Cleaning up the atmosphere with quantum computing

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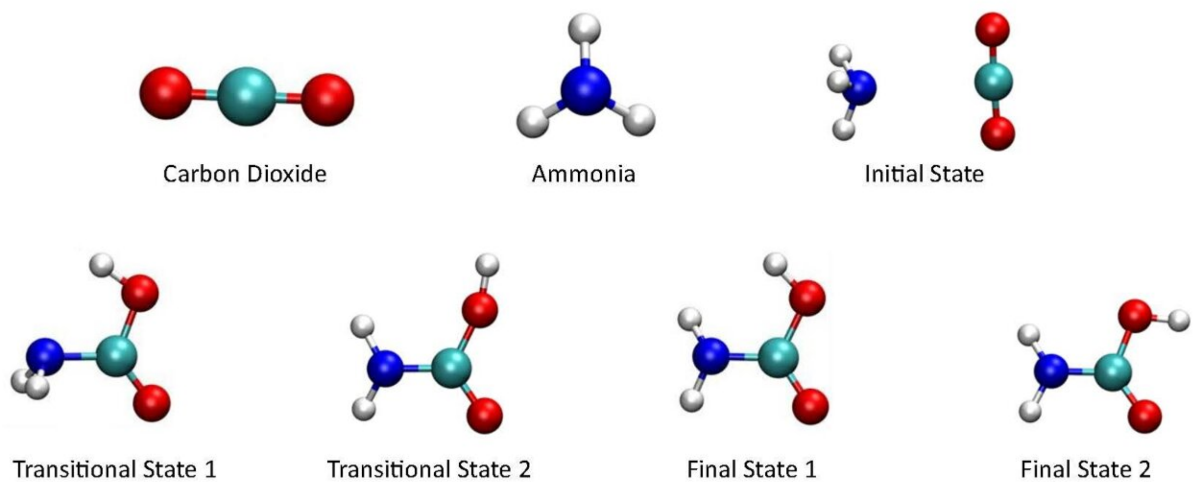

Molecular representations of a simple reaction involving carbon dioxide and ammonia. Credit: Nguyen et al

The amount of carbon dioxide in the atmosphere increases daily with no sign of stopping or slowing. Too much of civilization depends on the burning of fossil fuels, and even if we can develop a replacement energy source, much of the damage has already been done. Without removal, the carbon dioxide already in the atmosphere will continue to wreak havoc for centuries.

Atmospheric carbon capture is a potential remedy to this problem. It would pull carbon dioxide out of the air and store it permanently to reverse the effects of climate change. Practical carbon capture technologies are still in the early stages of development, with the most promising involving a class of compounds called amines that can chemically bind with carbon dioxide. Efficiency is paramount in these designs, and identifying even slightly better compounds could lead to the capture of billions of tons of additional carbon dioxide.

In an article published in *AVS Quantum Science* on March 14, researchers from the National Energy Technology Laboratory and the University of Kentucky deployed an algorithm to study amine reactions through quantum computing. The algorithm can be run on an existing quantum computer to find useful amine compounds for carbon capture more quickly.

"We are not satisfied with the current amine molecules that we use for this [carbon capture] process," said author Qing Shao. "We can try to find a new molecule to do it, but if we want to test it using classical computing resources, it will be a very expensive calculation. Our hope is to have a fast algorithm that can screen thousands of new molecules and structures."

Any computer algorithm that simulates a chemical reaction needs to account for the interactions between every pair of atoms involved. Even a simple three-atom molecule like carbon dioxide bonding with the simplest amine, ammonia, which has four atoms, results in hundreds of atomic interactions. This problem vexes traditional computers but is exactly the sort of question at which quantum computers excel.

However, quantum computers are still a developing technology and are not powerful enough to handle these kinds of simulations directly. This is where the group's algorithm comes in: It allows existing quantum computers to analyze larger molecules and more complex reactions, which is vital for practical applications in fields like carbon capture.

"We are trying to use the current quantum computing technology to solve a practical environmental problem," said author Yuhua Duan.

More information: Manh Tien Nguyen et al, Description of reaction and vibrational energetics of CO2–NH3 interaction using quantum computing algorithms, *AVS Quantum Science* (2023). DOI: 10.1116/5.0137750

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