Syllabus - Fall 2019

Computational Chemistry [CHEM-UA 752]

Instructor:

Professor Yingkai Zhang, 1166D Waverly Building, 212-998-7882, yz22@nyu.edu
TA: Jocelyn Lu, 1167 Waverly Building, jl8570@nyu.edu

Lecture/lab Time and Place:

Monday, 2:00 PM - 3:15 PM at LSTC_MACLB (Lecture)
Wednesday, 2:00 PM - 4:30 PM at LSTC_MACLB (Lab)

Office Hour Time and Place:

Friday, 4:00 PM – 5:00 PM, 1166 Waverly Building

Course website: Class

Course Goal:

• This course is a brief introduction to computational chemistry and biomolecular modeling.
• to assist you in developing a practical understanding of computational methods (strengths, limitations, applicability)
• to assist you in developing competence in applying these computational methods to molecular modeling.

Reference books

• Molecular Modeling: Principles and Applications, second edition by Andrew R. Leach (Pearson Education EMA, January 2001

Grading

<table>
<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Labs</td>
<td>(25%)</td>
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<tr>
<td>Exams</td>
<td>(50%)</td>
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<tr>
<td>Final project</td>
<td>(25%)</td>
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Late lab report/Final Project policy: each late day deducts 20% of total points. It will not be graded if it is more than 5 days past the due date.
Tentative Course Schedule

**Week 1:**
- Sep. 4  Introduction to molecular structure modeling, and protein structure, and Lab1

**Week 2:**
- Sep. 9  Introduction to Computational Quantum Chemistry
- Sep. 11 Lab2 on biomolecular visualization with Chimera

**Week 3:**
- Sep. 16 MM force field
- Sep. 18 Lab3 on QM calculations with Gaussian

**Week 4:**
- Sep. 23 QM/MM and energy minimization methods
- Sep. 25 Lab4 on Amber tutorial 1a: protein preparation and minimization

**Week 5:**
- Sep. 30 Molecular dynamics simulation
- Oct. 2 Lab5 on Amber tutorial 1b: MD simulation and analysis

**Week 6:**
- Oct. 7 Introduction to ensemble and monte carlo simulation
- Oct. 9 Exam I, finishing Lab 5 or starting Lab 6

**Week 7**
- Oct. 14 Fall Recess
- Oct. 16 Lab 6, modeling of the protein JAK2

**Week 8**
- Oct. 21 Simulation protocol, boundary condition, solvation modeling
- Oct. 23 Lab7 on Antechamber tutorial

**Week 9**
- Oct. 28 Free energy calculations: biomolecular recognition
- Oct. 30 Lab8 on Simulation of the JAK2-SKE complex

**Week 10**
- Nov. 4 Binding pocket analysis
- Nov. 6 Lab 9 on binding pocket analysis

**Week 11**
- Nov. 11 Molecular modeling, machine learning and drug design
- Nov. 13 Lab10 on ligand docking

**Week 12**
- Nov. 18 Course project discussion
- Nov. 20 Exam II and course project

**Week 13**
- Nov. 25 Course project
- Nov. 27 Thanksgiving Recess, no class

**Week 14**
- Dec. 2 Course project
- Dec. 4 Course project presentation

**Week 15**
- Dec. 9 Course project
- Dec. 11 Course project
- Dec. 16 Course project report will be due on Dec. 16.
Letter Grades

Final grades will be awarded on a 100-point scale:

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<tr>
<th>Letter Grade</th>
<th>Points</th>
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