

Reliable Quantum Computation of Molecular Energies

By combining quantum error correction with fault-tolerant techniques, researchers have improved how accurately a quantum computer estimates a molecule's energy.

By **Ryan Wilkinson**

Quantum computers could one day simulate molecules with a level of detail beyond the reach of even their most powerful classical counterparts. But today's quantum computers remain highly error prone because of unwanted interactions with their environment and imperfect implementations of quantum operations. Now Kentaro Yamamoto and his colleagues at Quantinuum, a quantum-computing company, have incorporated continuous error correction in an end-to-end quantum computation of a molecule's lowest energy [1]. Their work marks a key step toward using quantum machines to solve otherwise intractable chemistry problems.

The researchers considered the task of determining the ground-state energy of the smallest possible molecule, hydrogen. This task relies on sophisticated numerical methods and, for a classical computer, requires millions of computing bits for an accurate energy estimate. Yamamoto and his

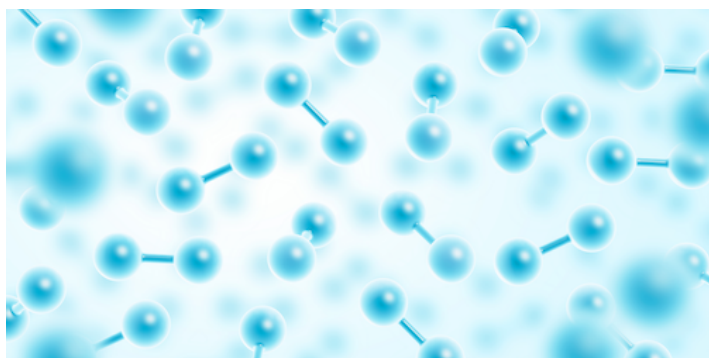
colleagues instead ran the calculation on a quantum computer using just 23 qubits, embodied by the quantum states of trapped ions. To improve the calculation's reliability, the researchers applied real-time error correction to find and fix errors. Moreover, they used state-of-the-art, partially fault-tolerant implementations of crucial quantum operations to make the calculation more resilient to hardware imperfections.

Yamamoto and his colleagues found that their computed ground-state energy was in close agreement with the value calculated on the leading classical computers, albeit with a much lower precision. The researchers also ran numerical simulations to determine which types of hardware errors most strongly affected the result. The findings suggest that further improvements in performance could come from increasing protection against errors accrued during extended idling and ion transport. If such a modest quantum computer can calculate the ground-state energy of a simple molecule, the team's results hint at what larger devices might accomplish for complex molecules.

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REFERENCES

1. K. Yamamoto *et al.*, "Quantum error-corrected computation of molecular energies," *PRX Quantum* **7**, 020319 (2026).



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