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### **Quantum Computation for Quantum Chemistry**

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The calculation time for the energy of atoms and molecules scales exponentially with system size on a classical computer, but polynomially using quantum algorithms. We demonstrate that such algorithms can be applied to problems of chemical interest using modest numbers of quantum bits. Calculations of the H<sub>2</sub>O and LiH molecular ground-state energies have been carried out on a quantum computer simulator using a recursive phase estimation algorithm. The recursive algorithm reduces the number of quantum bits required for the read-out register from approximately twenty to four. Mappings of the molecular wave function to the quantum bits are described. An adiabatic method for the preparation of a good approximate ground-state wave function is described and demonstrated for stretched H<sub>2</sub>. The number of quantum bits required scales linearly with the number of basis functions used and the number of gates required grows polynomially with the number of quantum bits.