Syllabus - Spring 2020

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, 9:30 AM - 10:45 AM at Silver 506

Office Hour Time and Place:
Friday, 4:00 PM – 5:00 PM, 1166D Waverly Building

Course website: Class

Course Goal:

- This course is a full-scale introduction to computational chemistry, biomolecular modeling and related informatics tools, 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

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<tr>
<th>Component</th>
<th>Weight</th>
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<tbody>
<tr>
<td>Homeworks</td>
<td>25%</td>
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<tr>
<td>Exams</td>
<td>50%</td>
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<tr>
<td>Course Projects</td>
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Late HWs/Projects 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. 27  Introduction to molecular modeling and visualizations.
Jan. 29  Biomolecular structure and interaction

Week 2:
Feb. 3   Introduction to sequence comparison and homology modeling
Feb. 5   Introduction to cheminformatics and molecular representation

Week 3:
Feb. 10  Introduction to Computational Quantum Chemistry I (HF and basis set)
Feb. 12  Introduction to Computational Quantum Chemistry II (DFT, MP2, Semi-QM)

Week 4:
Feb. 17  President’s day, no class
Feb. 19  Fundamental bioinformatics and cheminformatics data processing

Week 5:
Feb. 24  MM force field
Feb. 26  QM/MM and Energy Minimization Techniques

Week 6:
Mar. 2   Energy Minimization Techniques, conformation analysis, and Transition state
Mar. 4   Molecular dynamics simulations

Week 7:
Mar. 9   Introduction to Statistical Mechanics
Mar. 11  Exam I

Week 8
Mar. 16  Spring Break, No class.
Mar. 18  Spring Break, No class

Week 9
Mar. 23  Monte Carlo Simulation and boundary condition
Mar. 25  Solvation modeling: implicit solvent

Week 10
Mar. 30  Molecular Trajectory Analysis
April 1  Free energy calculations: FEP/TI and MM/PB(GB)SA

Week 11
April 6  Introduction to enhanced sampling techniques
April 8  Computational aided inhibitor design

Week 12
April 13 AlphaSpace and binding pocket analysis
April 15 Ligand docking

Week 13
April 20 Machine learning and molecular modeling
April 22 course project discussion

Week 14
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<thead>
<tr>
<th>Date</th>
<th>Event</th>
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<tbody>
<tr>
<td>April 27</td>
<td>Exam II</td>
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<tr>
<td>April 29</td>
<td>Course project discussion</td>
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<td><strong>Week 15</strong></td>
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<td>May 4</td>
<td>Course project discussion</td>
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<td>May 6</td>
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<td><strong>Week 16</strong></td>
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<td>May 11</td>
<td>Course project presentation</td>
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<td>May 17</td>
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