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 commands 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*

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