Course Schedule of TIGP Program
Semester: Fall, 2008

Course: Advanced Physical Chemistry (I)-高等物化一
Time: 9:1 0~12:00 am, Tuesday
Room: 311 IAM
Required, credit: 3
Course No.: TIGP727100

Date	lecturer	Date	lecturer
9/16	Prof. Sheng-Hsien Lin	11/11	Prof. Michitoshi Hayashi
9/23	Prof. Sheng-Hsien Lin	11/18	Prof. Michitoshi Hayashi
9/30	Prof. Sheng-Hsien Lin	11/25	Prof. Michitoshi Hayashi
10/07	Prof. Sheng-Hsien Lin	12/02	Prof. Michitoshi Hayashi
10/14	Prof. Sheng-Hsien Lin	12/09	Prof. Michitoshi Hayashi
10/21	Prof. Sheng-Hsien Lin	12/16	Prof. Michitoshi Hayashi
10/28	Prof. Sheng-Hsien Lin	12/23	Prof. Michitoshi Hayashi
11/04	Prof. Michitoshi Hayashi		

Speaker	Part 1 (Week 1-week7) Prof. Sheng-Hsien Lin 林聖賢教授
Class Outline	1. Classical Mechanics 2. Schrödinger Equation 3. Some Simple Systems 4. Hydrogen Atom 5. Approximation Methods
Introduction	First present the methods of Newton equations of motion, Lagrange's equations of motion and Hamilton equations of motion and show how to employ these methods to treat dynamical problems. These will then be compared with quantum mechanical treatments. Particle in a box, harmonic oscillator rigid rotator and hydrogen atom will be solved Approximation methods like perturbation method and variational method will be presented.
Grading	Homeworks Quizzes Examinations
Textbook	Lecture Notes

Speaker	Part 2 (Week 8-week 15) Prof. Michitoshi Hayashi 林倫年教授
Class Outline	1. Many Electron Systems -- Hamiltonian -- Tight-binding systems -- Nearly free electron systems -- Born Oppenheimer approximation -- Molecular Hamiltonian -- Basis set approach -- Localized basis set -- Plain wave -- Many electron wave functions -- Slater determinant -- Exchange correlation of two electrons -- The Hartree-Fock self-consistent Field Method -- Exchange energy 2. Ab initio Implementations of Hartree-Fock Molecular Orbital Theory -- Basis sets -- Hartree-Fock limit 3. Electron Correlation -- Dynamical & non-dynamical correlations -- Configuration interaction -- Many-body perturbation theory -- Coupled cluster theory -- Multi-configuration Self-consistent Field Theory 4. Density Functional Theory -- The Hohenberg-Kohn theorems -- Kohn-Sham self-consistent field theory -- Exchange-correlation functionals --LDA, LSDA, GGA, Post-GGA 5. Time-dependent density functional theory -- Runge-Gross theorem -- Time-dependent Hartree-Fock -- Linear response theorem -- Random phase approximation -- Tamm-Dancoff approximation 6. Applications

Introduction	This course focuses on the quantitative introduction to the major concepts of many-body theory for electrons and its applications to modern quantum chemistry. To some extent, the course also aims at bridging the gap between quantum chemistry and many electrons in solid state. The course teaches many-electron theory, molecular orbitals with atomic basis sets and density functional theory. The Pauli exclusion principle and the Slater determinant will be introduced. Based on the solution of the Hartree-Fock equation, the electron-electron interaction (correlation effects) will be discussed. Configuration interaction and multi-configuration Hartree-Fock theories will also be introduced. Time-dependent density functional theory will be discussed in comparison with configuration interaction and random-phase approximation based on Hartree-Fock reference systems (non-interacting systems).
Grading	Homeworks Quizzes Examinations
Textbook	Lecture Notes References 1. Essence of computational chemistry: theories and models Second Edition Christopher J. Cramer, Wiley 2. Modern Quantum Chemistry A. Szabo, N. S. Ostlund, Dover 3. Electron correlations in molecules and solids P. Fulde, Springer 4. A. Dreuw and M. Head-Gordon Chem. Rev. 2005**,** 105, 4009-4037 5. M.A.L. Marques and E.K.U. Gross Annu. Rev. Phys. Chem. 2004. 55:427–55 6. M. E. Casida “Time-dependent density functional response theory for molecules” in Recent Advances in Computational Chemistry Vol.1 Ed. D. P. Chong, page 155 (1995, World Scientific)