Researchers find way to extract more water from air using a metal-organic framework

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Chemists and engineers find innovative ways to access water—including by pulling it out of thin air. Now, University of Chicago researchers found a way to extract even more water.

In 2021, Prof. Laura Gagliardi of the Pritzker School of Molecular

Engineering and the Department of Chemistry was part of a cross-institutional team developing a new device to extract water from air. The key innovation was a designed material called a metal-organic framework, a hybrid structure of metal ions and organic linkers that can be tuned at the molecular level.

MOFs have a structure of empty pores that adsorb water molecules from air. Gagliardi and her team used theoretical and computational methods to better understand how the material worked at the atomic level.

Now, Gagliardi's team has helped guide the design of an optimized MOF that adsorbs 50% more water from the air than the previous version. The material will ultimately be incorporated into a device built to demonstrate this potentially game-changing technology.

"It is a true breakthrough," Gagliardi said. "It shows that theory, modeling and prediction can guide new experiments and new technology." The research was published in *ACS Central Science*.

Though the original MOF worked well, the team wanted to improve it by increasing the material's pore volume, but at the same time keeping a similar binding strength to water. The MOF framework consists of tiny aluminum-based rods connected by "linker" molecules. This structure creates pores that are lined by alternating hydrophilic (water-binding) and hydrophobic (water-avoiding) pockets.

These pockets are ideally suited for the initial binding of water—when the MOF is exposed to air, water molecules naturally bind themselves to it. Once the initial water molecules are bound, then the following molecules attach themselves to the initial water molecules.

The result is a "sponge" full of water. But the researchers wanted to increase the pore volume (which would allow space for more water to be extracted from the air) while still keeping this special environment needed to attract the initial water molecules. The team also had to find the right sweet spot in design: water needed to bind to the MOF, but not too strongly, or else it could never be desorbed (squeezed out of the sponge).

Gagliardi's team ran computer simulations to find what was ultimately the answer: adding in special linker extension, essentially a long arm on the structure made from two carbon atoms, that would increase the pore size while retaining the special water-binding properties the MOF originally had.

They collaborated with experimentalists at University of California, Berkeley to ensure the material was synthesizable at a relatively low cost. The team—which also includes researchers at the University of Minnesota, General Electric and Humboldt University in Berlin—is now scaling up the production of this new MOF and incorporating it into their prototype water-collecting device. If it works as well in the device as it does in the lab, it means the device could collect significantly more water than before.

"It was a true collaboration of discussions, modeling and experiments," Gagliardi said.

Next, the team is considering more changes to the design and will integrate machine learning that can sift through the data they've gained through their modeling and experiments to give new suggestions for improvement. Ultimately, the device could be used to help soldiers in combat in arid areas or civilians in water-scare regions.

"Hopefully we will continue these discoveries that will ultimately help people capture water in arid climates," she said.

More information: Nikita Hanikel et al, MOF Linker Extension Strategy for Enhanced Atmospheric Water Harvesting, *ACS Central Science* (2023). DOI: 10.1021/acscentsci.3c00018

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