New nano trap protects environment

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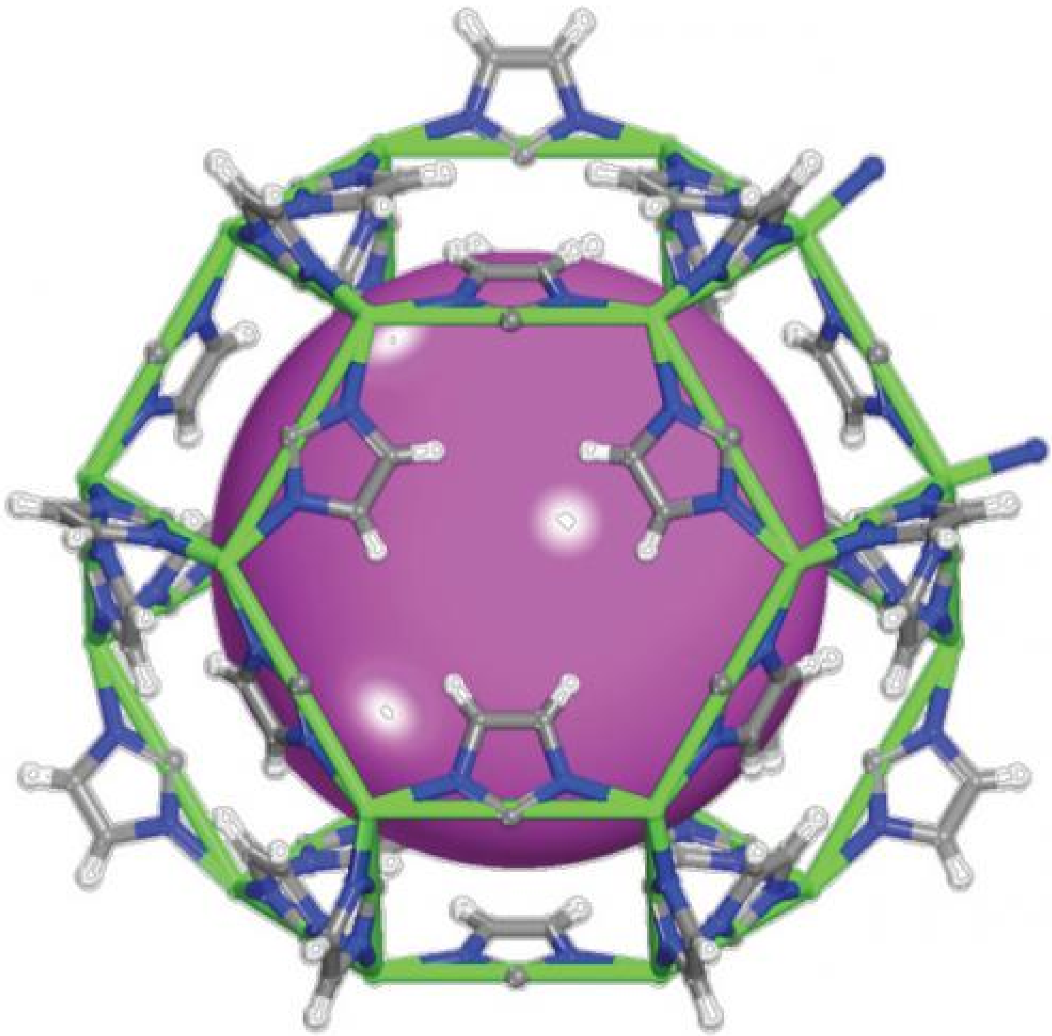

This illustration of a metal-organic framework, or MOF, shows the metal center bound to organic molecules. Each MOF has a specific framework determined by the choice of metal and organic.

A new type of nanoscale molecular trap makes it possible for industry to store large amounts of hydrogen in small fuel cells or capture, compact and remove volatile radioactive gas from spent nuclear fuel in an affordable, easily commercialized way.

The ability to adjust the size of the trap openings to select for specific molecules or to alter how molecules are released at industrially accessible pressures makes the trap uniquely versatile. The trap is constructed of commercially available material and made possible through collaborative work at Argonne and Sandia national laboratories.

"This introduces a new class of materials to nuclear waste remediation," said Tina Nenoff, a chemist at Sandia National Laboratories. "This design can capture and retain about five times more iodine that current material technologies."

Organic molecules linked together with metal ions in a molecular-scale Tinker Toy-like lattice called a metal-organic-framework, or MOF, form the trap. Molecules of radioactive iodine or carbon dioxide or even hydrogen for use as fuel can enter through windows in the framework.

Once pressure is applied, these windows are distorted, preventing the molecules from leaving. This creates a cage and a way of selecting what to trap based on the molecule's shape and size.

The compression also turns the MOF from a fluffy molecular sponge that takes up a lot of space into a compact pellet. The ability to compress large amounts of gas into small volumes is a crucial step to developing hydrogen gas as an alternative fuel for engines.

But what makes this MOF, called ZIF-8, dramatically different from designs created during the past decade is its ability to distort the windows in the framework and trap large volumes of gas at relatively low pressures. ZIF-8 takes about twice the pressure of a junkyard car compactor, which is about 10 times less pressure than is needed to compress other comparable zeolite MOFs.

This creates an environmentally friendly process that is within the reach of existing industrial machinery, can be produced on a large scale and is financially viable.

The ZIF-8 is composed of zinc cations and organic imidazolate-based linkers. The topology of the framework is analogous to sodalite – a well-known zeolite.

The use of other available porous MOFs is limited to small batches because specialized scientific equipment is needed to apply the large amount of pressure they require to compress to a position that will maintain the new shape that traps the gas. This makes them not commercially viable.

Chapman and her colleagues at Argonne used X-rays from the Advanced Photon Source to perfect the low-pressure technique of making the MOFs into dense pellets. The distortion of the molecular framework that occurs during the process does not significantly reduce the gas storage capacity.

"These MOFs have wide-reaching applications," said Karena Chapman, a scientist at Argonne National Laboratory, who was inspired to explore low-pressure treatments for MOFs by her experiences working with flexible MOFs for hydrogen storage. Prior to this work, most high-pressure science research, such as the development of MOFs, took its cue from earth studies, where extensive pressures cause transitions in geological materials.

With the pellet process worked out, the scientists tapped Nenoff at

Sandia to find a just the right type of molecule for the MOF's structure to expand its use from hydrogen and carbon dioxide capture. Nenoff and her team had identified the ZIF-8 MOF as being ideally suited to separate and trap radioactive iodine molecules from a stream of spent nuclear fuel based on its pore size and high surface area.

This marks one of the first attempts to use MOFs in this way. This presents opportunities for cleaning up nuclear reactor accidents and for reprocessing fuel. Countries such as France, Russia and India recover fissile materials from radioactive components in used nuclear fuel to provide fresh fuel for power plants. This reduces the amount of nuclear waste that must be stored. Radioactive iodine has a half-life of 16 million years.

The research team is continuing to look at different MOF structures to increase the amount of iodine storage and better predict how environmental conditions such as humidity will affect the storage lifetime.

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