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Towards Quantum Chemistry on a Quantum Computer BENJAMIN LANYON, University of Queensland, JAMES WHITFIELD, Harvard University, GEOFFREY GILLETT, University of Queensland, MICHAEL GOGGIN, Truman State University, MARCELO ALMEIDA, University of Queensland, IVAN KASSAL, Harvard University, JACOB BIAMONTE, Oxford University, MASOUD MOHSENI, Harvard University, BENJAMIN POWELL, University of Queensland, MARCO BARBIERI, Institut d'Optique, ALÁN ASPURU-GUZIK, Harvard University, ANDREW WHITE[1], University of Queensland — Exact first-principles calculations of molecular properties are currently intractable because the number of conventional computational resources required grow exponentially with molecular size. A solution is to build a quantum computer, which would suffer only a polynomial resource-scaling. In this work, we experimentally realize the calculation of molecular properties on a small-scale photonic quantum computer—obtaining the complete energy spectrum of the hydrogen molecule (H2) in a minimal basis, to 20 bits of precision. We detail how the technique can be expanded to solve large-scale chemical problems that lie beyond the reach of modern supercomputers. Our results represent an early practical step toward a powerful tool for a broad range of quantum-chemical applications.

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