Chemistry 4450/6450: Molecular Modeling Methods
2016

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 (**Sybyl**, **Spartan**, **VMD, Hyperchem, 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: >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 webfolder.
Student Login:
http://lithium.gsu.edu/courses/MolecularModeling
user: MM
passwd: Chem6450

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: http://www2.gsu.edu/~wwwfhb/sec400.html#409

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) (Sybyl), (*solvation*)
→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

•Atropisomerism
• add topic depending on students input

Lecture Modules:

1. What is molecular modeling. Introduction to Sybyl and Spartan
2. Sybyl & Force Fields Minimization Methods
3. Chemical Applications of Molecular Modeling
4. Visualization tools (Sybyl/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