Workshop on Building a HF program with Python

Abstract:

In this workshop, we plan to go over the basics for electronic structure theories, including a short introduction for python, and the Hartree-Fock Theory. Through the guidance, participants will be able to write a program for doing Hartree-Fock calculation for H2, the simplest molecule.

- This workshop includes practical sessions. Please bring a laptop to the event.
- The materials of the practical session on 2/9 can be downloaded from the link
- https://drive.google.com/drive/folders/1CqieBRd_dPe1ptEnJm3S_HZttK8vCH90?usp=sharing
- We will use colab in the practical session on 2/9. If colab is new to you, please refer to https://colab.research.google.com
- If Python is new to you, before attending the course, please download and install Anaconda on your computer.
- Download Anaconda: https://www.anaconda.com/products/individual

Invited Speakers:

Dr. Hung-Hsuan Lin
Dr. Ching-Cher Sanders Yan

Program:

Tuesday - 2/8	
9:30 – 10:20	Introduction to the theoretical background of Hartree-Fock method Oral Session Dr. Hung-Hsuan Lin
10:20-10:30	Coffee Break
10:30-11:20	Introduction to Basis set approximation Oral Session Dr. Hung-Hsuan Lin
11:20 – 13:00	Lunch Break
13:00 – 16:00	The basics of Python and the coding Skills Oral and Practical Session Dr. Ching-Cher Sanders Yan

Wednesday - 2/9	
9:00 – 12:00	Building a Hartree-Fock program with Python Practical Session Dr. Hung-Hsuan Lin