METAL-ORGANIC FRAMEWORKS

MOF boasts impressive gas-storage properties

Sorbent may boost clean-burning transportation fuels

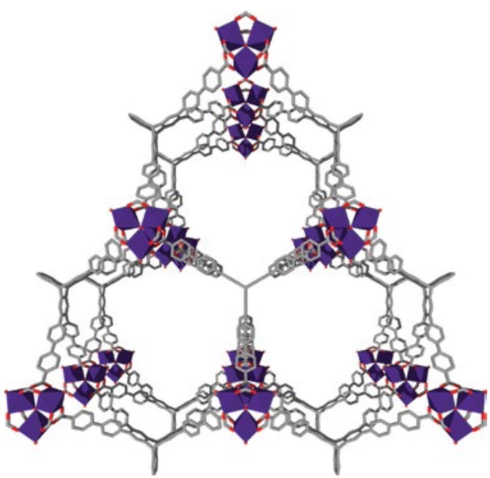
A new solid sorbent could pave the way toward inexpensive and safe storage of hydrogen and methane, which could serve as environmentally friendlier alternatives to conventional liquid transportation fuels. The material balances many of the properties that researchers have been looking for in gas sorbents (*Science* 2020, DOI: 10.1126/science.aaz8881).

Replacing gasoline and diesel fuel with clean-burning hydrogen, which can power zero-emission fuel-cell vehicles, or with methane, which generates relatively low levels of combustion products, could go a long way toward reducing atmospheric levels of carbon dioxide, a greenhouse gas. One challenge impeding broad implementation of such low-emission vehicles is coming up with a low-cost onboard fuel system that can store enough gas at moderate pressure to enable practical driving distances between fill-ups. In principle, gas-adsorbing solids such as metal-organic frameworks, or MOFs, could help in this quest because ordinary fuel tanks containing these spongelike materials could hold more gas at low pressure than costly specialized tanks can hold at high pressure.

MOFs are a large family of porous crystalline solids composed of metal ions or clusters joined by organic linkers. By tailoring the molecular building blocks, which control internal pore sizes and other features, researchers have previously made MOFs with extremely high internal surface areas.

A team led by Zhijie Chen, Penghao Li, and Omar K. Farha of Northwestern University set out to balance several gas-storage properties in a single MOF by combining various computational and experimental methods. For example, the team evaluated thousands of MOFs to explore trade-offs between properties such as internal empty space—or void fraction—pore diameter, and the strength of host-guest interactions.

The study led them to NU-1501-Al, which is composed of trinuclear aluminum centers and triptycene-like organic ligands (the researchers also made an iron analog). The new MOF exhibits surface-area values and reversible, or deliverable, gas-uptake values that, taken individually, are outstanding but not record setting. The combination of these properties in a single material, however, is unprecedented.



This metal-organic framework soaks up exceptional amounts of hydrogen and methane on a per-weight and per-volume basis. C = gray; Al and Fe = purple polyhedra; O = red.

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The Al-based MOF has a surface area of 7,310 m^2/g (one of the highest) and 2,060 m^2/cm^3. Its methane uptake is 0.66 g per gram of MOF, which exceeds the Department of Energy's gravimetric target value (0.5 g/g), and it nearly meets the DOE's volumetric target, 263 cm^3/cm^3. The new material also exhibits one of the highest capacities for deliverable hydrogen on both a weight and a volume basis—roughly 14% by weight and 46 g/L.

"This is a spectacular demonstration of how being able to control matter on the atomic, molecular, and framework levels in one extended chemical structure leads to amazing properties not achievable without such precise control," says MOF pioneer Omar M. Yaghi of the University of California, Berkeley.—MITCH JACOBY