

## TRANSFORMING INDUSTRIAL SEPARATION OF GASES

Separating one gas from another—removing carbon dioxide from power plant emissions, for example—is not easy. To do so would prevent carbon dioxide, a greenhouse gas, from entering the atmosphere, but present methods are very expensive. Carbon dioxide is also a contaminant found in the methane from natural gas wells. And in submarines or space capsules, carbon dioxide from human respiration must be removed from the air the crew breathes before it reaches toxic levels.

That challenge, to find new and more efficient ways of separating gases, prompted the U.S. Department of Energy's Office of Science to fund an Energy Frontier Research Center (EFRC) based at the University of California at Berkeley. The Center for Gas Separations research team decided to explore the potential of metal organic frameworks—metal atoms bound together by organic molecules to form a porous, sponge-like material. In this case, the researchers intended to also coat the metal atoms with another organic chemical that bonds readily with carbon dioxide.

About the image: NASA Flight Engineer Reid Wiseman and two other astronauts spent five months onboard the International Space Station, which would not be possible without removing excess carbon dioxide from the air they breathe. (NASA / Bill Ingalls)



*Top:* Coal-fired power plants are a major source of carbon dioxide entering the atmosphere; "cooperative adsorption" may enable a low-cost way of removing it from exhaust gases. (*Heidi Besen / Shutterstock*)

*Bottom:* Drilling in the Texas Permian Basin is now a major source of U.S. natural gas. (*GB Hart / Shutterstock*)

Tom McDonald, a new graduate student, was assigned to test a wide variety of organic chemicals called amines as part of the metal organic framework to see how well the material could bond with, or capture, carbon dioxide gas. One particular amine showed promise. But the metal organic framework had small pores that became easily blocked, inhibiting the carbon dioxide molecules from entering. McDonald spent time learning how to make different metal organic frameworks with larger pores and more potential binding sites for carbon dioxide. In addition, instead of adding the amine molecules to the material used to make the metal organic framework, he added amines after the metal organic framework was already formed. When he tested the resulting material, it was able to absorb and release large amounts of carbon dioxide and to do so with a very small change in conditions, almost like an on-and-off switch—an unexpected and dramatically different behavior.

At this point, the collaborative nature of an EFRC became important. The materials were studied theoretically

with computational chemistry models and analyzed in the laboratory with several different techniques. These were repeated in materials with slightly altered compositions. But the data didn't seem to make any sense—the material's ability to absorb carbon dioxide defied understanding—at least under the long-standing assumption that each potential binding site operated independently of the others.

McDonald finally asked himself: suppose that the behavior of one site (binding to a carbon dioxide molecule) influenced the next site? There were no known examples of such behavior in physical chemistry systems, but there is a well-known biological example: the hemoglobin system in human blood that carries iron to cells. When the metal organic framework data were analyzed as "cooperative adsorption" (in which the binding of a carbon dioxide molecule to one site activated a neighboring site), the data suddenly made sense. And once that cooperative or self-catalytic model was understood, it became possible to design materials and industrial separation processes that were more efficient, much less energy intensive, and potentially far less costly. In particular, McDonald's material absorbed large amounts of carbon dioxide even at relatively low temperatures and, equally important, could be regenerated (to release the carbon dioxide) with a small drop in pressure or a small increase in temperature, thus enabling efficient reuse of the material.

This fundamental discovery led to formation of a U.S.based startup company—Mosaic Materials—which will focus initially on commercializing cooperative adsorption for human life-support systems that remove carbon dioxide from air targeting the naval and space markets. A number of companies are now exploring the potential of cooperative adsorption for scrubbing carbon dioxide from electric power plant exhausts. Perhaps the largest existing market is in removing carbon dioxide from methane, given the rapidly growing U.S. production of natural gas. Moreover, it is already clear that metal organic frameworks can potentially be used to separate carbon monoxide and other commonly used gases, so this EFRC research provides a pathway to develop new materials and separation processes that could lower costs and save energy use for a broad cross-section of industry.

Center for Gas Separations (CGS) Winner — Scientific Ideas Award www.science.osti.gov/bes/efrc/Centers/CGS