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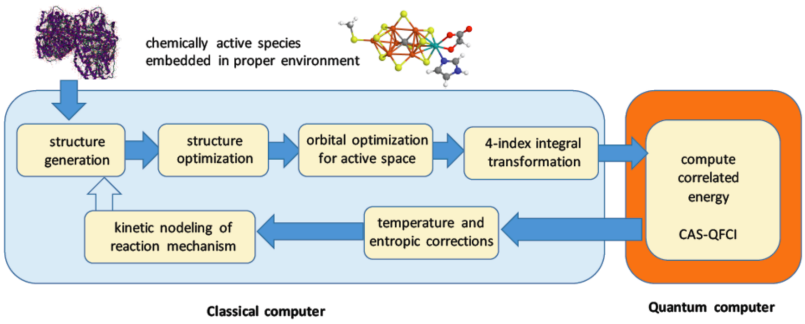
Master's thesis project at the Quantum Technology Laboratory, Department of Microtechnology and Nanoscience

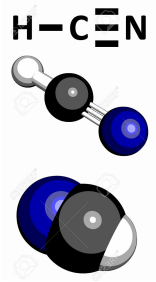
Quantum computation of molecular electronic structure of HCN

for applications on existing and near-future quantum computers

Motivation:
One of the "killer applications" for quantum computers is to calculate the electronic structures and binding energies of large molecules, e.g. biological enzymes, much faster than classical high-performance computers (HPC). The goal is to achieve "quantum supremacy" in a few years, i. e. for quantum accelerators to compute molecular energies that is beyond HPC.



Project description:
The goal of this master's thesis is to calculate the ground state energy surface of the pre-biotic hydrogen cyanide molecule, HCN [1] using a quantum computer, both simulated on an HPC, and implemented on real quantum processor hardware.
The first part of this master's thesis project involves studying recent papers of direct importance for the thesis work [1-3] and, simultaneously, to access and get acquainted to the QISKit quantum program package [4] (IBM Q Experience) in some "simple" standard cases, like LiH.
The second part of the project consists in setting up a quantum calculation of the HCN molecule on (a) an HPC simulator of a quantum computer, and (b) on available quantum hardware. The project lies at the very frontline, globally. The mission is to see how far one can go. HCN is the primary challenge, but it may be necessary also to consider simpler molecules to match available computational local resources.



More information on quantum computing is available at http://www.chalmers.se/en/centres/wacqt/Pages/default.aspx

Prerequisites:
a. Course in Quantum Mechanics and/or Quantum Information Processing
b. Course in Physical Chemistry is not required, but is considered an asset.

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References:
1. Polymorphism and electronic structure of polyimine and its potential significance for prebiotic chemistry on Titan
M. Rahm, J. I. Lunine, D. A. Usher, and D. Shalloway, PNAS **113**, 8121-8126 (2016).
2. Quantum optimization using variational algorithms on near-term quantum devices
N. Moll et al., Quantum Sci. Technol. **3**, 030503 (2018).
3. Quantum information processing with superconducting circuits: a review
G. Wendin, Rep. Prog. Phys. **80**, 106001 (2017).
4. QISKit: IBM's quantum applications work package: https://qiskit.org/aqua; https://github.com/QISKit

Job opportunities:
R&D in industry requiring advanced skills in classical and quantum computing, modelling, optimisation, machine learning. There will be opportunities for industry PhD studies at several companies in the near future.