Course Schedule of MST Program ,TIGP

Semester: Fall, 2010(99 學年度上學期)

Course(科目): Advanced Physical Chemistry (I)-高等物化(I)
Time(時間): 9:1 0~12:00 am, Tuesday(T2T3T4) or 10:00~11:30 am, Tuesday , 10:00~11:30 am, Thursday(T3T4,R3R4)
Room(教室): 311 IAMS 中研院原分所 R311(台大校園)
NTHU coordinator(清大教師): 倪其焜

Course speakers(授課老師): Michitoshi Hayashi 林倫年、Kaito Takahashi 高橋開人、Yen-Chu Hsu 許豔珠
Required(必修課), credit(學分): 3
Course No.(科號): TIGP727100

Date	lecturer	Date	lecturer
9/14 Tuesday 9:1 0~12:00	Prof. Kaito Takahashi	12/07 Tuesday 10:00~11:30	Prof. Yen-Chu Hsu
9/21 Tuesday 9:1 0~12:00	Prof. Kaito Takahashi	12/09 Thursday 10:00~11:30	Prof. Yen-Chu Hsu
9/28 Tuesday 9:1 0~12:00	Prof. Kaito Takahashi	12/14 Tuesday 10:00~11:30	Prof. Yen-Chu Hsu
10/5 Tuesday 9:1 0~12:00	Prof. Kaito Takahashi	12/16 Thursday 10:00~11:30	Prof. Yen-Chu Hsu
10/12 Tuesday 9:1 0~12:00	Prof. Kaito Takahashi	12/21 Tuesday 10:00~11:30	Prof. Yen-Chu Hsu
10/19 Tuesday 9:1 0~12:00	Prof. Kaito Takahashi	12/23 Thursday 10:00~11:30	Prof. Yen-Chu Hsu
10/26 Tuesday 9:1 0~10:30	Prof. Michitoshi Hayashi	12/28 Tuesday 10:00~11:30	Prof. Yen-Chu Hsu
11/02 Thursday 9:1 0~10:30	Prof. Michitoshi Hayashi	12/30 Thursday 10:00~11:30	Prof. Yen-Chu Hsu
11/09 Tuesday 9:1 0~12:00	Prof. Michitoshi Hayashi	1/04/2011 Tuesday 10:00~11:30	Prof. Yen-Chu Hsu
11/16 Tuesday 9:1 0~12:00	Prof. Michitoshi Hayashi	1/06/2011 Thursday 10:00~11:30	Prof. Yen-Chu Hsu
11/23 Tuesday 9:1 0~12:00	Prof. Michitoshi Hayashi	1/11/2011 Tuesday 10:00~11:30	Prof. Yen-Chu Hsu
11/30 Tuesday 9:1 0~12:00	Prof. Michitoshi Hayashi	1/13/2011 Thursday 10:00~11:30	Prof. Yen-Chu Hsu

Speaker	Part 1 (Week 1-week6) Prof. Michitoshi Hayashi 林倫年教授

Class Outline	<The first 3 weeks> Quantum mechanical principles →Uncertainty principle and relations →The principle of superposition The dynamics of microscopic systems →Schrödinger equation →Wave function →Operator algebra →Eigenvalues and eigenvectors →Observables →Stationary states →The Virial Theorem <The last 3 weeks> Approximations →Perturbation method →Variational principle Simple applications → Harmonic oscillator → Diatomic systems Introduction to many electron systems → Independent particle approximation → Correlation effects
Introduction	This course consists of two parts: introduction of (1) the basic principles of quantum mechanics and (2) the essentials of the solving methods of Schrödinger equation and its applications to simple and important systems. The first 3 weeks, we will discuss the dynamics of microscopic systems and quantum mechanical principles. The last 3 weeks, we will see how quantum mechanics works for some of the simplest systems including hydrogen atom, hydrogen molecules using several approximation techniques.
Grading	Problem sets will be provided weekly to trace understanding of the materials. The final grade will be determined by Problem sets (60%) Exam (40%)
Textbook	Lecture Notes Reference Atkins' Physical Chemistry

Speaker	Part 2 (Week 7-week12) Prof. Kaito Takahashi 高橋開人教授

Class Outline	<week 7-9> Atomic electronic structure • Hydrogen like atom wave function • Atomic orbitals and ionization energy • Spectra and selection rules <week 10-12> Molecular Structure and electronic properties • Born-Oppenheimer approximation • Molecular orbitals of diatomic molecule • Molecular orbitals of polyatomic molecule • Prediction on molecular properties
Introduction	This class will use the basis techniques learned in the previous weeks to understand (1) atomic electronic structure and (2) molecular structure and electronic properties. In the first three weeks we will study the electronic wave functions of the hydrogen like wave functions and learn the effect of shielding and electron repulsion. Furthermore, selection rules for atomic structure will also be studied. In the last three weeks we extend the study to include nuclear motion and study molecules. After learning the Born-Oppenheimer approximation, molecular orbitals of diatomic and polyatomic molecules will be studied. The possibility to predict molecular properties from calculation will be mentioned at the end.
Grading	Home work (30%) Class room quiz (30%) Test (40%)
Textbook	Atkin&DePaula, “Physical Chemistry”

Speaker	Part 3 (Week 13-week18) Prof. Yen-Chu Hsu 許豔珠教授

Class Outline	1. Symmetry and symmetry classification 2. Group theory 3. Symmetry in Quantum Theory 4. Rotational spectroscopy: selection rules, line width and stark effect. 5. Rotational spectroscopy and Astrophysics
Introduction	This part will follow closely the textbook (chapter 12 and section 1-8 of chapter 13). Additional handout will be given in the classes.
Grading	1. Homework (40%). 2. Attendance (25%). 3. Examination (35%).
Textbook	Atkin's Physical Chemistry, 8^{th} edition(Oxford Univ., 2006)