Programmable synthetic materials

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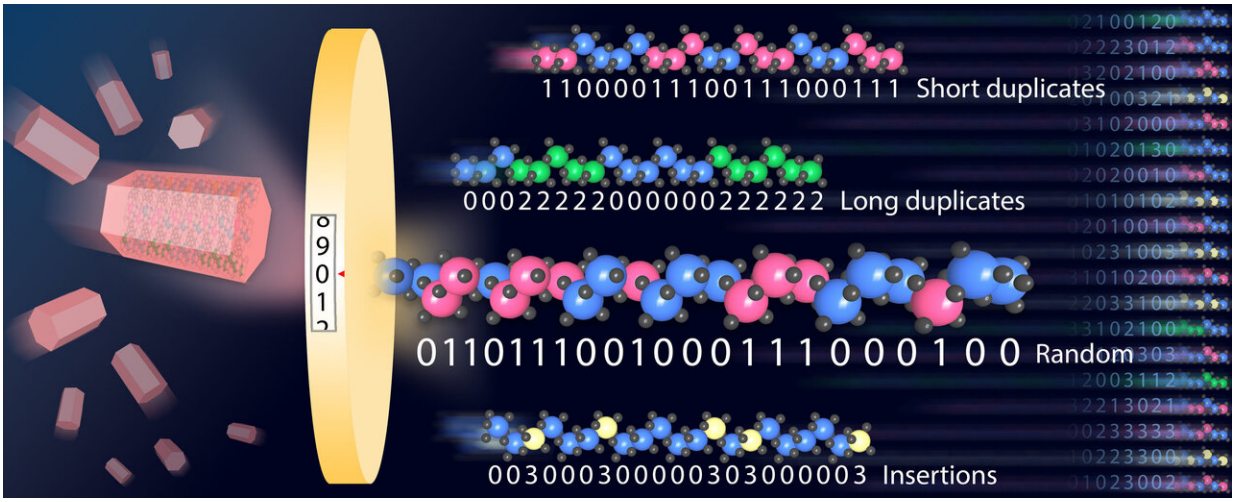

Rods of multivariate MOFs (left) can be programmed with different metal atoms (colored balls) to do a series of chemical tasks, such as controlled drug release, or to encode information like the ones and zeros in a digital computer. Credit: UC Berkeley image by Omar Yaghi and Zhe Ji

Artificial molecules could one day form the information unit of a new type of computer or be the basis for programmable substances. The information would be encoded in the spatial arrangement of the individual atoms—similar to how the sequence of base pairs determines the information content of DNA, or sequences of zeros and ones form the memory of computers.

Researchers at the University of California, Berkeley, and Ruhr-

Universität Bochum (RUB) have taken a step towards this vision. They showed that atom probe tomography can be used to read a complex spatial arrangement of metal ions in multivariate metal-organic frameworks.

Metal-organic frameworks (MOFs) are crystalline porous networks of multi-metal nodes linked together by organic units to form a well-defined structure. To encode information using a sequence of metals, it is essential to be first able to read the metal arrangement. However, reading the arrangement was extremely challenging. Recently, the interest in characterizing metal sequences is growing because of the extensive information such multivariate structures would be able to offer.

Fundamentally, there was no method to read the metal sequence in MOFs. In the current study, the research team has successfully done so by using atom probe tomography (APT), in which the Bochum-based materials scientist Tong Li is an expert. The researchers chose MOF-74, made by the Yaghi group in 2005, as an object of interest. They designed the MOFs with mixed combinations of cobalt, cadmium, lead, and manganese, and then decrypted their spatial structure using APT.

Li, professor and head of the Atomic-Scale Characterisation research group at the Institute for Materials at RUB, describes the method together with Dr. Zhe Ji and Professor Omar Yaghi from UC Berkeley in the journal *Science*, published online on August 7, 2020.

Just as sophisticated as biology

In the future, MOFs could form the basis of programmable chemical molecules: for instance, an MOF could be programmed to introduce an active pharmaceutical ingredient into the body to target infected cells and then break down the active ingredient into harmless substances once

it is no longer needed. Or MOFs could be programmed to release different drugs at different times.

"This is very powerful, because you are basically coding the behavior of molecules leaving the pores," Yaghi said.

They could also be used to capture CO_2 and, at the same time, convert the CO_2 into a useful raw material for the chemical industry.

"In the long term, such structures with programmed atomic sequences can completely change our way of thinking about material synthesis," write the authors. "The synthetic world could reach a whole new level of precision and sophistication that has previously been reserved for biology."

More information: Sequencing of metals in multivariate metal-organic frameworks, *Science* (2020). DOI: 10.1126/science.aaz4304 , science.sciencemag.org/content/369/6504/674

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