The quantum and classical cost of reliable assessments of electronic structure

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An accurate assessment of how quantum computers can be used for chemical simulation, especially their potential computational advantages, provides important context on how to deploy these future devices. In order to perform this assessment reliably, quantum resource estimates must be coupled with classical simulations attempting to answer relevant chemical questions and to define the classical simulation frontier. In this talk we describe cost estimates for phase estimation compiled into the surface code quantum error correction protocol and compare these timings against flagship quantum chemistry simulations for cytochrome P450 models which reveals a potential quantum advantage problem.