UC San Diego

JACOBS SCHOOL OF ENGINEERING NanoEngineering

UC SAN DIEGO NANOENGINEERING SEMINAR Wednesday, October 10, 2018 Seminar Presentation: 11:00am – 12:00pm SME 248

"Quantum Computation for Chemistry and Materials"

Dr. Jarrod McClean

Google Quantum Artificial Intelligence Lab

Abstract: 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, he 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. He will begin with an introduction to quantum computation appropriate for individuals with backgrounds in electronic structure to make the talk generally accessible. He 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. He will briefly review the original VQE approach and introduce a simple extension requiring no additional coherence time to approximate excited states. Moreover, he will show exciting results related to recent developments in dramatically reducing the scaling of chemistry algorithms for quantum computers.

Biosketch: Jarrod McClean is a senior research scientist in Google's Quantum Artificial Intelligence Lab working on the development of practical quantum algorithms for quantum simulation and other problems. He received his PhD in Chemical Physics from Harvard University specializing in quantum chemistry and quantum computation supported by the US Department of Energy as a Computational Science Graduate Fellow. His research interests broadly include quantum computation, quantum chemistry, numerical methods, and information sparsity.