جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology

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	2016/2017
Semester Start Date	01/22/2017
Semester End Date	05/18/2017
Class Schedule (Days & Time)	01:00 PM - 02:30 PM | Wed Thu

Instructor(s)

Name	Email	Phone	Office Location	Office Hours
Luigi Cavallo	Luigi.Cavallo@kaust.edu.sa	+966128080709		Send an email to fix an appointment

Teaching Assistant(s)

Name	Email
Mohit Chawla	mohit.chawla@kaust.edu.sa

Course Information

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.

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.

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.

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	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	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	**50.00**% - Midterm exam **50.00**% - Final exam
Nature of the assignments	Assigments will be focused on linking theoretical classes to the tutorials. Most of the assignemnts will be via hands on tutorials
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 01/25/2017 Thu 01/26/2017	**Week 1.** Introduction to the course. Overview of the potential of computational chemistry. Goals of the course. Suggested textbook. Grading assessment. Concept of potential energy surface. The empirical force field approximation.
2	Wed 02/01/2017 Thu 02/02/2017	**Week 2**. Algorithms for locating stationary points on the potential energy surface. Introduction to Molecular Dynamics methods. Time evolution of a system. Algorithms for integrating the equations of motion.
3	Wed 02/08/2017 Thu 02/09/2017	**Week 3.** Molecular dynamics in different ensembles. Temperature and pressure control. Concepts of thermostat and barostat. Algorithms for temperature and pressure control. Periodic boundary conditions. Concept of radial distribution function.
4	Wed 02/15/2017 Thu 02/16/2017	**Week 4.** Overview of Monte Carlo methods and algorithms. Sampling configurations space with Molecular Dynamics and Monte Carlo methods. Comparison between the two methods.
5	Wed 02/22/2017 Thu 02/23/2017	**Week 5**. **Tutorials:** Introduction to LINUX; Basic shell commands; Introduction to programs for visualizing molecular dynamics simulations. Visualizing proteins structure.
6	Wed 03/01/2017 Thu 03/02/2017	**Week 6. Tutorials:** Modeling small systems using a molecular dynamics code.
7	Wed 03/08/2017 Thu 03/09/2017	**Week 7**. Preparation for the exame and Middle term exam.
8	Wed 03/15/2017 Thu 03/16/2017	**Week 8.** Short overview of fundamental concepts of quantum mechanics; Overview of the Hartree-Fock method; The MO-LCAO approximation; Atom centered basis sets; Overview of post-HF methods.
9	Wed 03/22/2017 Thu 03/23/2017	**Week 9**. Introduction to Density Functional Theory; The Hohenberg-Kohn theorems; The Kohn-Sham equations; The machinery of DFT; Classes of density functionals.
10	Wed 03/29/2017 Thu 03/30/2017	**Week 10.** Introduction to spectroscopy; Vibrational analysis; From internal energy to free energy; Performance of DFT methods.
11	Wed 04/05/2017 Thu 04/06/2017	**Week 11.** Introduction to solvation and solvation free energy; Calculation of pKa and of RedOx potentials.
12	Wed 04/12/2017 Thu 04/13/2017	**Week 12.** Reactivity, locating intermediates and transition states; Improving the energetics of a reaction pathway; Assembling a reaction pathway; Thermodynamic and kinetic analysis of a reaction pathway.
13	Wed 04/19/2017 Thu 04/20/2017	**Week 13. Tutorials:** Introduction to building an input geometry; Optimizing an input geometry. Analyzing the output; Evaluation of the water dimer interaction energy; Improving the energetics. Adding solvent effects.
14	Wed 04/26/2017 Thu 04/27/2017	**Week 14. Tutorials:** Setting the input and analyzing the output of vibrational analysis; Evaluating free energies; Calculating the pKa of a simple organic acid; Calculating the RedOx potential of a simple organometallic compound.
15	Wed 05/03/2017 Thu 05/04/2017	**Week 15. Tutorials:** Locating intermediates and transition states along a simple reaction pathway; Refining the energetics of a reaction pathway; Assembling the complete reaction pathway from intermediates and transition states; Analyzing the thermodynamics and the kinetics emerging from a reaction pathway characterization. Final considerations over the course.
16	Wed 05/10/2017 Thu 05/11/2017	**Week 16**. Preparation for the exame and Final term exam.
17	Wed 05/17/2017 Thu 05/18/2017	
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Note

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