Using computational research methods to make carbon capture viable

Carbon capture technologies remove CO_2 from industrial gases and are among the technologies being pursued to reduce greenhouse-gas emissions. Carbon capture is also essential for removing unavoidable and historic carbon emissions. One prominent large-scale carbon capture technology relies on solid materials that can selectively bind CO_2 from the air or from the gases produced when fossil fuels are burned. After capture, the materials are coaxed into releasing the CO_2 for permanent storage or utilization — after which the materials are continuously reused to capture more CO_2. The process of capturing and releasing the CO_2 requires significant energy, and if new materials can be found that do it more efficiently, the cost of CO_2 capture can be brought down. Dr. Tom Woo and his research team at the University at Ottawa are among the many innovators who have been working to solve this problem. Through partnerships with other Canadian research groups, industry and government, they are achieving significant advances in carbon capture technology.

The Woo Lab, University of Ottawa.
Left to Right: Tom Woo, Grace Cosby, Sydney O'Shaughnessy, Yan Oueis, Ohmin Kwon, Marco Gibaldi, Raikhan Zakarina, Jun Luo.
Missing: Andrew White, Jake Burner, Rosa Cicciarelli, Olivier Marchan
Photo courtesy of Tom Woo.

Dr. Woo says computational research methods, supported by publicly funded DRI resources, are essential to solving the technological problems he studies. These include developing new materials for energy storage and conversion, gas separations and carbon capture. "Synthesizing and testing a new material represents a huge investment of time and money so it's only possible to evaluate a small number of candidate materials by traditional research methods alone," says Dr. Woo. "Computational methods allow us to, for example, rapidly screen 50,000 materials and predict their performance in order to better focus the arduous synthesis efforts to accelerate the discovery process." Dr. Woo's research team uses machine-learning, data mining and multi-scale simulations to predict the performance of materials when used in specific industrial processes to understand the energy use and operating costs of the carbon capture.

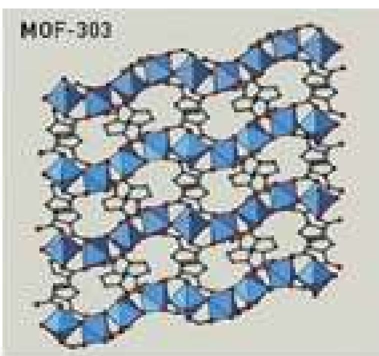
Dr. Woo's team focuses on metal-organic frameworks (MOFs) which are amongst the most studied materials for carbon capture. The architects of MOFs — Susumu Kitagawa, Richard Robson and Omar Yaghi — were awarded the 2025 Nobel Prize in Chemistry.

MOFs can be extremely porous at the molecular level, giving them extraordinary internal surface areas to allow the materials to selectively capture CO_2. "A teaspoon of MOF, which you can imagine would look like a teaspoon of sugar, can have two soccer fields of internal surface area inside of it!" says Dr. Woo.

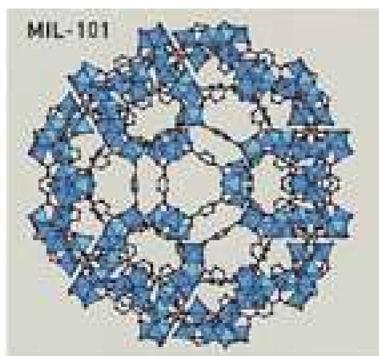
A key challenge is that many MOFs bind better with water than with CO_2, so they do not work as well in filtering combustion gases with a high moisture content, such as gases produced by cement-making. This means the gases must be dried before they can be filtered, which comes at a high energy cost. Dr. Woo's team helped solve this problem by computationally designing new MOFs that were successfully made in the lab. Dr. Woo's lab started by data mining a screening library containing over 300,000 computer-generated materials to identify structures that would bind CO_2 effectively in the presence of water. They then worked with chemists in Switzerland to synthesize new materials that were shown to effectively capture CO_2 from real combustion gases with high moisture content.

Dr. Woo's team has also been involved in the development of CALF-20, the first MOF to be commercialized for carbon capture. CALF-20 was first synthesized in the lab of Professor George Shimizu at the University of Calgary. Early in its development, atomistic simulations in Dr. Woo's lab showed that CALF-20 could capture CO_2 from wet flue gases, years before it was confirmed experimentally. Since then, CALF-20 has been adopted by Svante, a Vancouver-based startup, where it is at the heart of their carbon capture technology. Svante has used CALF-20 to remove CO_2 from cement making gases at the pilot scale continuously for more than 3 years. The pilot system captures about 1 ton of CO_2 per day and now Svante is scaling the technology to full size to capture more than 5000 tons per day from a Lafarge cement plant.

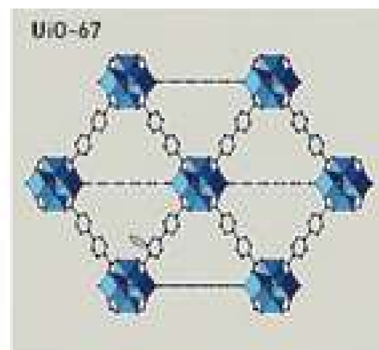
The CALF-20 project is only one of many collaborative projects in which Dr. Woo's research team is engaged. The team also works, for example, with France-based Total Energies, to evaluate the cost effectiveness and practicality of existing and new carbon capture technologies with MOFs. His lab also is working with Natural Resources Canada and other partners to decarbonize steel production with carbon capture technologies. All collaborations require compute-intensive research methods, which in turn critically depend on publicly funded DRI infrastructure. Dr. Woo's research team has used as much as 2000 CPU years of resources in recent years from Ontario's Niagara platform and other national computing platforms. "Without these resources provided by Compute Ontario and the Digital Research Alliance of Canada we could not tackle these important problems," he says.



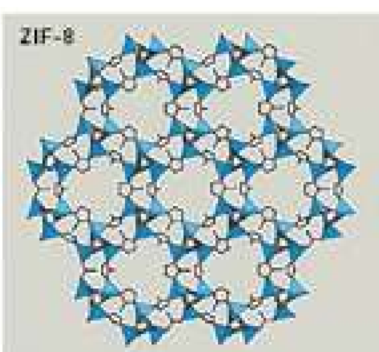
MOF-303 can capture water vapour from desert air during the night. When the sun heats up the material in the morning, potable water is released



MIL-101 has gigantic cavities. It has been used to catalyse the decomposition of crude oil and antibiotics in polluted water. It can also be used to store large quantities of hydrogen or carbon dioxide.

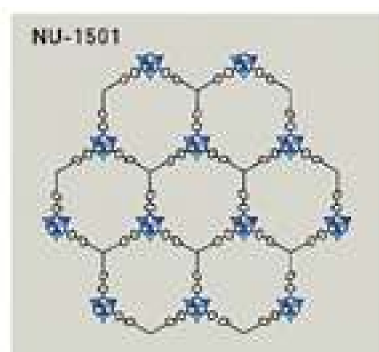


UiO-67 can absorb PFAS from water, which makes it a promising material for water treatment and the removal of pollutants.



ZIF-8 has been used experimentally for mining rare-earth elements from wastewater.

CALF-20 has an exceptional capacity to absorb carbon dioxide. It is being tested in a factory in Canada.



NU-1501 has been optimised to store and release hydrogen at normal pressure. Hydrogen can be used to fuel vehicles, but in ordinary high-pressure tanks the gas is extremely explosive.

Illustration of CALF-20 from the Nobel press kit.
Photo courtesy of Johan Jarnestad/The Royal Swedish Academy of Sciences.