step. Alternatively, supercritical carbon dioxide can be used to purge the pores. In the case of NU-100, a delicate combination of techniques, which included the use of supercritical CO_2, enabled successful activation of the material[1].

The high gas-sorption abilities of NU-100 are in good agreement with previous experimental work carried out on the other members of this (3,24) family, which have all shown gas-uptake properties superior to that of most MOF materials, owing to their high surface area and non-interpenetrating porous domain, as mentioned above. The H_2 uptake (99.5 mg g^{-1} at 56 bar, 77 K) exceeds that of any currently reported MOF material, and the high-pressure CO_2 uptake (2,315 mg g^{-1} at 40 bar, 298 K) and surface area (6, 143 m^2 g^{-1}) are exceeded only by those of the recently reported MOF-210 (ref. 9).

Both the structure and gas-uptake properties of NU-100 were therefore accurately predicted *in silico* prior to experiment. The excellent correlation between the predicted properties shows not only that the modelling is of very high standard but also that the experiments have been accurately performed. Often, pores are not fully activated experimentally, and computational gas-sorption models therefore overestimate experimental data. Although, in this particular case, the structure obtained might have been intuitively anticipated, the stability of the framework and the observed gas-sorption phenomena were not a foregone conclusion. Indeed, the studies on PCN-610, whose pores had collapsed on solvent evacuation, highlight the challenges and subtleties in activation of MOFs.

Recently, the stability of one form of a zeolitic polyoxometalate-based MOF over other possible polymorphs had been successfully predicted through computational studies[10]. Now, the work carried out by Snurr, Hupp and colleagues on NU-100 serves as a calibration for the suite of computational methods used to model the structure and properties of a MOF. One can envisage further expanding the (3,24) topology, but before making the synthetic investment in preparing the linker, computational foresight into the expected stability and properties would certainly be reassuring. Obviously, the methodology can be extended to MOFs beyond the (3,24) topology, and the potential assistance that both explanatory and predictive computation can provide to MOF synthesis is far-reaching. In this regard, it would be ideal if computational methods could be employed to predict not only the structure and properties of a MOF but also the specific preparative conditions the experimentalist would need to use to form the desired, phase-pure crystals. ❐

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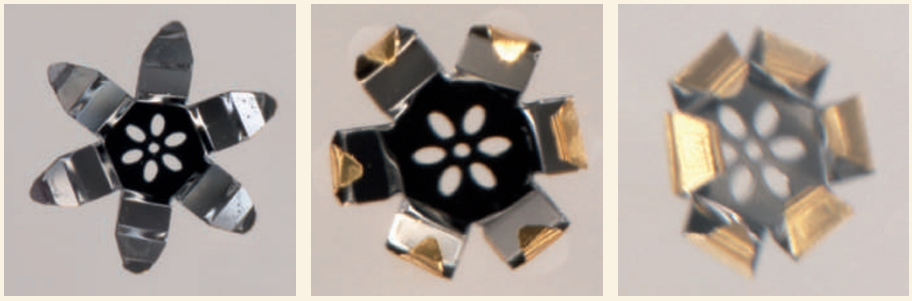
MICROMECHANICS

Enzymatic actuators

Chemical reactions can be used to change the physical properties of a material, and such processes are widely used in nature to drive movement. This form of chemical signalling is, however, rarely applied artificially — most micromechanical devices rely on electrical, hydraulic or pneumatic signals. The development of devices that operate in response to biological cues, such as a disease biomarker, would be of particular interest. Now, David Gracias and co-workers from Johns Hopkins University have fabricated miniaturized grippers that can collect and release biological material in response to being sequentially exposed to two different enzymes (pictured; *J. Am. Chem. Soc.* doi: 10.1021/ja106218s; 2010).



The miniature gripper consists of a petal-shaped assembly of three metals — nickel, chromium and gold. Each 'petal' contains rigid flat sections and two sections of pre-stressed metal that at equilibrium would cause the structure to bend. These two pre-stressed sections are, however, held flat by layers of crosslinked biopolymer — one by gelatin (a polypeptide) and one by carboxymethylcellulose (a polysaccharide). Adding a protease enzyme caused the layer of gelatin to degrade, thus making the first set of hinges bend and close the gripper. The action of a second enzyme — this time a cellulase — causes the second hinge to actuate. This hinge is designed to fold the structure in the opposite direction and amounts to opening the gripper.

Gracias and co-workers built a model liver, and were able to guide a gripper to the desired location within it using magnetic forces. Addition of the enzyme by injection caused the gripper to close and obtain a tissue sample.

STEPHEN DAVEY

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