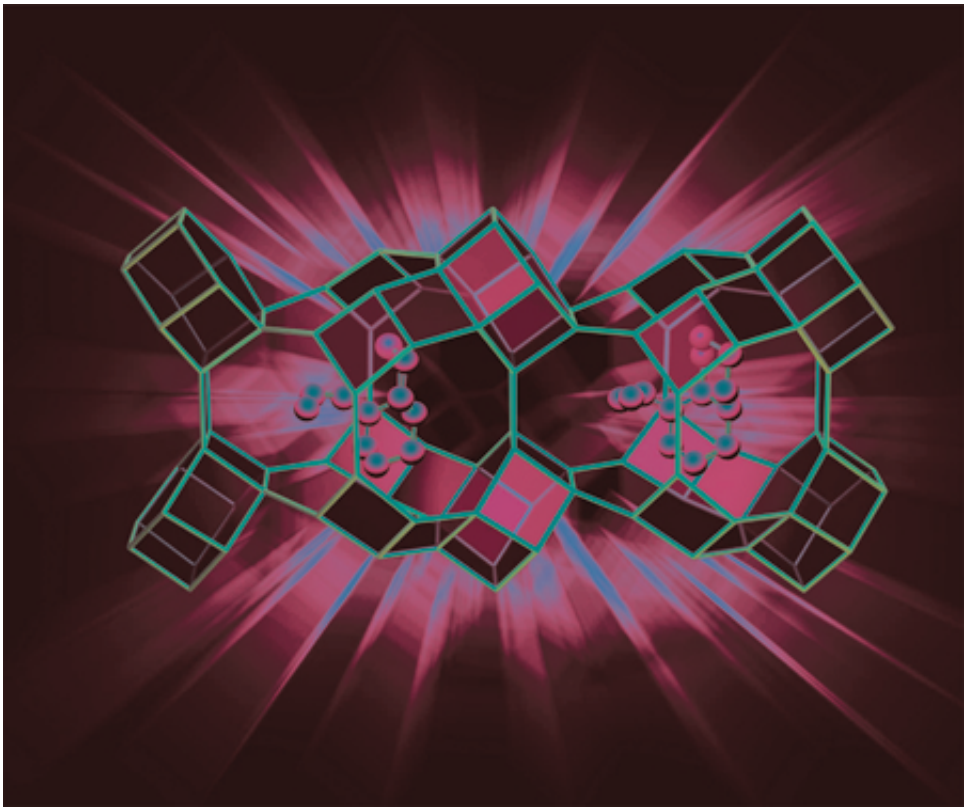
Working backward: Computer-aided design of zeolite templates

June 18 2013, by Jade Boyd



Rice University scientists have created a computational procedure to identify small organic molecules (purple) that can be used to guide the growth of zeolite crystals (yellow). Credit: Kelly Harvey

(Phys.org) —Taking a page from computer-aided drug designers, Rice University researchers have developed a computational method that chemists can use to tailor the properties of zeolites, one of the world's

most-used industrial minerals.

The research is available online and will be featured on the June 21 cover of the Royal Society of Chemistry's *Journal of Materials Chemistry A*. The method allows chemists to work backward by first considering the type of zeolite they want to make and then creating the organic template needed to produce it.

The findings are the latest from the laboratory of Michael Deem, Rice's John W. Cox Professor of Bioengineering and professor of physics and astronomy. Deem's group has previously identified the zeolites best-suited for removing carbon dioxide from power plant exhaust, and they have also used supercomputers to create a database of potentially synthesizable zeolites—some 2.6 million in all.

In the new study, Deem and co-authors Ramdas Pophale and Frits Daeyaert created a computational procedure to identify small organic molecules that can be used to synthesize zeolites.

"We began working on this three years ago," Deem said. "It's basic research, and we illustrated it by applying it to known zeolites. The approach could be used by industry to produce new types of zeolites."

Zeolites are common minerals. About 40 varieties occur naturally, and there are more than 150 man-made types. All zeolites are made of silicon, oxygen and aluminum, but the atomic arrangement of the three varies slightly in each type. These subtle molecular differences lead to significant variations in the chemical properties of each zeolite. As a result, several million tons of zeolites are used each year in processes such as refining of petroleum into gasoline or separation of air into oxygen and nitrogen and products as diverse as cat litter, cement, laundry detergent, water filters, animal feed and chemical separators.

Several million tons of natural zeolites are mined globally each year, but industry also uses a number of synthetic varieties. Producers create these in large process tanks.

"The silicon is either in a gel or in solution, and it condenses to make the zeolite crystal," Deem said. "The current thinking is that the crystal nucleates from an amorphous cluster of silicon oxide that's maybe 3-5 nanometers in size. Once the nucleus of the crystal forms, it continues to grow, and producers regulate the crystalline pattern by including organic molecules in the original solution.

These molecules are called "organic structure directing agents," or OSDAs. The zeolite crystal grows around the OSDAs. Intense heat is used to burn away the OSDAs and open the pores that give the zeolite its characteristic chemical properties.

In the new study, Deem, Pophale and Daeyaert created a procedure for designing OSDAs that would make a particular type of zeolite.

"We begin with a library of organic fragments—molecules that you could buy from a chemical supplier," Deem said. "Next, we have the computer apply a range of chemical reactions to each of the molecules in the library to build up an OSDA from these individual fragments. We then evaluate each candidate OSDA based upon a number of criteria. For example, is it easy to synthesize? Is it stable in solution? Can it withstand the conditions in the zeolite production vessel? How well, energetically, does it stabilize the zeolite?"

Deem said the method was designed to be practical for industry.

"Our inspiration for this is what people have done in drug design," he said. "Drug designers learned the hard way that they could build perfectly shaped molecules, atom by atom, but that it was completely

impractical to produce those ungainly molecules in bulk. As a result, they pioneered this idea of searching whole libraries of known compounds and feasible reactions to find drugs that are both efficacious and practical to produce. There are at least 55 drug candidates that have been discovered by this approach."

Deem's new method for designing OSDAs is similar, and he hopes it may one day allow researchers to produce one of the 2.6 million theoretically possible zeolites that his group identified in its 2011 study. For example, the crystalline structure of some zeolites features a chiral, twisting pattern that can be either right- or left-handed. The resulting zeolite crystals are mirror opposites. Researchers can make mixtures of these materials today, but they can't make pure right-handed or left-handed crystals. With Deem's new method, it may be possible to create an OSDA to make only left- or right-handed varieties.

"Breaking that chiral symmetry would be very exciting," Deem said. "It would highlight the broad range of possibilities of this OSDA design method."

More information: pubs.rsc.org/en/content/articl … g/2013/ta/c3ta10626h

Provided by Rice University