Hunting for new zeolites

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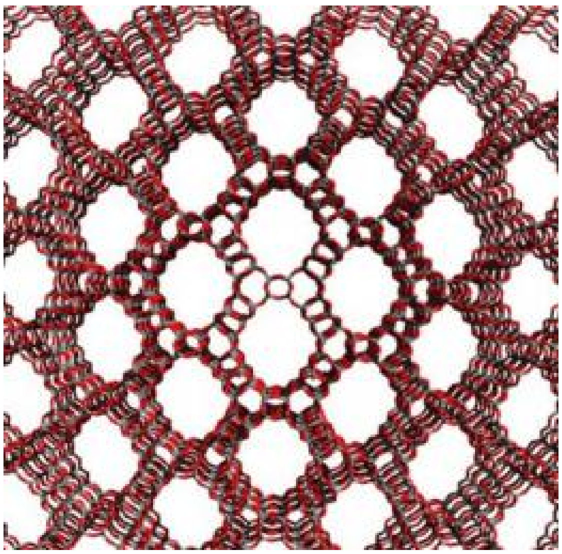

Zeolites are a fine lattice, a molecular sieve that can let molecules of a certain size pass while blocking others. Credit: Rice University

In all the world, there are about 200 types of zeolite, a compound of silicon, aluminum and oxygen that gives civilization such things as laundry detergent, kitty litter and gasoline. But thanks to computations by Rice University professor Michael Deem and his colleagues, it appears there are -- or could be -- more types of zeolites than once thought.

A lot more.

A project that goes back 20 years came to fruition earlier this year when

Deem, Rice's John W. Cox Professor in Biochemical and Genetic Engineering and a professor of physics and astronomy, and his team came up with a list that shows the structures of more than 2.7 million zeolite-like materials.

Of those, they found the thermodynamic characteristics of as many as 314,000 are near enough to currently known zeolites that it should be possible to manufacture these materials.

Creation of the public database is the focus of a new paper, "Computational Discovery of New Zeolite-Like Materials," posted online by the American Chemical Society's *Journal of Physical Chemistry C* and planned as the cover of the Dec. 24 print edition. The paper's authors include Ramdas Pophale, a postdoctoral research associate in Deem's lab; Phillip Cheeseman, senior scientific applications analyst at Purdue's Rosen Center for Advanced Computing; and David Earl, an assistant professor of chemistry at the University of Pittsburgh.

Zeolites can be viewed as "a membrane that will only let molecules of a certain size pass through," Deem said. "But they also do other things. They have an affinity for some molecules, so they're used to absorb odors, for instance, in flower shops."

In laundry detergents, zeolites trade soft ions for hard ones in the water, and the petrochemical industry uses zeolites to crack petroleum into gasoline, diesel and other products. After the accident at the Three Mile Island nuclear power plant, zeolites were used to adsorb radioactive ions.

Zeolites are a fine lattice, a molecular sieve that can let molecules of a certain size pass while blocking others. They can also adsorb molecules, attracting and gripping certain substances -- for which cats and their owners are grateful.

Natural zeolites are often the product of volcanic activity, as rocks, ash and alkaline water combine and crystallize over thousands of years. "The term zeolite comes from the combination of two Greek words that mean 'boiling' and 'stone,'" Deem said.

About a third of zeolites used for commercial purposes are mined, while the rest are synthesized into custom configurations that tend to be more pure, he said.

The fact that only 200 or so zeolites are known makes the creation of Deem's database a real breakthrough, as it gives industries new clues to optimizing their techniques. "That's one possibility, to look for related materials," he said. "In many catalytic applications, there's only one material that currently works."

It took serious computer time to figure out all the possibilities, said Deem, who has lately gained a measure of fame for his study of viruses, particularly H1N1. He began looking at zeolites two decades ago while at Exxon and published his first paper on the subject in the journal Nature. With support from the National Science Foundation (NSF) and the use of the Deem lab's Zefsa II software, researchers needed three years to complete the computations on the NSF's TeraGrid node at Purdue. "I think we were the biggest user of computer time there in 2006, and the fifth- or sixth-largest on the TeraGrid," Deem said. "At Purdue, we were making use of unused computer cycles, like the SETI@home project that searches for extraterrestrial life using people's home computers. We finished around the start of 2009."

The "big question," he said, is how to turn theoretical zeolites into real ones, a project his lab plans to pursue. "A couple of things have to happen. One is that we have to identify materials that look like they would have good properties, and then we have to find a synthesis mechanism to make those materials."

But how does one narrow the practicalities from 2.7 million possibilities? "It depends on the properties we're looking for," Deem said. "We have some ideas of what's practical, but of course we would love to work with other people."

More information:

• View the paper online at pubs.acs.org/doi/abs/10.1021/jp906984z
• The database is available at sdpd.univ-lemans.fr/cod/pcod/

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