

Variational quantum eigensolvers for quantum chemistry simulations

Sophia Economou

Virginia Tech

Quantum chemistry is one of the most interesting applications of quantum computers. Prior to the development of a universal quantum computer, near-term quantum simulators could implement the solution of chemistry problems that are beyond the capabilities of classical computers. To achieve this ambitious goal, it is paramount to develop algorithms that exploit the strengths of the quantum processor while also making use of classical resources. A notable example of such algorithms is the variational quantum eigensolver (VQE). A crucial aspect of VQE is the creation of a good variational ansatz, which allows for relatively shallow circuits and a low number of classical optimization parameters. In this talk, I will give an overview of VQEs for chemistry applications and present ADAPT-VQE, a novel algorithm which realizes efficient ansätze on quantum computers.