Strategies for quantum chemistry on a quantum computer using a factorized form of the unitary coupled cluster method

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Quantum Chemistry has been viewed as one of the most likely fields of science to benefit from quantum computing. In this talk, I will discuss some of the different strategies that can be employed to calculate electronic structure of molecules with quantum computers. Most algorithms need to balance the number of qubits against the depth of the circuit in order to be able to be run on current hardware. We will describe the different ways in which the unitary coupled-cluster approximation can be implemented on a quantum computer including describing techniques to simulate only part of the molecule on the quantum computer and to use Green's functions in the analysis. We also will discuss how to make efficient circuits and the differences between electronic encoding versus hardware efficient ansatze. While most calculations of electronic structure on quantum computers have been simple demonstrations or proofs of principle, it is possible that we will be seeing real calculations initiated over the next few years using ideas discussed in this presentation.