# Elucidating Reaction Mechanisms on Quantum Computers

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We show how a quantum computer can be employed to elucidate reaction mechanisms in complex chemical systems, using the open problem of biological nitrogen fixation in nitrogenase as an example. We discuss how quantum computers can augment classical-computer simulations for such problems, to significantly increase their accuracy and enable hitherto intractable simulations. Detailed resource estimates show that, even when taking into account the substantial overhead of quantum error correction, and the need to compile into discrete gate sets, the necessary computations can be performed in reasonable time on small quantum computers. This demonstrates that quantum computers will realistically be able to tackle important problems in chemistry that are both scientifically and economically significant.

[1] M. Reiher *et al.* PNAS **114** 7555-7560 (2017).