Advanced Physical Chemistry II - Course Syllabus

Course Number: ChemS 370

Course Title: Advanced Physical Chemistry II

Academic Semester:	Spring	**Academic Year:**	2015/ 2016
Semester Start Date:	Jan 24, 2016	**Semester End Date:**	May 19, 2016

Class Schedule: Monday and Wednesday 1.00pm-2.30pm

Classroom Number: 3135

Instructor(s) Name(s): Luigi Cavallo
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Office Location: Bldg. 3 R-4237

COURSE DESCRIPTION FROM PROGRAM GUIDE

Review of quantum mechanics from a postulational viewpoint; variational and matrix methods; time independent and time-dependent perturbation theory; applications to molecular systems including potential energy surfaces and reaction pathways.

COMPREHENSIVE COURSE DESCRIPTION

Applied quantum chemistry is becoming a standard technique to assist the research, and especially to rationalize catalytic behavior. This course is designed to give an overview of frequently applied computational methods. This includes the underlying theoretical approach as well as hands-on tutorials. The course is split into two units, at the end of the first is the middle term exam, and at the end of the second is the final term exam.

The first unit will cover basic concepts, such as that of molecular structure, connection between geometry and energy, the concept of the potential energy surface. Methods for locating a stationary point on the potential energy surface are also introduced. Next a brief separation between methods based on empirical force fields and quantum mechanics, for the calculation of the energy of a system, is introduced. Once this separation is given, details on the empirical force field approach are given, together with a physical explanation of the various terms. Next the concepts of static and dynamics methods are introduced. The concepts of configurations space and exhaustive sampling of the configurations space are provided, with the limitations of current methods. This part of the course terminates with the introduction of Monte Carlo based methods. Hands-on tutorials are fundamental part of this

section of the course. First an introduction to UNIX and to programming in FORTRAN is given. Then, the tutorials focus on the molecular dynamics simulation of a small protein, and of a salt dissolved in water, with an introduction of the most classic tools for the analysis of these systems.

The second unit of the course starts with a brief introduction of quantum mechanics and of the fundamental postulates, and moves then to the introduction of classic wavefunction based methods, with an overview of the Hartree-Fock method. Next the molecular orbital (MO) model and its application to molecules will be introduced, together with expansion of the MO in terms of the linear combination of atomic orbitals (LCAO-MO). Post Hartree-Focks methods are then rapidly overviewed. The course moves then to density functional theory (DFT) methods, since DFT is the workhorse of current applications of quantum chemistry. After introduction of the Honenberg-Kohn theorems and of the Kohn-Sham machinery, attention is focused on a description of the most used functionals, together with their accuracy in predicting chemical behavior. The last classes focus on deriving properties, and rationalizing reactivity using DFT based methods. The hands-on tutorials will teach to control a user friendly quantum mechanics program to build a small molecule, to optimize its geometry, to evaluate its potential and free energy, to study a small reaction.

By the end of the course a clear understanding of how computational tools can be used to derive properties that can explain experimental behavior should have been acquired, together with the ability to run basic calculations, and finally with the proper knowledge to read the computational section of papers.

GOALS AND OBJECTIVES

1. Introduce the student to concepts and basic principles of thermodynamics and kinetics.

2. Enable the student to have a physico chemical approach to perform and analyze experiments.

3. Present a variety of applications of the concepts of physical chemistry, showing their usefulness.

REQUIRED KNOWLEDGE

Basic knowledge of quantum mechanics

REFERENCE TEXTS

The official textbook for the course is: Christopher Cramer “Essentials of Computational Chemistry 2nd Ed.”, Wiley

The textbook will mostly be used as a reference for the material presented in the course, and to provide additional reading material. Lecture notes will be the fundamental source of information when preparing for the exams or working on the assignments. The textbook will also provide detailed derivations of fundamental equations, plus numerous examples,

problems and answers. Handout is posted on the blackboard before each class. It is strongly recommended that the handout material is studied before the lectures.

METHOD OF EVALUATION

Graded content
Grading: 30% - Attendance to classes and to the hands-on tutorials 30% - Middle term exam 40% - Final exam Exam: All exams will be open-book exams, where only the reference book and handout distributed during the class can be used.

COURSE REQUIREMENTS

Assignments

The course will include hands-on tutorials. Participation to these tutorials is mandatory.

Course Policies

No more than 2 absences is allowed before the middle term exam. The same holds for the second section of the course, from the middle term to the final exam.

Additional Information

NOTE
The instructor reserves the right to make changes to this syllabus as necessary.