

Quantum computers could excel in modeling chemical reactions

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Quantum computers would likely outperform conventional computers in simulating chemical reactions involving more than four atoms, according to scientists at Harvard University, the Massachusetts Institute of Technology, and Haverford College. Such improved ability to model and predict complex chemical reactions could revolutionize drug design and materials science, among other fields.

Writing in the *Proceedings of the National Academy of Sciences*, the researchers describe "software" that could simulate chemical reactions on quantum computers, an ultra-modern technology that relies on quantum mechanical phenomena, such as entanglement, interference, and superposition. Quantum computing has been heralded for its potential to solve certain types of problems that are impossible for conventional computers to crack.

"There is a fundamental problem with simulating quantum systems -- such as chemical reactions -- on conventional computers," says Alán Aspuru-Guzik, assistant professor of chemistry and chemical biology in Harvard's Faculty of Arts and Sciences. "As the size of a system grows, the computational resources required to simulate it grow exponentially. For example, it might take one day to simulate a reaction involving 10 atoms, two days for 11 atoms, four days for 12 atoms, eight days for 13 atoms, and so on. Before long, this would exhaust the world's computational power."

Unlike a conventional computer, Aspuru-Guzik and his colleagues say, a

quantum computer could complete the steps necessary to simulate a chemical reaction in a time that doesn't increase exponentially with the reaction's complexity.

"Being able to predict the outcomes of chemical reactions would have tremendous practical applications," says Ivan Kassal, a graduate student in chemical physics at Harvard. "A lot of research in drug design, materials science, catalysis, and molecular biology is still done by trial and error. Having accurate predictions would change the way these types of science are done."

The researchers demonstrate in PNAS that quantum computers would need to attain a size of about 100 qubits -- which are to quantum computers as bits are to conventional computers -- to outperform current classical supercomputers at a chemical simulation.

"This is still far beyond current prototype quantum computers," Kassal says. "And although it might take millions of quantum elementary operations on a few hundred quantum bits, our work suggests that with quantum computers that are as fast as modern conventional computers, one could simulate in seconds a chemical reaction that would take a conventional computer years."

Rather than using binary bits labeled as "zero" and "one" to encode data, as in a conventional computer, quantum computing stores information in qubits, which can represent both "zero" and "one" simultaneously. When a quantum computer is put to work on a problem, it considers all possible answers by simultaneously arranging its qubits into every combination of "zeroes" and "ones."

Since one sequence of qubits can represent many different numbers, a quantum computer would make far fewer computations than a conventional one in solving some problems. After the computer's work is

done, a measurement of its qubits provides the answer.

Source: Harvard University

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