Syllabus - Spring 2018

Computational Chemistry [CHEM-GA 2627]

Instructor:

Professor Yingkai Zhang, 1166D Waverly Building, 212-998-7882, yz22@nyu.edu

Lecture/lab Time and Place:

Monday/Wednesday, 11:00 AM - 12:15 PM at LSTC_MACLB

Office Hour Time and Place:

Thursday, 4:00 PM – 5:00 PM, 1166D Waverly Building

Course website: Class

Course Goal:

- This course is a full-scale introduction to computational chemistry and biomolecular modeling, including special topics on computational-aided drug design.
- 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>
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<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Homework</td>
<td>(30%)</td>
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<tr>
<td>Exam</td>
<td>(40%)</td>
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<tr>
<td>Final project</td>
<td>(30%)</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 Schedule

**Week 1:**
- Jan. 22 Introduction to molecular modeling, visualizations.
- Jan. 24 Biomolecular structure introduction

**Week 2:**
- Jan. 29 homology modeling
- Jan. 31 Introduction to Computational Quantum Chemistry I (HF)

**Week 3:**
- Feb. 5 Introduction to Computational Quantum Chemistry II (HF and basis set)
- Feb. 7 Introduction to Computational Quantum Chemistry III (DFT, MP2)

**Week 4:**
- Feb. 12 MM force field.
- Feb. 14 QM/MM

**Week 5:**
- Feb. 19 Energy Minimization Techniques and conformation analysis
- Feb. 21 Molecular dynamics simulations

**Week 6:**
- Feb. 26 Introduction to Statistical Mechanics
- Feb. 28 Monte Carlo Simulation and boundary condition

**Week 7**
- Mar. 5 EXAM 1
- Mar. 7 Solvation modeling: explicit vs. implicit

**Week 8**
- Mar. 12 Spring Break, No class.
- Mar. 14 Spring Break, No class

**Week 9**
- Mar. 19 Computational characterization of protein interaction surfaces
- Mar. 21 AlphaSpace tutorial

**Week 10**
- Mar. 26 Solvation modeling: implicit solvent
- Mar. 28 Free energy calculations: FEP/TI and MM/PB(GB)SA

**Week 11**
- April 2 Ligand docking
- April 4 molecular modeling and machine learning

**Week 12**
- April 9 introduction to machine learning
- April 11 Biomolecular modeling literature discussion

**Week 13**
- April 16 Biomolecular modeling literature discussion
- April 18 Biomolecular modeling literature discussion and course project discussion

**Week 14**
<table>
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<tr>
<th>Date</th>
<th>Event</th>
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<tbody>
<tr>
<td>April 23</td>
<td>Exam II</td>
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<tr>
<td>April 25</td>
<td>Course project discussion</td>
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<td><strong>Week 15</strong></td>
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<td>April 30</td>
<td>Course project discussion</td>
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<td>May 2</td>
<td>Course project discussion</td>
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<td><strong>Week 16</strong></td>
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<td>May 7</td>
<td>Course project presentation</td>
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<td>May 13</td>
<td>Course project report due</td>
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