Implementing the Variational Quantum Eigensolver for Materials

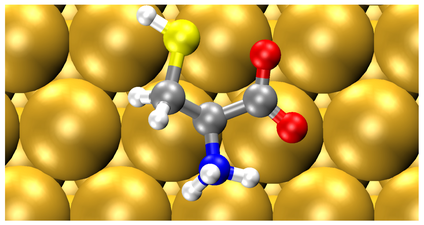
Clayton Smith, Irina Paci

Department of Chemistry, University of Victoria

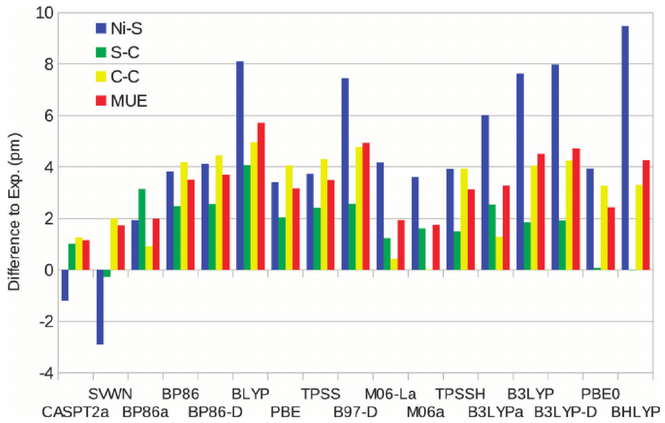
University of Victoria

Background and Motivation

The field of computational chemistry is in no small part a response to the lack of an analytical solution to the Schrödinger equation for nearly all systems in chemistry (i.e. those with more than one electron). A very large number of methods exist to numerically approximate solutions at a wide range of levels of theory.



Deciding what method to use for a project is usually a balance of efficiency and accuracy. Density functional theory (DFT) has become a general purpose method for computational chemistry, but the best functional for a given job is not always clear.



Delcey, M. G. et al. Physical chemistry chemical physics : PCCP ***2014****, 16, 7927–7938*

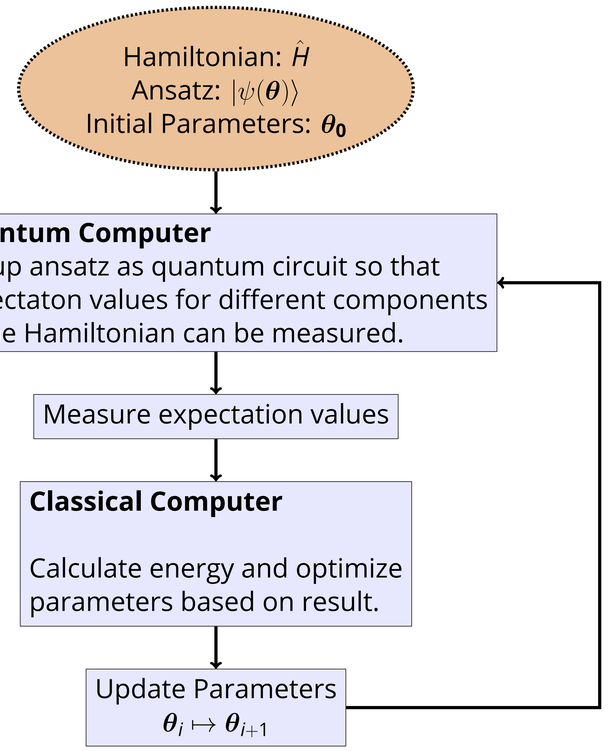
One direction for new methods that could strike the balance between cost and accuracy come in the form of algorithms for quantum computers. One reason for this is that there are natural mappings from chemical systems to qubits, the unit of information used in quantum computers (analogous to bits in classical computers).

An important adjustment from classical computers is that the Hamiltonian of the system is written in a formalism known as the second quantization.

$$\hat{H} = E_{\text{nuc}} + \sum_{ij} h_{ij}\hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\sum_{ijkl} g_{ijkl}\hat{a}_i^\dagger \hat{a}_k^\dagger \hat{a}_j \hat{a}_l$$

VQE

The variational quantum eigensolver (VQE) is currently one of the most popular methods for chemisty calculations on quantum computers. It attempts to solve some of the difficulties of using current or near-term quantum computers (such as noise or lack of computational resources) by offloading some parts of the calculation onto a classical computer.



An important part of using VQE is the selection of the ansatz, since it fixes the form that the wavefunction of the system can take. This can be thought of as similar to basis set selection for other methods, however it is significantly more dependent on the system.

Since VQE is a relatively new method, there is not as wide of a selection of ansätze as say DFT functionals. Moreover, fewer are implemented in existing software packages. As such, most studies involving VQE will require an ansatz to be implemented which can be a complex process.

Scope and Progress

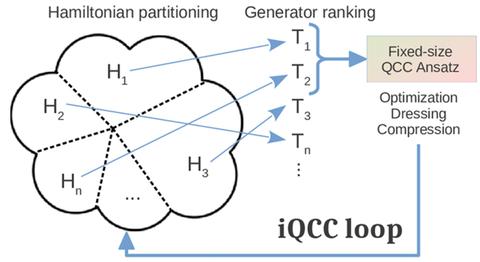
The main goal of this research is to modify the implementation of VQE that exists in the python package Tangelo so that it works for periodic systems. These are systems which have some unit that repeats in space, for example a perfect gold surface. Usually when materials are being studied, the system is modelled as periodic to give a more accurate picture of its properties in bulk.

Currently, we have implemented a technique of computing the necessary coefficients for the Hamiltonian and performing a VQE calculation from this operator. With a non-periodic hydrogen molecule and the built-in UCCSD ansatz, very good agreement with FCI results was seen (with a simulated quantum computer).

However, when doing the same for a periodic string of hydrogen atoms using the same ansatz, the results are quite far from those computed with a method for classical computers. One likely source of this inconsistency is that the ansatz is not designed for a periodic system and so won't model the system as well as one that is tailored for such systems.

Future Work

The most obvious next step with this work is to find an ansatz that works with periodic systems and construct it in code in a form that Tangelo can use. Previous studies have identified some potential ansätze, but the step of implementation will still be time-consuming.



Ryabinkin, I. G. et al. Journal of chemical theory and computation ***2020****, 16, 1055–1063*

A longer term goal of this work would be to expand to the use of other quantum computing algorithms for periodic calculations such as the iterative qubit coupled cluster method. This method is less widely used, but shows promise for use on near term quantum devices.

This research was supported by the Jamie Cassels Undergraduate Research Awards, University of Victoria
Supervised by Dr. Irina Paci