Chemistry 4450/6450: Molecular Modeling Methods
2020

Location: PSC 311 Tuesday + Thursday 2:30-5pm
Instructor: Dr. Markus W. Germann 412 NSC, 404 651-1576, mwg@gsu.edu
Office Hours: TBA

Prerequisites: Chemistry 3410, Organic Chemistry II and Chemistry 4110, Physical Chemistry I or equivalent course work and consent of instructor.

Objective: An introduction to molecular modeling methods with an emphasis on the use of molecular mechanics methods to solve structural problems in organic, bioorganic, and biophysical chemistry. Software packages used/discussed (**Spartan**, **Maestro (Schrödiner package)**, **VMD, Chimera**, Pymol, Amber). Some of these programs require UNIX/LINUX skills. They are invoked via command line often via telnet or ssh (ftp, sftp). Basic unix commads are found at: http://mally.stanford.edu/~sr/computing/basic-unix.html

Assignments and requirements: There **will** be homework assignments. Late homework will be penalized 5% per day. Note that the homework is the **main** determinant of the overall score; please plan accordingly. The lowest HW score will be dropped. Midterm and final exams are also compulsory. Academic honesty policies are in effect.

Grading policy:
Percent of course grade: Homework 80%, Midterm 10%, Final 10%
Course grades will be assigned by the following scheme: >95% =A+, >90%=A, >86.6%=A-, >83.3%=B+, >80%=B, >76.6%=B-, >73.3%=C+, >70%=C, >66.6%=C-, >60%=D, below 60% = F.

Attendance: Punctual attendance for each and every class period is expected.
Materials: Required materials will be provided to the student during class or via drop box.

Policy on Academic Honesty: The University's Policy on Academic Honesty and will be adhered to. The Policy on Academic Honesty is also on the web at: https://codeofconduct.gsu.edu/files/2013/03/2014-2015-Section-II-Academic-Conduct-Student-Code-of-Conduct.pdf

Students will learn

→Construction and evaluation of molecular models
→Measure distances and angles, compare molecules
→Predict NMR spectra (lookup and *ab initio*), predict 3-bond couplings
→Using experimental data to support modeling studies
→Visualization and tools
→Electrostatic maps
→Compare stabilities of conformers and estimate equilibrium constants.
→Conformational searching, grid, MC, dynamics
→Molecular Dynamics (basics) (Macromodel)

→Introduction to Unix systems/trajectory analysis
→3D QSAR
→Virtual Screening and Docking (Schrödinger SW)
→QM models and reactivity. HOMO/LUMO, electron & spin density, spectroscopy (IR, UV,VIS)

Additional Stuff to include this year
→additional topic depending on student input

Lecture Modules:

1. What is molecular modeling. Introduction to Maestro and Spartan
2. Force Fields &Minimization Methods
3. Chemical Applications of Molecular Modeling, comparing Molecules
4. Visualization tools (Maestro/Spartan/VMD etc)
5. Conformational searches, Monte Carlo Methods
6. Chemical Shift calculations, Coupling constants
7. Molecular Dynamics I
8. Molecular Dynamics II
9. Introduction to 3D QSAR
10. Virtual Screening and Docking
11. QM models, QM and reactivity
12. Trajectory analysis & Introduction to Unix systems

The course syllabus provides a general plan for the course; deviations may be necessary

10/13 Module 1
10/15 Module 2, 3
10/20 Module 3, 4
10/22 Module 4, 5
10/27 Module 5, 6
10/29 Module 6, 7
11/3 Module 7, 8
11/5 Module 8, 9
11/10 Module 9
11/12 Module 10
11/17 Module 10
11/19 Module 11
11/24 TG Break
11/26 TG Break
12/1 Last Class Module 12
12/3 Final (hand in final assignment)