Chemistry Beyond the Reach of Exact Solutions of the Schroedinger Equation on a Quantum-centric Supercomputer

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Abstract

We present quantum computations of chemistry that go beyond problem sizes amenable to current state-of-the-art exact diagonalization methods. Our results are obtained in a quantum-centric supercomputing architecture, using 6400 nodes of the Fugaku supercomputer to assist an IBM Heron quantum processor. We simulate the N2 triple bond breaking in a correlation-consistent cc-pVDZ basis set, and the active-space electronic structure of [2Fe–2S] and [4Fe–4S] clusters, using 58, 45 and 77 qubits respectively, with quantum circuits of up to 10570 (3590 2-qubit) quantum gates.. The experiments performed establish an unconditional quality metric for quantum advantage, certifiable by classical computers at polynomial cost. We believe these results will redefine the exploration of quantum advantage for chemistry, and more broadly for applications of quantum computing in general.