But all the prior researchers used a heavy hand, with a lot of ozone exposure. When you do that, you destroy the favorable optical characteristics of the nanotube. It basically turns off the fluorescence. In our work, we only add about one oxygen atom for 2,000–3,000 carbon atoms."

The researchers add small amounts of gaseous or dissolved ozone to a suspension of nanotubes in water and then induce a photochemical reaction by exposing the sample to light — even light from an ordinary desk lamp. Most sections of the nanotubes absorb infrared light and form excitons, which are quasiparticles that tend to jump along the tube. When the excitons encounter oxygen atoms in the nanotube, however, they tend to remain there because that state is energetically more stable. The excitons become trapped and emit light at a longer wavelength.

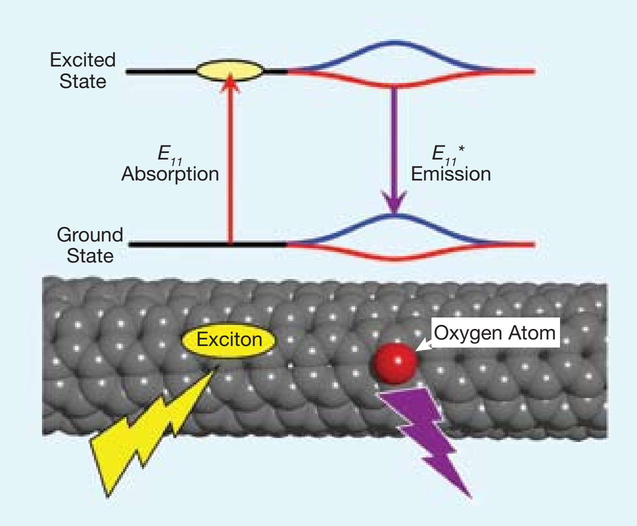
"Essentially, most of the nanotube is turning into an antenna that absorbs light energy and funnels it to the doping site. We can make nanotubes in which 80–90% of the emission comes from doped sites," notes Weisman.

By exciting cells in the infrared, instead of the visible, range, the researchers have reduced background emissions. They added their nanotubes to cultures of human uterine adenocarcinoma cells to study them in a biological environment. When viewed in the NIR spectrum, the nanotubes shined brightly against a dark background, but when illuminated with visible light, the nanotubes in the same sample were dimmer and more difficult to see because of background haze.

Weisman notes that this is not an expensive or an elaborate process, and he is convinced of the potential of this research. "If you want to see a single tube inside a cell, this is the best way to do it," he says.

Oil and Water Do Mix — Just Add Nanofibers

Using vigorous agitation of water, dense oil, and polymer nanofibers, a team of chemists and engineers at the Univ. of California, Los Angeles (UCLA) has developed a new



▲ Rice Univ. researchers add ozone to the carbon atoms in nanotubes, and then expose the sample to light. When excitons, which are quasiparticles that jump along the tube, come in contact with oxygen, they become trapped and emit light at a longer wavelength. Image courtesy of Rice Univ.

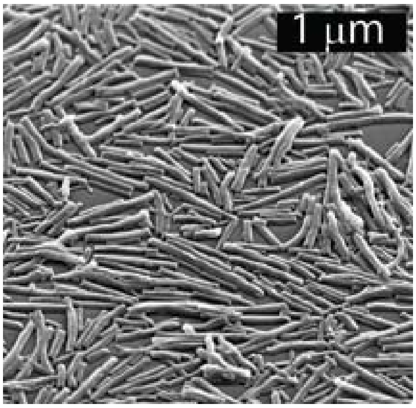
method for coating large surfaces with nanofiber thin films that are both transparent and electrically conductive. The solution spreads over virtually any surface and could lead to conductive plastic coatings for use in new solar cells, windows, and sensors.

"The beauty of this method lies in its simplicity and versatility," says California NanoSystems Institute (CNSI) researcher Richard B. Kaner, a professor of chemistry and biochemistry and of materials science and engineering. "The materials used are inexpensive and recyclable, the process works on virtually any substrate, it produces a uniform thin film that grows in seconds, and it can be done at room temperature."

Although conducting polymers have been proposed for applications ranging from printed electronic circuits to supercapacitors, they have failed to gain widespread use because of difficulties processing them into films.

The researchers discovered the solution-based technique when a transparent film of polymer spread up the walls of a container while nanofibers in water were being purified with chloroform. "What drew me in immediately was the eerie phenomenon of what appeared to be self-propelled fluid flow," says Julio M. D'Arcy, senior graduate student in Kaner's UCLA lab. "Now I can tell people that I make films in L.A."

When water and oil are mixed, a blend of droplets forms, which creates a water-oil interface that

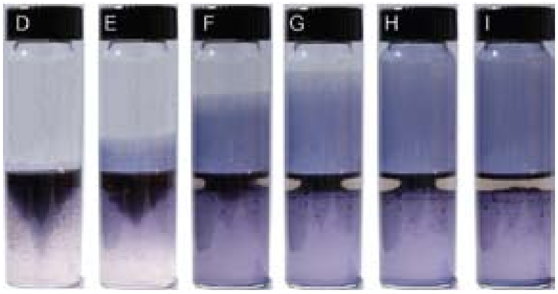


▲ Inexpensive, recyclable nanofiber thin films are both transparent and electrically conductive. Photo courtesy of UCLA.

serves as an entry point for trapping polymer nanofibers. As the droplets unite, the concentration of blended solids at the water-oil interface changes and causes the surface tension to change as well. An interfacial surface-tension gradient develops, which in turn causes the fluid film to spread over the solid surfaces as a result of the Marangoni effect — that is, a fluid of lower surface tension (*e.g.,* oil) will always spread over a fluid of higher surface tension (*e.g.,* water). In this way, the oil film can effectively carry dispersed organic nanostructures across an aqueous layer on the surface of glass.

Directional fluid flow produces a continuous conductive thin film comprised of a single layer of polymer nanofibers. The uniformity of the film surface is due to the particles being drawn out of the water-oil interface, sandwiched between two fluids of opposing surface tensions.

Other techniques for creating thin films of conducting polymers tend to work for only a limited number of applications or are not feasible for



◀ A polymer film grows in tubes in this sequence of images taken over 35 seconds. Photo courtesy of UCLA.

scaling up. A method has long been sought that would overcome the limitations of the previous methods. The water-and-oil technique, with a bit of nanotechnology thrown in, might provide a scalable, universal method for creating large, thin films of conducting polymers.

One potential application for such films is smart, or switchable, glass that changes between states when an electric current is applied, such as switching between transparent and opaque states to let light in or block it.

The UCLA group is applying the technique to other nanomaterials in the hopes of expanding the range of applications.

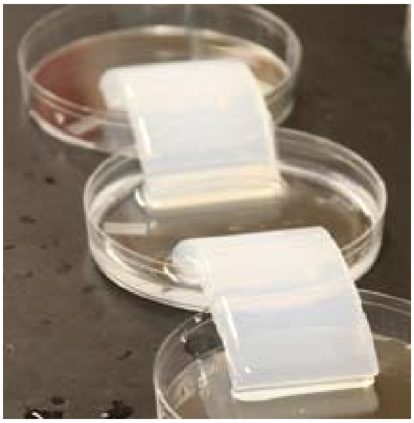
BIOTECHNOLOGY

Cartilage Cells Stem from Cues Found in Nature

Engineers at the Univ. of California, San Diego (UCSD) have scored a hat-trick in stem cell science — they created an artificial environment for stem cells that simultaneously provides the chemical, mechanical, and electrical cues necessary for stem cell growth and differentiation.

Other researchers have created artificial environments that provide only two cues — chemical, and either mechanical or electrical — to support adult stem cell culture. The UCSD team, led entirely by undergraduate bioengineering students, says that its approach is the first reported in the scientific literature to simultaneously provide all three cues.

Stem cells communicate with other cells and with the extracellular matrix through chemical, electrical, and mechanical signals. "We mimicked all these cues that the native environment provides to the cells," explains bioengineering professor Shyni Varghese, who advised the students working in her lab. By creating a more-realistic environment for stem cells, researchers can not only culture the cells, but also study cell



▲ The translucent materials bridging the dishes in the photo are agarose salt bridges — part of the electrochemical cell used to subject hydrogels to an electric field. Photo courtesy of UCSD Jacobs School of Engineering.

function, signaling pathways, disease progression, and tissue growth and development.

The stem cells are embedded in a gelatin-like hydrogel immersed in an electrolyte solution compatible with cell growth. An electric potential is passed through the hydrogel. "Our hydrogel provides the chemical cues, and when you expose the cell-laden hydrogel to an electric field, the hydrogel surrounding the stem cells bends, which provides mechanical strain to the cells," said Varghese.

Using the new technique, the engineers grew mesenchymal stem cells derived from human bone marrow in the new environment. The combination of the three cues directed the cells to differentiate into cartilage cells.

Although the technique has not yet been perfected, the team continues to make strides toward coaxing healthy tissue from stems cells in an effort to eventually save lives. Building better microenvironments for nurturing stem cells is critical for realizing the promises of stem-cell-based regenerative medicine, including cartilage for joint repair, cardiac cells for damaged hearts, and healthy skeletal myoblasts for muscular dystrophy patients.

In addition, the team is working to gain further control over the cues that the stem cells receive, so that future regenerative therapies will be more effective.

For a detailed discussion of stem cell engineering, see the SBE special supplement in the Nov. 2010 issue. — Editor

E. coli Produce Antibiotics

Engineers at Tufts Univ. have successfully produced the antibiotic erythromycin A as well as two variations using *E. coli* as the production host. The new technique offers the potential for a more cost-effective way to make both erythromycin A and new drugs that will combat the growing incidence of antibiotic-resistant pathogens.

Used to treat bacterial infections, erythromycin A is the most common and most biologically active of several variants of erythromycin that are produced naturally by the soil bacterium *Saccharopolyspora erythraea*.

Because *S. erythraea* is difficult to engineer, the Tufts team turned to *E. coli*. However, the genetic and biochemical complexity — more than 20 enzymes must work in concert to create the erythromycin A molecule — makes synthesis difficult.

"To transfer and reconstitute these biosynthetic pathways is very difficult. In fact, erythromycin A poses nearly every challenge that must be addressed in the quest for heterologous biosynthesis of complex natural products," says Blaine Pfeifer, assistant professor of chemical and biological engineering. Such challenges include the active expression of substantially foreign or large genes that produce multi-unit enzyme complexes requiring posttranslational modification. Pfeifer's group overcame these problems through a combination of metabolic and process engineering, particularly featuring the overproduction of enzymes that limit final product formation.

Previously, erythromycin A intermediates had been manufactured in *E. coli*, but not the final product. In the current work, the Tufts engineers reconstituted and manipulated the compound's original biosynthetic pathway — an approach that differed from previous attempts, which used analogous biosynthetic enzymes from closely related biological sources.

The *E. coli* production platform offers numerous opportunities for the production of other natural products with complex biosynthetic pathways. "Our ability to fully manipulate erythromycin A's biosynthetic pathway to expand molecular diversity and antibiotic activity helps set a precedent for producing other similarly complex and medicinally relevant natural products," Pfeifer adds.

CATALYSIS

From Greenhouse to Green Tech: Scientists Transform Carbon Dioxide into Useful Compounds

Scientists at the Institute of Bioengineering and Nanotechnology (IBN) have developed a new environmentally friendly technique to transform carbon dioxide into propiolic acids — a breakthrough in their quest to develop green technologies for pharmaceutical synthesis.

Carbon dioxide is an abundant and renewable carbon source. The researchers have devised a technique to transform it into more useful compounds — propiolic acids, which are basic building blocks for the synthesis of a wide range of pharmaceuticals, such as cholesterol-reducing drugs and small molecule inhibitors that may be used, for instance, to destroy cancer cells.

"Our research is focused on converting sustainable resources such as carbon dioxide into useful pharmaceuticals through environmentally benign processes," says team leader and principal research scientist Yugen Zhang.

The harsh and severe reaction conditions necessary for most carbon dioxide transformation protocols, in addition to their poor catalytic performance and limited substrate scope, pose major obstacles for their practical application. So the team developed a copper and copper-N-heterocyclic carbene catalyst to use in the reaction. This organo/organometallic bifunctional catalyst is highly active and easy to synthesize. The approach involves the direct activation of the C-H bond and carboxylation of the terminal alkynes, with both steps using their catalyst. The synergetic effect of free carbene species and the copper center in the catalyst enables the reaction.

The reaction was carried out under ambient conditions without the use of any organometallic reagents. Organometallic reagents are expensive and very sensitive to air and moisture, thus limiting the synthesis of a wide scope of functionalized propiolic acids.

Because the reaction produced excellent yields (70–95%), this elegant and economically viable protocol has great potential for practical applications, and it is flexible enough to be used with a wide variety of substances, including alkyl alkynes, aryl alkynes, and alkynes with functional groups, Zhange says.

He notes that a main goal of the research is to provide new and powerful tools to help pharmaceutical companies bring medicines to patients with minimal impact on the environment. The team also intends to further develop this technology for the large-scale synthesis of industrial chemicals from carbon dioxide.

Converting Wood into Plastic

Chemical engineers at the Univ. of Massachusetts, Amherst (UMass), have developed a process that could reduce or eliminate industry's reliance on fossil fuels to make industrial chemicals. They have devised a way to produce high-volume chemical feedstocks, including benzene, xylenes, and olefins, from pyrolytic bio-oils, the least-expensive biomass-derived liquid fuel available.

▲ UMass Amherst researchers have developed a method of producing commodity chemical feedstocks entirely through the processing of pyrolysis oils. Photo courtesy of Phil Badger, Renewable Oil International.

"Thanks to this breakthrough, we can make commodity chemical feedstocks entirely through the processing of pyrolysis oils. We are making the same molecules from biomass that are currently being produced from petroleum, with no infrastructure changes required," says associate professor George Huber.

The team devised a two-step, integrated catalytic approach that consists of a tunable, variable-reaction hydrogenation stage followed by a zeolite-catalyzed step. The zeolite catalyst has the proper pore structure and active sites to convert biomass-based molecules into aromatic hydrocarbons and olefins.

The engineers' findings indicate that "the olefin-to-aromatic ratio and the types of olefins and aromatics produced can be adjusted according to market demand," Huber says. He and his team have performed economic calculations for determining the optimal mix of hydrogen and pyrolytic oils, depending on market prices, to yield the highest-grade product at the lowest cost. By choosing from three options, including low- and high-temperature hydrogenation steps, and the type of zeolite used, chemical manufacturers can adjust the carbon content from biomass they need, as well as hydrogen amounts.

The development will allow chemical manufacturers to use pyrolysis oils made from waste wood, agricultural waste, and non-food energy crops, instead of petroleum, to produce the same high-value materials for making products ranging from solvents and detergents to plastics and fibers. The plant biomass is renewable, and will also provide U.S. farmers and landowners a large additional revenue stream.

The engineers have achieved yields three times higher than have been previously achieved for pyrolysis. "We've essentially provided a roadmap for converting low-value pyrolysis oils into products with a higher value than transportation fuels," Huber adds.

Using the new method, these chemicals are now being produced on a liter-quantity scale in a pilot plant on the UMass Amherst campus. The technology has been licensed to Allentech Corp., cofounded by Huber and David Sudolsky of New York City.

"There are several companies developing technology to produce pyrolysis oils from biomass. The problem has been that pyrolysis oils must be upgraded to be useable. But with the new UMass Amherst process, Anellotech can now convert these pyrolysis oils into valuable chemicals at higher efficiency and with very attractive economics," says Sudolsky. CEP

CHEM ECONOMICS

The Role of Chemistry in Today's Economy

Chemistry is essential to the global economy. In fact, chemistry directly touches just about everything we consume or come into contact with each day. Using data from the U.S. Census Bureau's Bureau of Economic Analysis (BEA), the American Chemistry Council (ACC) determined that 96% of all goods manufactured for consumer use contain chemistry. When the scope is widened to include packaging and ancillary uses of chemicals in processing, it is clear that all manufactured goods contain or were processed with some form of chemistry products.

Based on the BEA input-output tables, which provide a detailed accounting of inter-industry purchases, ACC calculated the percentage of chemistry contained in more than 80 classes of manufactured products in everyday use. Dubbed the "ChemFactor," this percentage represents the amount of chemical materials used to make a wide range of consumer, industrial, and packaging products.

During 2011, the International Year of Chemistry (see p. 3 and pp. 51–52), Chem Economics will look at some of the impacts of chemistry and chemical engineering on modern living. The following vignettes present ChemFactors for a few products that most of us consider essential. Look for more of these stories throughout IYC 2011. For more information on the benefits of chemistry, visit ACC's website, www.americanchemistry.com. (This month's regular Chem Economics column is replaced by Kevin Swift's article, "Capital Spending in the Chemical Industry," pp. 39–43).

— Martha Gilchrist Moore
American Chemistry Council
martha_moore@americanchemistry.com

Motor Vehicles

- Chemistry contributes 12% of the value of the materials used in the production of a typical motor vehicle
- Polyvinyl chloride (PVC) is used to insulate electrical components
- Tires, fan belts, and hoses are manufactured of synthetic rubber
- Carpeting is made from synthetic styrene-butadiene rubber (SBR), for the backing, and nylon and polypropylene, for the fibers
- Impact-resistant polymers such as polyvinyl butyral are combined with regular glass to make shatter-resistant safety glass
- Polyurethane foams make seats comfortable and fenders durable and shock-absorbent
- Paints protect the automobile's underlying steel frame from corrosion
- Ethylene glycol and propylene glycol antifreeze agents protect engine parts from freezing in cold weather

Gaming Systems

- Acrylonitrile-butadiene-styrene (ABS) plastic shells protect the internal components and give controllers their shape
- Keypad buttons on controllers are made from silicone rubber
- Epoxy novolac compounds shield integrated circuits and semiconductors from overheating
- Circuit boards inside the console are produced from phenolic resins because of their outstanding electrical resistance
- Game discs are comprised of polycarbonates (bisphenol A and carbonyl chloride) and a thin aluminum layer for storing data
- Polyvinyl chloride (PVC) plastics sheathe internal wires for insulation, safety, and added strength

Magazines

- Chemistry contributes 29% of the value of materials used to produce magazines
- Chlorine dioxide is used to bleach wood pulp during the manufacturing of paper
- Titanium dioxide whitens paper, making the text sharper and magazines easier to read
- Precipitated calcium carbonate and alumina trihydrate are used as fillers and paper coatings
- The pages of glossy magazines get their shine from the acetate-based lacquers in paper coatings
- Inks made from various organic and inorganic chemicals make the printed word possible

AIChE JOURNAL Highlight

Minimizing Risk and Systemic Failures

In the history of chemical plant accidents, a few disasters have served as wake-up calls. In 1974, the Flixborough accident killed 28 people in a chemical plant explosion in the U.K. The worst was Union Carbide's Bhopal, India, tragedy in 1984, in which more than 2,000 people were killed and an estimated 100,000 or more others were seriously injured by the accidental release of methyl isocyanate. Another important incident involved the Piper Alpha offshore oil platform operated by Occidental Petroleum in the North Sea, U.K., which exploded in 1988, killing 167 people and causing about $2 billion in losses. Even though the human casualties were low, this list should also include the 1989 Exxon Valdez oil spill and, now, the BP oil spill — both of which are very serious from an environmental damages perspective, says Venkat Venkatasubramanian in the January *AIChE Journal* Perspective, "Systemic Failures: Challenges and Opportunities in Risk Management in Complex Systems."

Such systemic failures are not limited to the chemical and petrochemical industries. The electrical power blackout in the Northeast U.S. in 2003 and the recalls of numerous consumer products ranging from toys to medicines to tires and automobiles are systemic failures. Financial disasters involving such companies as Enron and WorldCom, the subprime mortgage derivatives market, and the Madoff Ponzi scheme, as well as some other events also belong to the same class, says the author.

Although these are different disasters that occurred in different domains and facilities, triggered by different events and involving different (or no) chemicals, they share certain common underlying patterns. "These patterns teach us important fundamental lessons that we must learn to avoid such disasters in the future," Venkatasubramanian says.

"To understand these patterns and learn from them, we need to go beyond analyzing them as independent one-off accidents, and instead, examine them from the broader perspective of the potential fragility of all complex engineered systems. We need to study all these disasters from a common systems-engineering perspective to be able to thoroughly understand the commonalities as well as the differences, and to better design and control such systems in the future." Furthermore, he says, such studies need to be carried out in concert with public policy experts so that all the scientific and engineering lessons get translated into effective policies and regulations.

Typically, systemic failures occur due to fragility in complex systems. Modern technological advances are rapidly creating an increasing number of complex engineered systems, processes, and products, and ensuring their proper design, analysis, control, safety, and management for successful operation over their lifecycles involves many challenges. Their scale, nonlinearities, interconnectedness, and interactions with humans and the environment can make these systems-of-systems fragile. The cumulative effects of multiple abnormalities can propagate in numerous ways to cause systemic failures. In particular, the nonlinear interactions among a large number of interdependent components, and the environment, can lead to emergent behavior — *i.e.,* the behavior of the whole is more than the sum of its parts — which can be difficult to anticipate and control. This is further compounded by human errors, equipment failures, and dysfunctional interactions among components and subsystems that make systemic risks even more likely if one is not vigilant all the time.

Post-mortem investigations have shown that major disasters rarely occur due to a single failure of equipment or personnel — layers of failures of equipment, systems, processes and people are usually at fault. And often, Venkatasubramanian says, the responsibility for the accident rests with the top levels of company management and a poor corporate culture regarding safety.

Universities can play a role in creating and disseminating knowledge about the management of abnormal events in complex engineered systems, as well as their public and corporate policy implications. According to the author, it is imperative that chemical engineering academics rise to the challenge and responsibility in fostering the education of the next generation of chemical engineers with higher sensitivity to the importance of safety, sustainability, and ethics.

Venkatasubramanian concludes: "No contemporary engineered system with ever-increasing complexity can be risk-free. Minimizing inherent risks in our products and processes is a wonderful intellectual challenge for creative science and engineering and one that could provide substantial differentiating competitiveness. This takes vigilance and effort all the time and across the board. In the long run, considerable technological help would come from progress in taming complexity, which would result in more-effective prognostic and diagnostic systems for monitoring, analyzing, and controlling systemic risks. Getting there will require innovative thinking, bolder vision, and overcoming some misconceptions in and about the process systems engineering community."