Course Outline

Course: Computational Chemistry

Year: 114 Semester: 2

Credit: 3

Course Number: 2708003

Teacher: Prof. Wei-Ping Hu (E-mail: chewph@ccu.edu.tw)

Department: Chemistry and Biochemistry

Classroom: Chemistry 313

Web Page: http://deptche.ccu.edu.tw/Chemistry/Comp_Chem/

Contents:
- History of Computation
- Atomic Structure
- Introduction to Computational Chemistry
- Coordinate Systems and Model Building
- Basic Principles of Quantum Mechanics
- Methods of Quantum Chemistry
- Basis Sets
- Atomic Calculation
- Molecular Structure and Potential Energy Surface
- Chemical Thermodynamics
- Chemical Dynamics
- Electronic Excited States
- Solvation Effects

Evaluation: Reports 40%, Mid-Term Exam. 30%, Final Exam. 30%

References:

Ira N. Levine, Quantum Chemistry, 5th Edition, Prentice Hall, 2000.

Frank Jensen, Introduction to Computational Chemistry, 2nd Edition, Wiley 2006.

Christopher J. Cramer, Essential of Computational Chemistry, Theories and Models, 2nd Edition, Wiley 2004.

Andrew R. Leach, Molecular Modelling, 2nd Edition, Prentice Hall 2001.

Mark A. Ratner, George C. Schatz, Introduction to Quantum Mechanics in Chemistry, Prentice Hall 2001.

Encyclopedia of Computational Chemistry, Wiley.