# Genetic algorithm can rapidly pinpoint top candidates for pre-combustion carbon capture

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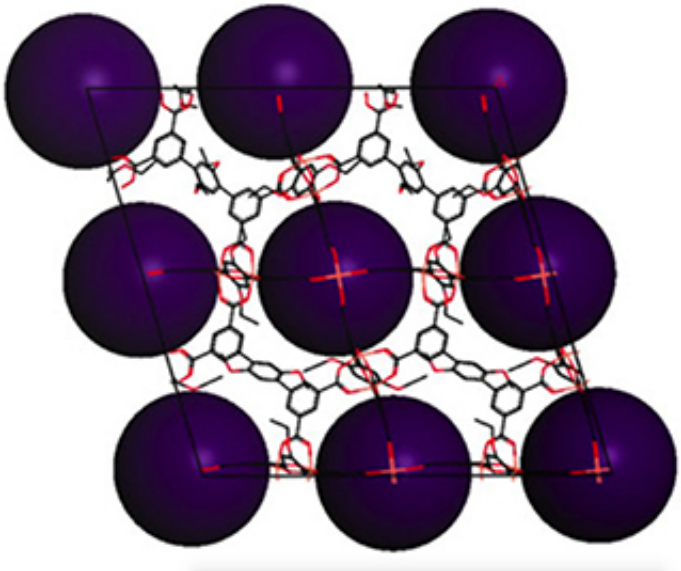

A schematic of the variant of NOTT-101. Credit: Northwestern University

In recent years, a class of highly absorbent, nanoporous materials called metal-organic frameworks (MOFs) have emerged as a promising material for carbon capture in power plants. But finding the optimal MOF to do the best job is another story.

"People are really excited about these materials because we can make a huge variety and really tune them," said Northwestern University's

Randall Q. Snurr. "But there's a flip side to that. If you have an application in mind, there are thousands of existing MOFs and millions of potential MOFs you could make. How do you find the best one for a given application?"

Snurr, who is the John G. Searle Professor of Chemical and Biological Engineering, and his group have discovered a way to rapidly identify top candidates for carbon capture—using just 1 percent of the computational effort that was previously required. By applying a genetic algorithm, they rapidly searched through a database of 55,000 MOFs.

"In the past, we had to evaluate all 55,000 candidates one at a time," Snurr said. "We just marched through them and calculated all of their properties. This genetic algorithm allows you to avoid that."

One of the identified top candidates, a variant of NOTT-101, has a higher capacity for carbon dioxide (CO2) than any MOF reported in scientific literature for the relevant conditions. This information could lead to designs for newly commissioned, cleaner power plants.

"The percentage of carbon dioxide that the MOF can absorb depends on the process," Snurr said. "The Department of Energy target is to remove 90 percent of carbon dioxide from a power plant; it's likely that a process using this material could meet that target."

Supported by the US Department of Energy, the research appeared online today in the journal *Science Advances*. Yongchul G. Chung and Diego A. Gomez-Gualdron, former postdoctoral fellows in Snurr's laboratory, were the paper's co-first authors. Northwestern chemistry professors J. Fraser Stoddart, Joseph Hupp, and Omar Farha contributed to the work as well as Fengqi You, former professor of chemical and biological engineering at Northwestern.

With their nanoscopic pores and incredibly high surface areas, MOFs are excellent materials for gas storage. MOFs' vast internal surface areas allow them to hold remarkably high volumes of gas. The volume of some MOF crystals might be the size of a grain of salt, for example, but the internal surface area, if unfolded, could cover an entire football field.

Snurr's previous work has explored how to use MOFs to capture carbon from existing power plants during the post-combustion process. About 10 to 15 percent of power plant exhaust is CO2; the rest is mainly nitrogen and water vapor. Snurr and Hupp designed a MOF that can sort these gases to capture CO2 before it enters the atmosphere.

Recently, Snurr recalled that the method is a lot easier after a little chemical processing. Chemically processing the fuel before it enters the power plant can turn it into CO2 and hydrogen. After the MOF captures the CO2, the hydrogen is burned and the only byproduct is water. This extra chemical processing step would need to be built into new power plants as a pre-combustion process.

"In places like China, where they are still building a lot of power plants," Snurr said, "this would make a lot of sense."

An optimization technique that mimics natural selection, the genetic algorithm takes a random population of candidate solutions and evolves them toward better solutions through mutation, crossover, and selection. Snurr said this technique has been applied to material screening in the past but not in a search for top candidates for the pre-combustion process, which he describes as a "new challenge."

To tackle carbon capture in pre-combustion, the genetic algorithm pinpointed NOTT-101 as a top candidate. (The material is named after Nottingham, the place where the MOF was first discovered.) Hupp and Farha created the NOTT-101 variant and tested it in the laboratory. Out

of all of the MOFs that have been evaluated for pre-combustion, this material had the highest capacity for capturing carbon and good selectivity for grabbing CO2 to sort it from hydrogen.

"Initially, I wasn't sure how well this algorithm would work," Snurr said. "But using just 1 percent of the usual computational effort is a significant improvement in speed. It's very exciting."

**More information:** Y. G. Chung et al. In silico discovery of metal-organic frameworks for precombustion CO2 capture using a genetic algorithm, *Science Advances* (2016). DOI: 10.1126/sciadv.1600909

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