Fundamental researchers offer new ways to sort molecules for clean energy

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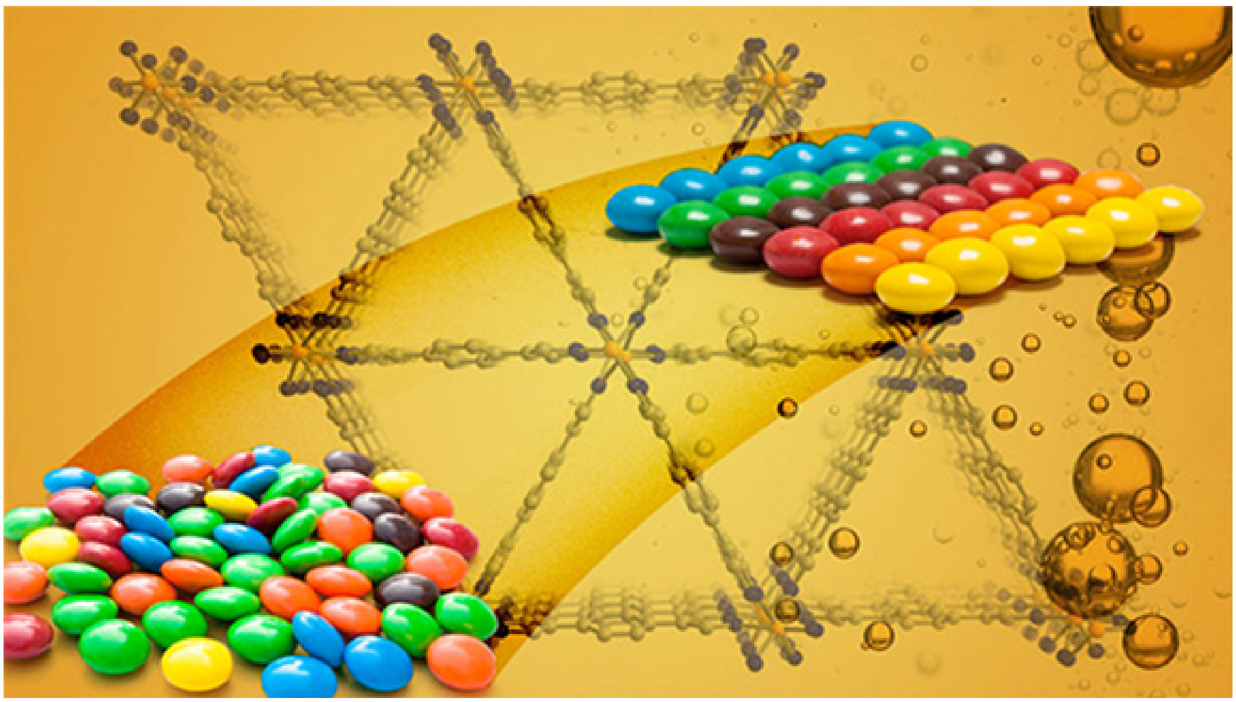


It's the candy dish problem, but rather than picking the desired flavors, scientists must pick impurities from complex mixes. Scientists funded by the Office of Science at the Department of Energy are creating new materials and answering fundamental questions that could improve separations. Credit: US Department of Energy

It's called the office candy dish problem. You grab a jellybean, but it's not the flavor you want. Pawing through for your favorites is irritating in terms of time, energy, and efficacy. It also annoys your office mates. In an odd way, it's the same problem for those in manufacturing, power generation, and elsewhere. They want a specific subset of molecules or other bits; however, getting that subset can consume vast amounts of energy.

Chemical separation accounts for 10 to 15 percent of the nation's energy consumption, according to an article in Nature. Industries spend up to half of their energy budget on separations. The associated price tag is in the billions. That energy use has environmental costs, including tons of carbon dioxide released each year.

Researchers funded by the Department of Energy's (DOE) Office of Science are tackling the energy demands of separation by focusing on the underlying science. They are answering questions about "how" and "why" the targeted materials behave.

A cooler way to refine valuable chemicals. In today's oil refineries, engineers take crude oil and produce a mix of desirable chemicals. They then refine the mix to create separate streams of pure chemicals, rather like sorting the big bowl of candy into smaller dishes of desired sweets. New separation processes could reduce the economic and environmental costs of separations, making it faster and easier to get what you want.

How? An iron-based sieve, known as a metal-organic framework (MOF). By flowing gas through the sieve, the scientists saw the desirable hydrocarbons adhere to the MOF. Impurities passed through. In early tests, the material, designed at the Center for Gas Separations (CGS), resulted in streams of desirable hydrocarbons that can meet industry's requirements. More importantly, it works at room temperature, eliminating the need for extreme temperature changes.

"Separations can work either way—catching the desired product or letting it pass. Generally which of these is preferable depends whether the target is a minority species—catch—or the majority—let pass," says University of California, Berkeley's Jeffrey Long, who leads the CGS.

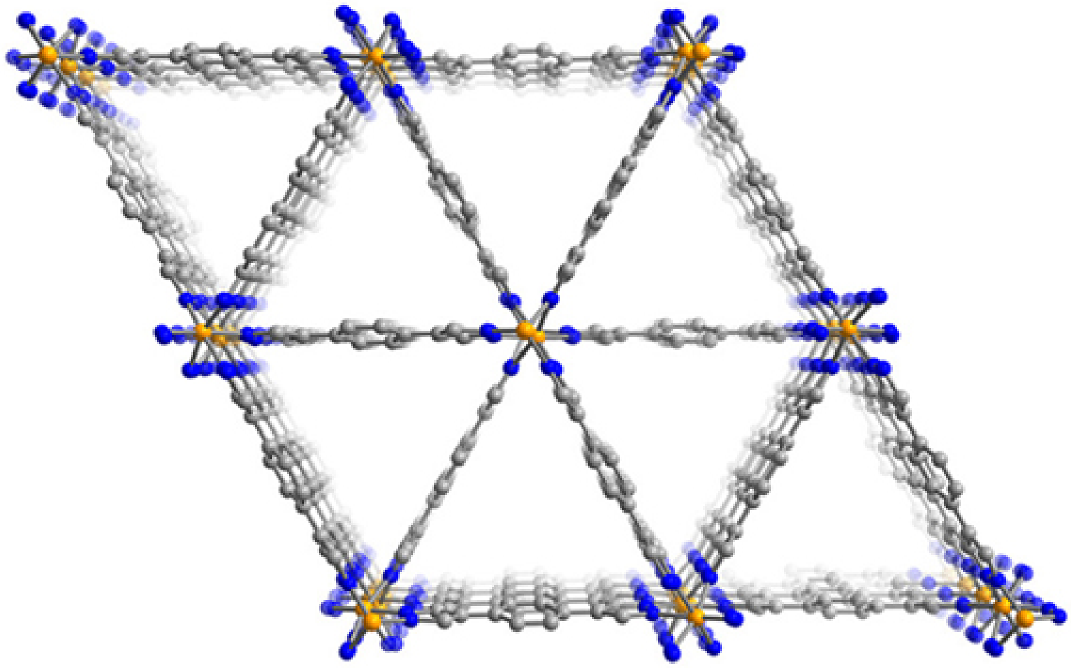
The center is one of DOE's Energy Frontier Research Centers, a collaborative center where teams from universities, laboratories, or industry converge on the scientific problems vital to our nation's future. DOE's Office of Science funds 36 such centers.

The group at CGS also showed how changing the shape of the "holes" in another porous MOF material lets scientists separate molecules by shape. Why does shape matter? Whether a six-carbon molecule called hexane has branches, looking like the letters "x" or "y", or is branch-free is the difference between your car running smoothly and hearing that expensive knocking sound.

X-shaped hexane molecules pass through first, then y-shaped molecules. Finally, the linear form passes through. By knowing when and how the different forms of hexane are passed through or are caught by the MOF's triangular pores, the team separated the troublemakers and purified the high-octane, x-shaped molecules.

Sort data, separate chemicals. Just as crude oil requires refining, so does the biofuel ethanol. Fermentation turns poplar trees, grasses, and other forms of biomass into a mix of the alcohol ethanol and water. Absorbent materials called zeolites pick out the ethanol molecules, but water can interfere with the separation process. Altering the chemical structure of the zeolite lets it better reject water. But which structure works best? There are many options.

Narrowing down options to just the best is the task taken up by researchers at the Nanoporous Materials Genome Center (NMGC) at the University of Minnesota. They knew that the challenge was the equivalent of finding a needle in a field of haystacks, so they turned to the Argonne National Laboratory's Leadership Computing Facility.



Scientists funded by DOE's Office of Science are examining the properties of different materials, such as this iron-based metal-organic framework, to find less expensive routes to separate chemicals we use every day. Credit: Jeffrey Long, University of California, Berkeley

The researchers performed millions of virtual experiments to screen 402 zeolites and find a promising ethanol-preferring, water-rejecting structure. The result is a process that can reduce the time and cost in finding a new separations material for ethanol.

Also, the team used this approach to sort through 386 variations to find the 16 best all-silica zeolites for removing hydrogen sulfide from natural gas reserves. High levels of hydrogen sulfide "sour" reservoirs, making their exploration unprofitable. Using zeolites for removing hydrogen sulfide and sweetening the natural gas may be an economical solution for this sour problem.

"We are making discoveries that could be huge for the fuel industries," says Ilja Siepmann, who leads the NMGC.

Separate the unseen. Because of its potential use in cancer treatment, having too little of the rare element astatine is a problem. The element decays away in mere hours. It's so rare and decays so fast that scientists can't produce enough to see it or weigh it. They rely on detectors to know if they've created and separated it.

Scientists delved into astatine's chemistry and improved a complex process to separate the desirable material from irradiated bismuth plates. The team is automating the separation process, making it easier to purify larger quantities. This process lets them produce enough to make the isotope available to others through the National Isotope Development Center.

"I want to get this to other people so even more studies can be done," says D. Scott Wilbur at the University of Washington. He is now leading studies that give a more nuanced view of the element. He is participating in planning clinical studies to evaluate astatine's tumor-fighting abilities in the near future.

Capture pollutants. Power plants fueled by coal and other fossil fuels produce energy and release tons of carbon dioxide; the climate-changing gas can be scrubbed out by flowing the gaseous mix through a special liquid. The liquid absorbs 2 to 3 percent of its weight in carbon dioxide.

The liquid is heated to wring out the carbon dioxide for reuse or storage.

Heat adds cost. While far less heat is used than in refining, heat adds operational cost that must be paid.

Back at CGS, scientists examined the underlying science of carbon dioxide and designed a material that pulls in 13 percent of its own weight in carbon dioxide. Releasing carbon dioxide uses less heat. Carbon dioxide is absorbed at 104°F and released at just 122°F.

"There are big potential advantages in terms of capital and operating costs," says Long.

The future and separation science. Separations matter, whether it's the quality of the fuel you pump in your car, the medicine you take, or the air you breathe. These separations processes come at an economic and environmental cost. To reduce these costs means answering questions about the complexities of removing the targeted materials quickly and efficiently.

Provided by US Department of Energy

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