Syllabus - Fall 2016

Computational Chemistry [CHEM-UA 752]

Instructor:

Professor Yingkai Zhang, 1166D Waverly Building, 212-998-7882, yz22@nyu.edu
TAs: Ms. Yuwei Yang (yy1274@nyu.edu), 1166 Waverly Building
   Mr. Haotian Li (haotian.li@nyu.edu), 1166 Waverly Building

Lecture/lab Time and Place:

Wednesday, 2:00 PM - 3:15 PM at LSTC_MACLB (Lecture)
Friday, 12:30 PM - 3:00 PM at LSTC_MACLB (Lab)

Office Hour Time and Place:

Tuesday, 4:00 PM – 5:00 PM, 1166 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

Lab (30%)
Exam (40%)
Final project (30%)

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:
Sep. 7 Introduction to molecular structure modeling, visualization, databases.
Sep. 9 Exploration of PDB database, Linux tutorial, and Hands on exercises.

Week 2:
Sep. 14 Protein structure
Sep. 16 Biomolecular visualization: Chimera and Hands-on exercises

Week 3:
Sep. 21 Introduction to Computational Quantum Chemistry
Sep. 23 High performance computing, Gaussian and Hands-on exercises

Week 4:
Sep. 28 MM force field.
Sep. 30 High performance computing, Amber and Hands-on exercises

Week 5:
Oct. 5 Energy Minimization Techniques and conformation analysis
Oct. 7 Biomolecular modeling I: Amber and Hands-on exercises

Week 6:
Oct. 12 Computational analysis of binding interfaces
Oct. 14 Hands-on binding pocket analysis exercise

Week 7
Oct. 19 EXAM 1

Week 8
Oct. 26 Molecular dynamics simulations
Oct. 28 Biomolecular Modeling III: simulation, analysis and hands-on exercises

Week 9
Nov. 2 Introduction to Statistical Mechanics
Nov. 4 Biomolecular Modeling IV: simulation, analysis and hands-on exercise

Week 10
Nov. 9 Solvation modeling: explicit vs. implicit
Nov. 11 Biomolecular Modeling V: Modeling solvation effects

Week 11
Nov. 16 Free energy calculations: biomolecular recognition
Nov. 18 Biomolecular Modeling VI: Ligand docking
Week 12
Nov. 23  No class Thanksgiving

Week 13
Nov. 30  Exam II
Dec. 2   Course project discussion and course projects

Week 14
Dec. 7   Course project
Dec. 9   Course project

Week 15
Dec. 14  Course project
Dec. 16  Course project presentation
Dec. 19  Course project report will be due on Dec. 19.