

Quantum computation for chemistry and materials

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Quantum computers promise to dramatically advance our understanding of new materials and novel chemistry. Recent advances in the technologies related to quantum computing hardware suggest that devices capable of so-called "quantum supremacy" may be available in the next few years. In this talk I will focus on the application of quantum computers to hard problems in the application area of chemistry and materials, and discuss the challenges and opportunities related to current algorithms. I will begin with an introduction to quantum computation appropriate for individuals with backgrounds in electronic structure to make the talk generally accessible. I will then describe one particular method of interest to overcome quantum resource requirements, the variational quantum eigensolver (VQE). This hybrid quantum-classical method provides a way of solving eigenvalue problems and more generic optimizations on a quantum device leveraging classical resources to minimize coherence time requirements. I will briefly review the original VQE approach and introduce a simple extension requiring no additional coherence time to approximate excited states. Moreover, I will show exciting results related to recent developments in dramatically reducing the scaling of chemistry algorithms for quantum computers.