**Syllabus**

Department of Chemistry and Biochemistry

National Chung Cheng University

Chia-Yi 621, Taiwan

**Course: Advanced Quantum Chemistry (**2605417**)**

**Academic Semester: 113-1 (2024-1)**

**Instructor: Prof. Wei-Ping Hu**

Classroom: Chem 313

Time: Tuesday 08:45-11:30

Textbook: Quantum Chemistry, Ira N. Levine

Evaluation: Weekly Report 40%, Mid-Term 30%, Final Report 30%

*This course encourages the use of generative AI tools, but this must be clearly noted in assignments and reports.*

**Scheduled Contents:**

1. Course Introduction, Historical Background
2. Fundamental Particles and Forces, Cosmology, and Nucleosynthesis
3. Postulates of Quantum Mechanics
4. Particle in a Box, Size Effects, and Tunneling
5. Harmonic Oscillator and IR Spectra
6. Rigid Rotor and Rotational Spectra
7. Hydrogen-Like Atoms and Periodic Tables
8. Many-Electrons Atoms and Atomic Spectra
9. Mid-Term Exam.
10. Scientific Computing and AI tools
11. Molecular Property Prediction
12. Electronic Transition and UV-VIS Spectra
13. Reaction Dynamics Calculation and Application to Atmospheric Chemistry
14. Presentation of Final Report

**References:**

1. Physical Chemistry: A molecular approach Donald A. Mcquarrie and John D. Simon
2. Molecular Quantum Mechanics, P.W. Atkins
3. Molecular Modelling: Principles and applications, Andrew R. Leach