Hidden atomic patterns discovered in mixed-metal MOFs

BY FERNANDO GOMOLLÓN-BEL | 17 AUGUST 2020

Layer-by-layer laser slicing of metal–organic frameworks (MOFs) has revealed that different metals in these materials arrange themselves in organised sequences – rather than randomly as researchers had assumed. The team behind the work envisions that materials with multi-metal patterns could encode instructions to carry out series of chemical reactions.

MOFs are porous structures assembled from metals and organic linkers. ‘Multivariate MOFs combine different types of metals, [and/or] linkers in their backbone, enabling new chemical properties that are not possible in simpler structures,’ explains Isabel Abánades Lázaro from the University of Valencia, Spain, who wasn’t involved in the work. Until now, most researchers believed that metal atoms in multivariate MOF were organised randomly. ‘It is truly surprising to see these sequences surface, and to discover that different synthetic conditions lead to different organised structures,’ she adds.
‘This is the future of materials chemistry,’ explains the study’s co-lead, Omar Yaghi from the University of California-Berkeley, US. ‘We show that MOFs can operate in a programmable way, following sequences superimposed onto their structure.’ These sequences, he says, transform otherwise dull and repetitive crystal structures. ‘We create highways across the lattice, enabling new paths for molecules and novel ways to store bits of information,’ Yaghi adds.

His team used a technique called atom probe tomography (APT) to analyse the sequence of metals within MOF-74, which combines cobalt, cadmium, lead and manganese. Laser pulses evaporate the crystalline sample layer by layer, ‘almost like cutting MOF slices,’ explains Deanna D’Alessandro from the University of Sydney, Australia. Then, the researchers analyse the composition of each vaporised layer using mass spectrometry. Unlike nuclear magnetic resonance or x-ray diffraction, ‘APT can construct a 3D map of the MOF crystals,’ she explains.

Tuning temperatures and metal ratios, Yaghi and co-workers created MOFs with different patterns, such as different length sequences of two metals, or a single metal atom in a long string of another metal. ‘This could determine the behaviour and properties of a material,’ says Yaghi. ‘Imagine cobalt, cadmium, lead and manganese behaving like the nucleotides in DNA – metals could catalogue instructions for processes such as catalysis, cascade reactions, gas separations and drug delivery.’

Potentially, ‘it can encode information to an unprecedented level,’ says D’Alessandro. ‘With knowledge
and control over the ion sequence within a MOF, we could design materials that perform a series of different functions.

Eventually, Yaghi hopes to programme a MOF to capture carbon dioxide and then transform it into chemical fuels. 'We aim to bring chemical synthesis to a level of precision and sophistication only known to biology,' he says.

References

Z Ji, T Li and O Yaghi, *Science*, 2020, **369**, 674 (DOI: [10.1126/science.aaz4304](https://doi.org/10.1126/science.aaz4304))