

# Chemistry 4450/6450: Molecular Modeling Methods 2019

**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**, **VMD**, **Sybyl**, PC model, Swisspdb, ACD, Pymol, Amber, Gromacs, Dyana). 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
- Practical use. Examples from the literature and from GSU
- 3D QSAR
- Virtual Screening and Docking (intro, Vina)*
- QM models and reactivity. HOMO/LUMO, electron & spin density, spectroscopy (IR, UV, VIS)*

*Italics are mainly introductions and some examples*

### **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
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
12. QM and reactivity
13. Trajectory analysis & Introduction to Unix systems

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

- 1/15 Module 1**
- 1/17 Module 2, 3**
- 1/22 Module 3, 4**
- 1/24 Module 4, 5**
- 1/29 Module 5,6**
- 1/31 Module 6,7**
- 2/5 Module 7,8**
- 2/7 Module 8,9**
- 2/12 Module 10**
- 2/14 Module 11**
- 2/26 Module 12,13**
- 2/28 Module 12**