

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Elucidating Reaction Mechanisms on Quantum Computers

NATHAN WIEBE, microsoft research, MARKUS REIHER, ETH Zurich, KRYSTA SVORE, DAVE WECKER, Microsoft Research, MATTHIAS TROYER, ETH Zurich — 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.

Nathan Wiebe
microsoft research

Date submitted: 08 Nov 2016

Electronic form version 1.4