Two simple building blocks produce complex 3-D material

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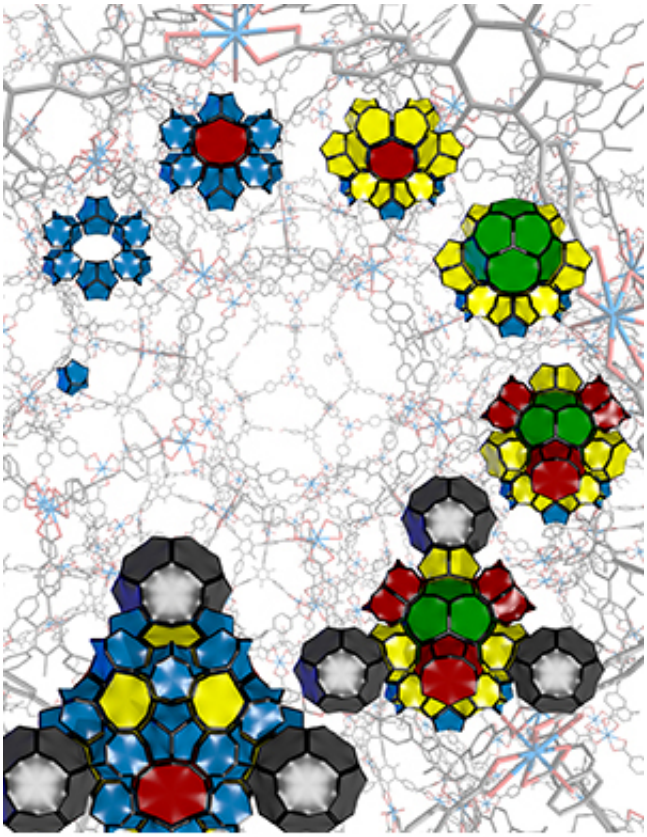

Self-assembly of a metal-organic framework. Credit: Northwestern University

Northwestern University scientists have built a structurally complex

material from two simple building blocks that is the lowest-density metal-organic framework ever made.

Directed by design rules developed by the scientists, uranium atoms and organic linkers self-assemble into a beautiful crystal—a large, airy 3-D net of very roomy and useful pores. The pores are so roomy, in fact, that the scientists have nestled a large enzyme inside a pore—no small feat. The material can act as a protective scaffold for enzymes.

"We are building with one-atom precision," said Omar K. Farha, a research professor of chemistry in the Weinberg College of Arts and Sciences who led the research. "Our material begins at the level of individual atoms, measured by angstroms, and ends on the hundreds of microns level, where we can hold the small crystal with a tweezers and see it with the naked eye."

The study was published in the May 12 issue of the journal *Science*.

The material is very light, despite being made from uranium, one of the heaviest elements in the periodic table. (The scientists used uranium 238, a nonradioactive isotope.) The uranium atoms are so far away from each other in the structure that the metal-organic framework (MOF) takes the lowest density title from any of the competition.

"It is counterintuitive," said Farha, who specializes in the rational design of MOFs for catalysis, sensing and storage applications.

"This material has not been seen or predicted before. Despite its simple beginnings, our MOF's structure has an unparalleled structural complexity. And we've just scratched the surface of building sophisticated structures using simple building blocks."

The discovery unveils the potential to create general design rules for self-

assembly of open, complex structures from simple building blocks while also highlighting the potential of actinides, such as uranium, in materials synthesis, Farha said.

Researchers now can apply the new set of design rules for bottom-up construction to synthesize various novel materials with pre-designed and predictable complex structures.

Metal-organic frameworks are well-ordered, lattice-like crystals. The nodes of the lattices are metals, and organic molecules connect the nodes. The new MOF, called NU-1301, is made up only of uranium oxide nodes and tricarboxylate organic linker units. This simplicity makes the MOF industrially relevant.

In addition to the structural complexity, NU-1301 has a very high surface area, pore volume and water stability and can be used to separate small organic molecules and large biological molecules, or enzymes, based on their sizes and charges.

Each unit cell—the basic unit that repeats in three dimensions to create the crystal structure—is composed of 816 uranium nodes and 816 organic linkers. One unit cell measures 173 angstroms across, and it keeps repeating itself. The unit cells assemble into pentagons and hexagons, eventually growing into a crystal that can reach a quarter of a millimeter wide.

The paper is titled "Bottom-up construction of a superstructure in a porous uranium-organic crystal."

More information: Peng Li et al. Bottom-up construction of a superstructure in a porous uranium-organic crystal, *Science* (2017). DOI: 10.1126/science.aam7851

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