



Course Syllabus: Advanced Physical Chemistry II - ChemS 370

Division	Physical Science and Engineering Division
Course Number	ChemS 370
Course Title	Advanced Physical Chemistry II
Academic Semester	Spring
Academic Year	2018/2019
Semester Start Date	01/27/2019
Semester End Date	05/23/2019
Class Schedule (Days & Time)	01:00 PM - 02:30 PM Wed Thu

Instructor(s)				
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Teaching Assistant(s)	
Name	Email
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Course Information	
Comprehensive Course Description	<p>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.</p> <p>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.</p> <p>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 short 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 Hohenberg-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.</p> <p>Hands-on tutorials are fundamental part of this course. First an introduction to UNIX and to shell commands and text editors is given. The tutorials cover the fundamental sections of the course, and the scope is to link the concepts provided in the theoretical classes with real life work. By the end of the course a basic understanding of how computational tools can be used to derive properties and to 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.</p>

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.
Goals and Objectives	<ol style="list-style-type: none"> 1. Introduce the students to the potential of computational chemistry. 2. Give an overview of the physics behind the various computational methods. 3. Provide the students the experience of running computations. 4. Provide the students the skills to read the computational section of a paper.
Required Knowledge	Knowledge of quantum mechanics is fundamental.
Reference Texts	<p>The official textbook for the course is: Christopher Cramer "Essentials of Computational Chemistry 2nd Ed.", Wiley</p> <p>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.</p>
Method of evaluation	<p>40.00% - Final exam 40.00% - Midterm exam 10.00% - Homework /Assignments 10.00% - Attendance and Participation</p>
Nature of the assignments	<p>Assignments will be focused on linking theoretical classes to the tutorials. Most of the assignments will be via hands on tutorials</p>
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	A tentative schedule of the weekly topics is listed below. This schedule can be changed to match progress of the students during the course and the hands on tutorials.

Tentative Course Schedule

(Time, topic/emphasis & resources)

Week	Lectures	Topic
1	Wed 01/30/2019	Intro and scope of course
1	Thu 01/31/2019	Computers and chemistry
2	Wed 02/06/2019	Potential energy surfaces
2	Thu 02/07/2019	The Empirical Force Field
3	Wed 02/13/2019	Geometry optimizations and algorithms
3	Thu 02/14/2019	Introduction to molecular dynamics
4	Wed 02/20/2019	MD Integration algorithms
4	Thu 02/21/2019	Temperature & Pressure control, PBC
5	Wed 02/27/2019	Analysis of MD trajectories, the RDF
5	Thu 02/28/2019	Space sampling with MD
6	Wed 03/06/2019	Monte Carlo methods and Space sampling with MC
6	Thu 03/07/2019	Tutorial 1 : Linux
7	Wed 03/13/2019	MD tutorial 1
7	Thu 03/14/2019	MD tutorial 2
8	Wed 03/20/2019	MD tutorial 3
8	Thu 03/21/2019	Middle term exam
9	Wed 03/27/2019	Spring Break
9	Thu 03/28/2019	Spring break
10	Wed 04/03/2019	Brief summary of Quantum Mechanics
10	Thu 04/04/2019	The Hamiltonian and the BO approximation
11	Wed 04/10/2019	The LCAO method - Basis sets
11	Thu 04/11/2019	Hartree-Fock method and brief intro to CI – MP2
12	Wed 04/17/2019	Density Functional Theory
12	Thu 04/18/2019	Density Functional Theory
13	Wed 04/24/2019	Vibrations ZPE Thermodynamics
13	Thu 04/25/2019	Solvent and solvation free energy
14	Wed 05/01/2019	Calculating pKa & RedOx potentials
14	Thu 05/02/2019	Calculating reaction Profiles
15	Wed 05/08/2019	DFT tutorial 1
15	Thu 05/09/2019	DFT tutorial 2
16	Wed 05/15/2019	DFT tutorial 3
16	Thu 05/16/2019	DFT tutorial 4
17	Wed 05/22/2019	Final Exam Week
17	Thu 05/23/2019	Final Exam Week

Note

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