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Designing better catalysts for cleaner, more efficient chemistry

Solid catalysts underpin many of the large-scale chemical transformations used to manufacture modern materials, converting hydrocarbons — including renewable or recycled forms of carbon — into the building blocks of fuels, polymers, solvents and medicines. Researchers who design these catalysts, such as UC Santa Barbara's Susannah Scott, a professor of chemistry and biochemistry and of chemical engineering in the Robert Mehrabian College of Engineering, are constantly looking for ways to make these catalytic processes more energy-efficient and more selective.

Recently, Scott was named the lead principal investigator of a new National Science Foundation (NSF)-funded collaboration with Stanford University and the University of Washington. The study is focused on understanding and controlling a little-understood phenomenon: the high mobility of positively charged ions — *cations* — in catalytic materials. The funding came through the NSF's Designing Materials to Revolutionize and Engineer our Future (DMREF), a program "to foster the design, discovery, and development of materials to accelerate their path to deployment by harnessing the power of data and computational tools in concert with experiment and theory."

"Some catalytically active materials are highly dynamic," Scott said, "It seems to be something every generation of researchers rediscovers. The reason the next generation overlooks it and then finds it again is that atom mobility can be very

difficult to observe directly. We often need to model our catalysts as if they were not dynamic materials."

That simpler approach, however, leaves a lot out. "We're now acknowledging that, in many cases, the dynamic behavior of atoms is critical to how catalysts function," Scott noted. "They can migrate to create *transient* ensembles of atoms capable of catalyzing reactions that would not be possible otherwise. In a process called *deactivation*, however, this dynamic behavior can also cause a catalytic material to gradually lose the original structure responsible for its desired behavior. When that happens, catalytic reactions start to take much longer, until it becomes necessary to discard the catalyst and replace it with fresh material. There are enormous environmental and economic ramifications for these consequences of dynamic behavior, which is why we need to understand and control it better."

Tracking the mobility of atoms requires the ability to diagnose specific signals. "Basically, we've found such a signal for metal ions; in this project, we will apply it to probe dynamic behavior," Scott explained. "The important thing is that we have a new way to detect ion mobility in materials while they are operating as catalysts. That's empowering, because it allows us to link the dynamics of a material to its performance as a catalyst."

Tracking metal ions requires very high energy X-rays that are much brighter than any normal lab instrument can produce, which is where the synchrotron at SLAC National Accelerator Laboratory, a U.S. Department of Energy national laboratory operated by Stanford University, comes in. "Absorption of those very-high-energy X-rays by the atom we're interested in triggers the emission of a photoelectron, which is scattered by neighboring atoms, providing a signal that contains information about the local environment," Scott said. "Our team has been using this technique for many years to probe *static* structures. What's new is that we are looking at parts of the signal that we weren't paying as much attention to previously, to extract detailed information about the *dynamic* behavior of the atoms."

Discussing a key aspect of the project, Scott noted, "An atom is never completely immobile; it's always moving around some equilibrium position, and sometimes those motions can become quite large. The extent of the displacement is reflected in a parameter called the Debye–Waller factor, which is a quantitative signature for atom mobility as a function of its environment.

“We want to be able to design more powerful catalysts intentionally,” an idea, Scott added, “that has been around for about twenty years, but mostly as an aspiration. Basically, we stumble across a material with interesting behavior and then try to understand how it works and improve it a little bit. Eventually, we might claim that we designed it, but that kind of retrospective approach usually doesn’t allow us to predict new behaviors. If we truly want to design catalysts, we can’t just design static structures; we have to target their dynamic properties as well.”

As a project-related example, Scott said, “Sometimes, a catalytic reaction requires two distant atoms in the catalyst to interact with each other briefly, so, presumably, the atoms have to be able to come together and then move apart. We know that this probably happens; the question is how to see that it *is* happening? In this project, we will watch atoms find each other. We have this very sensitive fingerprint that responds only to the dynamic part of the material, which allows us to know when and how fast that process is occurring, to measure what fraction of the atoms are involved, and also to know when it's blocked and which atoms are not able to move. Sometimes we can mobilize them to make the catalyst much more effective.”

Causing the atoms to move — Scott refers to ‘turning them on’ — depends on another process. “We have a catalyst that we’ve prepared in air,” she explains. “Everything is fully oxidized, so nothing moves. Then we reduce it by exposing it to hydrogen, activating the catalyst and causing some of the metal atoms to become mobile. The activation is partly a result of some atoms redistributing in the material and finding new places where they can interact in a better way to form the active sites.”

While that process applies to one family of catalysts the researchers have been studying, Scott says she believes that different treatments will lead to activation in other systems as well. She hopes, too, that this research will provide new insights into using the contributions of mobility to synthesize catalysts having a desired type of dynamic behavior, and to prolong their useful life. “Lifetime is a huge concern,” she said. “Most of the time, when academic researchers design a new material, we say, ‘Oh, it's a great catalyst that has these wonderful properties,’ but a company will look at it and say, ‘No thanks.’ And the reason they say no is that it doesn't ‘live’ long enough; its catalytic properties are not robust enough.

“A catalyst used in a big commercial industrial process has to be able to perform for months or even years,” she continued. “I don't do experiments on the time scale of

years, my graduate students don't have that much patience [or time], and neither do funding agencies. As a result, when we design catalysts, we test them for days. But this lifetime issue is really important for commercial applications."

By way of example, Scott said, "Imagine you use a catalyst in a process, and it behaves like it's supposed to for a few days but then slowly loses its ability to catalyze the reaction because of structural changes that occur in the material, so you briefly change the conditions to reactivate it. In most commercial processes where catalysts are used for years, they have to be reactivated in this way periodically. This project inspires us to believe that mobility could be critical to reactivating these materials."

The work is likely to have a spill-over effect into other areas of science and engineering, Scott noted: "The phenomenon of mobile ions is not specific to any one catalytic reaction or to any one component of the catalyst, and it could be useful in other fields where the key to materials properties is the mobility of atoms. We see this in batteries, for instance, which are, by their nature, conductors required to move ions when you want them to move and to keep them in place when you want them to stay where they are. We're starting to understand how, as you change the ability of the ion to move by changing its electronic structure, you can precisely control that process. Thus, the tools we're developing to study catalysts might also be useful to study battery materials."

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