**11120CHEM524500 Computational Chemistry (計算化學)**
**Instructor: Prof. Tzuhsiung Yang** (楊自雄). Office: R409 (Ext. 33359)
**Date:** 2/13(M) to 6/5(M)
**Time:** M5M6, Monday 13:20-15:10
**Location:** Computer Lab II, NTHU library second floor
**Prerequisite:** Must have taken physical chemistry II or equivalents
**Language:** English/Chinese
**Suggested textbooks:**

- Szabo, A.; Ostlund, N. S. **Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory**; Courier Corporation, 2012.
- Christopher J. Cramer, **Essentials of Computational Chemistry: Theories and Models**, 2nd Ed. Wiley & Sons, New York.

**Course description:** This is a hands-on course. This course will provide a survey of modern computational chemistry methods, with the focus on molecular systems. Routine job types such as single point calculations, geometry optimization, frequency, conformer, and excited states calculations will be covered. Emphasis will be given on the correct application of and analysis of results from computational simulations and troubleshoot calculations when unexpected outcomes are observed. Special topics on machine learning in chemistry will be covered.

**Software:** Pyscf, Orca, Gaussian 16, Gromacs
**Packages:** Pyscf, Openbabel, Pytorch, Scikit-learn
**Sites:** Github

**Grading:** Grades will be based on 1) attendance (20%), 2) midterm presentation (40%), and 3) a final project (40%). Missing 2 classes without excuses = fail.

- Presentation date: We will decide one of the nights on the week of April 10$^{th}$ for midterm presentations.
- Final project: Due on the week of June 12$^{th}$.

**Covid19 policy:** Online class will be available ONLY for people who are tested positive for covid19 or required to self-quarantine. Class link will be provided on the day of the class.

**Syllabus**

| Date | Class | Contents |
|---|---|---|
| **13-Feb** | 1 | Linux/bash commands, Text editors, HPC and schedulers, Molecular visualizers, Python |
| **20-Feb** | 2 | Slater determinant, Restricted/Unrestricted orbital, Self-consistent field (SCF), Hartree-Fock theory, |
| **27-Feb** | *No Class* | |
| **6-Mar** | 3 | Density Functional Theory, Basis sets, Dispersion, Integral approximations, Relativistic corrections |
| **6-Mar** | 3 | Population analysis, Orbital hessian, Close-lying electronic states, Broken symmetry |
| **13-Mar** | 4 | Conformer search, Geometry optimization, Frequency calculations, Implicit solvation models |
| **20-Mar** | 5 | Transition state search, Transition state optimization, Classical kinetic isotope effect |
| **3-Apr** | *No Class* | |
| **10-Apr** | 7 | Excitation energies, XAS pre-edge, Excited state optimization, Conical intersection |
| **17-Apr** | 8 | Spin-orbit coupling, g-Tensor, Hyperfine coupling, Zero-field splitting, Mossbauer parameters |
| **24-Apr** | 9 | Post-HF methods:<br>Perturbation Theory, Coupled-clusters, Complete active space |
| **1-May** | 10 | Revisit property calculations:<br>Excited state energies, Spin-orbit coupling, g-Tensor, Zero-field splitting |
| **8-May** | 11 | Quantum mechanics/molecular mechanics |
| **15-May** | 12 | Molecular dynamics |
| **22-May** | 13 | Special topic:<br>Machine learning in chemistry |
| **29-May** | 14 | Special topic:<br>Machine learning in chemistry |
| **5-Jun** | 15 | Special topic:<br>Machine learning in chemistry |