Computational Chemistry

CHEM-AD 315 Special Topics in Chemistry, Spring Semester 2015

Instructor: Serdal Kirmizialtin, 6855727, serdal@nyu.edu
Time: Tue-Thr 12:45pm-2pm
Number of Credit Hours: 4 credit hours
Location: East Administration 006
Prerequisites: FoS1-6, Multivariable Calculus
Office Hours: Monday 4-5pm, ERB, 114

Course Description

This course is an introduction to modern computational simulation techniques useful to model structure, dynamics and reactivity of molecular systems. The lectures will focus on the fundamental theory behind these methods and application of them to real life problems. You will gain hands-on experience in using some program packages such as GROMACS, VMD and Gaussian as well as gain some programming experience in Python. Each student will have remote access to our linux based High-Performance Computing facility where they can perform their simulations and analyze their data.

Recommended Texts

Reading assignments, homework, and lecture notes will be posted on NYU classes. No textbook is required but the following books are recommended:

- Understanding Molecular Simulation: From Algorithms to Applications, D. Frenkel, B. Smith, 2nd Edition, Computational Science Series (2002)
- Molecular Modelling Principles and Applications, Andrew R. Leach, Prentice Hall (2001)
- Introduction to Computational Chemistry, Frank Jensen, 2nd Edition, Wiley 2007

Course Outline

- Computational Modeling of Molecules: What is computer modeling and why it is needed, challenges and progress so far
- Elements of Classical Mechanics
- Basics of Statistical Mechanics
- Intermolecular Forces and Molecular Mechanics
- Optimization Techniques

- Basic Sampling Techniques
    - Monte-Carlo Simulations
    - Molecular Dynamics Simulations
- Free Energy Calculations
    - Thermodynamic Integration and Perturbation
    - Umbrella Sampling
- Advanced Sampling Techniques
    - Parallel Tempering
    - Metadynamics
- Basic Theory of Quantum Mechanics
- Computational methods to solve the Schrodinger's equation
    - Molecular Orbital Calculations
    - Hartee-Fock Equations
    - Basis Sets
    - Approximate Molecular Orbital Theories
- Advances Quantum Mechanics Methods
    - Open shell systems and Electron correlation
    - Density Functional Theory
- QM/MM Hybrid Methods

Requirements

- Some knowledge of scientific programing and ability to use UNIX is very helpful but not required. Similarly, programs such as Mathematica or Matlab will help with the theoretical assignments. Questions about these programs can be addressed during office hours or in a tutorial session as determined by the needs of the class.
- A personal laptop with Internet connection is needed in the application part of the class.

Knowledge and skills that students will gain from this course

Upon the completion of this course, students will understand the role of molecular modeling in studying science and medicine.

- Students will acquire knowledge about Molecular Mechanics force fields (functional forms and parameterization), optimization techniques.
- Students will learn theory, scope and limitations of Molecular Dynamics simulations, Monte Carlo Sampling Methods, analysis methods, and enhanced sampling techniques that are commonly used in condensed matter simulations.
- They will also learn the basics of Computational Quantum Mechanics and how to apply these techniques to study chemistry.
- The ability to set up a simulation of a real life problem, and be able to analyze the output by using theoretical and computational tools.

Grading

The grading policy will be as follows:

Homework Assignments	7 x 5 = 35pts
Pop Quizzes	5 x 1 = 5pts
Project	1 x 30 = 30pts
Comprehensive Final Exam	1 x 20 = 20pts
Attending to the lectures	10pts

For each missing class after 2 will reduce your Attendance score -1pts.
Attending to relevant seminars 1pt/per seminar (up to 3 is rewarded)

A = 92 - 100;	**A**$^{-}$ = 88 - 91	
B^{+}= 85 – 87;	**B** = 82 – 84;	**B**$^{-}$=78-81
C^{+}= 75 – 77;	**C** = 72 – 74;	**C**$^{-}$=68-71
D^{+}= 65 – 67;	**D** = 62 – 64;	
F = below 62		

Homework Assignments (35 pts)

Each assignment set will focus on lecture material and include application of a computational modeling problem as well as some numerical or theoretical problems. Answer Key will be posted online after the due date that falls one week from the date of the assignment. Homework assignment received after due date will be penalized with -1 x (number of days being late including weekends). Assignments can be turned electronically (preferred) or paper.

Pop Quizzes(5 pts)

There will be 5 short quizzes during class hours between the materials that are covered since the last quiz. Quiz time will be announced one week in advance.

Project (30 pts)

Students will have to create an original, instructive (nontrivial) computational problem and solution to it. The topic of the project should be related to the material covered in lectures. The instructor will provide a number of project ideas to consider; you can come up with your own idea too. At the end of the semester each student will give a 30-minute presentation of the project, followed by 5-minute questions/answer session. The results will also be submitted as a scientific paper.

Performance on the assignment will be graded accordingly to:

Correctness/Completeness (15 points)

Oral Presentation (5 points)

Scientific Report (10 points)

Final Exam (20 pts)

The final exam will be comprehensive. There will be four questions (5pts each) from the lecture notes covered in the class one of the questions will be from the homework assignments where computation is not needed.

Attendance (10 pts)

Attendance is highly recommended, as the course materials are not standard and selected from different subjects it will be really difficult to catch up if a class is missed. Every student starts with 10pt credit of attendance. Student missing the class more than two lectures will start to loose these points by 1 point for every class that is missed after two.

Important Dates

Class starts January 27
Deadline to add February 9
Deadline to drop February 16
Spring Break March 19-28
Class starts March 31
Withdrawal and change of grade April 28
Last day of class May 14
Final TBA

Disabilities and Religious Holidays

Please notify me of any modification/adaptation you may require to accommodate a disability related need. Students unable to take the final exam that are given on a religious holiday must notify me at least fourteen days in advance.

Academic Dishonesty

Academic dishonesty is a serious problem and my hope is that this dishonesty does not take place in this course. You can always discuss the problem with your friends but the work submitted must be your own. Copying other student's homework or allowing other students copy your answers will not be TOLERATED. If academic dishonesty is suspected, it will be dealt within adherence with the official guidelines of NYU Abu Dhabi. For additional information, please check out the links below
https://students.nyuad.nyu.edu/academics/academic-policies/the-nyuad-communitys-commitment-to-integrity/

http://www.nyu.edu/about/policies-guidelines-compliance/policies-and-guidelines/academic-integrity-for-students-at-nyu.html