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REACTION MECHANISMS

Computing reactions in a qubit

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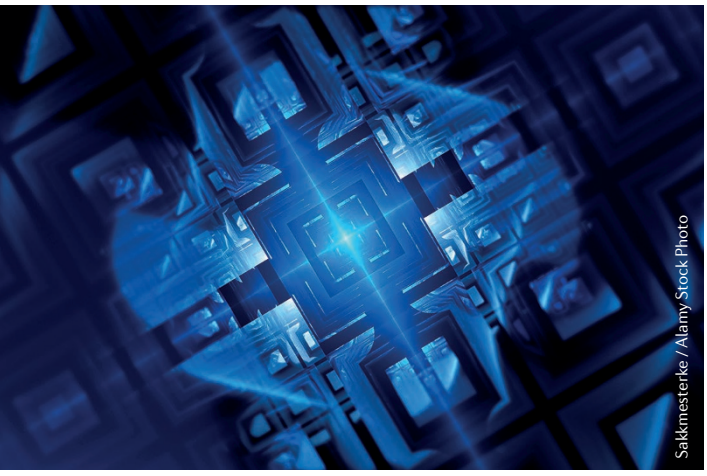
Understanding the thermodynamics and kinetics of a chemical reaction requires a thorough description of all the possible reaction intermediates and how they are energetically connected. The use of quantum computers might reduce the computational cost of such theoretical studies by several orders of magnitude. Matthias Troyer, Markus Reiher and co-workers, writing in *Proceedings of the National Academy of Sciences*, describe the use of quantum computers to predict the energy landscape of the nitrogenase enzyme.

The team studied the FeMo-cofactor in the nitrogenase enzyme, which possesses an electronic structure that is too complex to be studied at a quantum level using classical computers. Although accurate predictions of energetic profiles are achievable for small systems, the computational costs for strongly correlated molecules, such as those with a small bandgap and a dense frontier orbital region, increase exponentially. Several successful theoretical approaches have been proposed and tested to make the best possible use of classical computers; however, even these methods reach their limit for systems with more than about 50 orbitals in the frontier orbital region.



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Quantum computers were first proposed in the early 1980s by Richard Feynman. The main difference with respect to a classical computer is that bits are substituted by quantum bits or qubits. Whereas bits can assume only two values (0 or 1), qubits are two-state quantum systems — for example, particles with two nuclear spin states — and can assume any value corresponding to a superposition of the two states. This means that a qubit can store much more information than a 'classic' bit, reducing the resources necessary to store a molecular wavefunction. The number of bits required to store a wavefunction on a classical computer grows exponentially with the number of spin orbitals, whereas the number of qubits grows linearly. Therefore, quantum chemical calculations represent one of the best stages to demonstrate the value of quantum computers.

Troyer and co-workers analysed the reaction mechanism of the large nitrogenase system for several reasons. "Our goal was to anticipate one likely application of future quantum computers and determine the resources required," explains Troyer. "We also wanted to show that a classically intractable problem, which has much in common with other problems in catalytic chemistry, would be solvable on future quantum computers." Nitrogenase is an enzyme that reduces nitrogen under ambient conditions, and understanding its catalytic mechanism might lead to eco-friendly alternatives to the energy-intensive Haber–Bosch process for the production of ammonia. However, the enzyme-catalysed reaction involves strongly correlated species that test the limits of the approximate quantum chemistry methods available on classical computers. The FeMo-cofactor binds to dinitrogen and its reduced intermediates in different charge and spin states. Troyer and co-workers suggest that the energies related to all the possible intermediates can be accurately calculated at a quantum level using a quantum computer as an accelerator of classical computers. The quantum description of the active site would then consider the remainder of the protein with sufficient accuracy within the molecular mechanics framework.

This research also provided a clear estimate of the computational resources required for such a study. "Our approach builds on previous work on quantum algorithms for quantum chemistry but goes substantially beyond them by providing a full costing of resources, including quantum error correction, and presenting how quantum computers would be used to help explore chemical reaction mechanisms," says Troyer. Reducing the computational resources required for the study of nitrogenase has also been possible owing to the use of high-quality qubits, such as the topological qubits that Troyer's research group is developing. These new-generation qubits make use of 2D quasiparticles (anyons) and can substantially reduce the required size of a future quantum computer by several orders of magnitude. As a result, problems that would have taken years to solve using classical supercomputers might be solved in a matter of days using quantum computers.

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