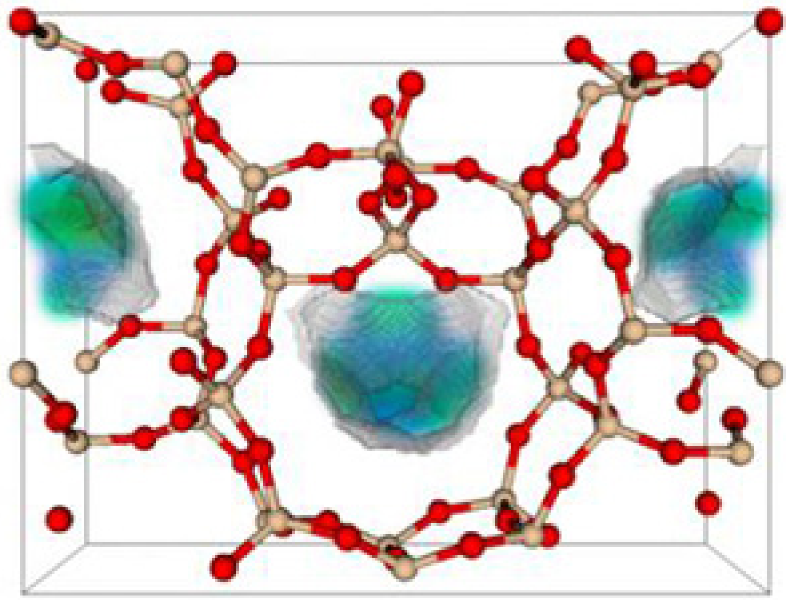
Computer model pinpoints prime materials for efficient carbon capture

Model vets millions of structures to find ones that will improve efficiency of current technology



This is an example of the 50 best zeolite structures for capturing carbon dioxide. Zeolite is a porous solid made of silicon dioxide, or quartz. In the model, the red balls are oxygen, the tan balls are silicon. The blue-green area is where carbon dioxide prefers to adsorb.

When power plants begin capturing their carbon emissions to reduce greenhouse gases – and to most in the electric power industry, it's a question of when, not if – it will be an expensive undertaking.

Current technologies would use about one-third of the energy generated by the plants – what's called "parasitic energy" – and, as a result, substantially drive up the price of electricity.

But a new computer model developed by University of California, Berkeley, chemists shows that less expensive technologies are on the horizon. They will use new solid materials like zeolites and metal oxide frameworks (MOFs) that more efficiently capture carbon dioxide so that it can be sequestered underground.

"The current on-the-shelf process of carbon capture has problems, including environmental ones, if you do it on a large scale," said Berend Smit, Chancellor's Professor in the departments of chemical and biomolecular engineering and of chemistry at UC Berkeley and a faculty senior scientist in the Materials Sciences Division at Lawrence Berkeley National Laboratory (LBNL). "Our calculations show that we can reduce the parasitic energy costs of carbon capture by 30 percent with these types of materials, which should encourage the industry and academics to look at them."

Smit and his colleagues at UC Berkeley, LBNL, Rice University and the Electric Power Research Institute (EPRI) in Palo Alto, Calif., who will publish their results online May 27 in advance of publication in the journal Nature Materials, already are integrating their database of materials into power plant design software.

"Our database of carbon capture materials is going to be coupled to a model of a full plant design, so if we have a new material, we can immediately see whether this material makes sense for an actual design," Smit said.

There are potentially millions of materials that can capture carbon dioxide, but it's physically and economically impossible for scientists and engineers to synthesize and test them all, Smit said. Now, a researcher can upload the structure of a proposed material to Smit's website, and the new computer model will calculate whether it offers improved performance over the energy consumption figures of today's best technology for removing carbon.

"What is unique about this model is that, for the first time, we are able to guide the direction for materials research and say, 'here are the properties we want, even if we don't know what the ultimate material will look like,'" said Abhoyjit Bhown, a co-author of the study and a technical executive at EPRI, which conducts research and development for the electric power industry and the public. "Before, people were trying to figure out what materials they should shoot for, and that question was unanswered until now."

Fossil fuel-burning power plants, in particular coal-burning units, are a major source of the carbon dioxide that is rapidly warming the planet and altering the climate in ways that could impact crops and water supplies, raise sea level and lead to weather extremes. Even with the move toward alternative, sustainable and low-carbon sources of energy, ranging from solar and wind to hydrothermal, coal- and natural gas-burning power plants are being built at an increasing rate around the world. At some point, Smit said, carbon capture will be the only way to reduce carbon emissions sufficiently to stave off the worst consequences of climate change.

Although no commercial power plants currently capture carbon dioxide on a large scale, a few small-scale and pilot plants do, using today's best technology: funneling emissions through a bath of nitrogen-based amines, which grab carbon dioxide from the flue gases. The amines are then boiled to release the $CO2$. Additional energy is required to compress the carbon dioxide so that it can be pumped underground.

The energy needed for this process decreases the amount that can go into making electricity. Calculations show that for a coal-fired power plant, that could amount to approximately 30 percent of total energy generated.

Solid materials should be inherently more energy-efficient than amine scrubbing, because the CO2 can be driven off at lower temperatures. But materials differ significantly in how tightly they grab CO2 and how easily they release it. The best process will be a balance between the two, Smit said.

Smit and his UC Berkeley group worked with Bhown and EPRI scientists to establish the best criteria for a good carbon capture material, focusing on the energy costs of capture, release and compression, and then developed a computer model to calculate this energy consumption for any material. Smit then obtained a database of 4 million zeolite structures compiled by Rice University scientists and ran the structures through his model. Zeolites are porous materials made of silicon dioxide, the same composition as quartz.

The team also computed the energy efficiency of 10,000 MOF structures, which are composites of metals like iron with organic compounds that, together, form a porous structure. That structure has been touted as a way to store hydrogen for fuel or to separate gases during petroleum refining.

"The surprise was that we found many materials, some already known but others hypothetical, that could be synthesized" and work more energy efficiently than amines, Smit said. The best materials used 30 percent less energy than the amine process, though future materials may work even better. The computer model will work for structures other than zeolites and MOFs, Smit said.

Bhown said that the theoretically best material will probably have a parasitic energy cost of about 10 percent, so processes that use 20 percent or less are more attractive.

Key to the team's success was using graphics processing units (GPUs) instead of standard computer central processing units (CPUs), GPUs reduced each structure's calculation, which involves complex quantum chemistry, from 10 days to 2 seconds.

Bhown noted that most people believe that some economic incentives or regulatory frameworks are needed to implement carbon capture, and the EPRI's goal is to help the industry identify the best technologies for doing so. A survey that EPRI conducted recently suggested that developing any new technology would take 10-15 years even with adequate funding.

"The collaboration between different parts of the Department of Energy is a nice illustration of the synergy that can be achieved if researchers working on the most fundamental aspects of carbon capture start to collaborate with their industry counterparts," said Karma Sawyer, DOE program director. "This study shows how engineering and fundamental science can speed-up the process of discovery and implementation of promising materials ready to test in the field."

"The hope is that there is a system set up such that, when someone comes up with a promising material, we can rapidly test it and get it to a readiness level pretty quickly," he said. "We are all excited by this work and look forward to pursuing it further."

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Other coauthors of the study are graduate students Li-Chiang Lin and Joseph A. Swisher of UC Berkeley; Adam H. Berger of the EPRI; Richard L. Martin, Chris H. Rycroft and Maciej Haranczyk of LBNL's Computational Research Division; post-doctoral fellows Jihan Kim and Kuldeep Jariwala of LBNL's Materials Science Division; and Michael W. Deem of the Departments of Bioengineering and Physics and Astronomy at Rice University.

This work has been supported by the Department of Energy through National Energy Technology Laboratory, Advanced Research Projects Agency—Energy (ARPA-E) and Office of Science, and through EPRI's Office of Technology Innovation. Smit is also director of the Department of Energy-funded Energy Frontier Research Center at UC Berkeley.

See original post [1].