## INTRODUCTION

Hartree–Fock (HF) method is a method of approximation for the determination of the wave function and the energy of a chemical system. The Hartree–Fock method assumes that the exact N-body wave function of the system can be approximated by a single Slater determinant or by a single permanent N spin-orbitals. By invoking the variational method, one can derive a set of N-coupled equations for the N spin orbitals. A solution of these equations yields the Hartree–Fock wave function and energy of the system.

In this project, I will implement a python notebook that will carry out Hartree-Fock calculations to reach Hartree-Fock energy.

## PROCEDURE

In this project I will:

- Introduce the overlap matrix
- Build an orthogonalization matrix
- Calculate the density
- Calculate the Coulomb and Exchange integral matrices
- Diagonalize the Fock matrix
- Implement an iterative procedure that converges to HF energy
- Test the code for different molecules and compare it with Psi4 results

After carrying out said calculations, I will make a table of comparison between the code I implemented and Psi4 results, I will compare both accuracy and time.

## EXPECTED OUTCOMES

A good iterative procedure capable of calculating Hartree-Fock energy for different molecules.