CHEM 343-001
Introduction to Modeling in Chemistry
Professor Metz
SSMB 150
College of Charleston
(843)953-8097
Fall Semester 2018
Course Syllabus
metzc@cofc.edu
http://metzc.people.cofc.edu
Office: MWF (~9:00 - ~noon)

Textbook and Website References
http://www.computationalscience.org/ccce
http://cccbdb.nist.gov/
http://chemistry.shodor.org/~webmo/cgi-bin/webmo/login.cgi

Meeting Schedule
M 12:00 - 12:50 pm SSMB 300

Class Schedule (tentative)
M 8/27 Introduction to Modeling
FF1
M 9/3 Background
FF1: 3-29; FF2: 35-48, 66, 67; FF10 (skim)
M 9/10 Basis Sets
FF2: 78-81
M 9/17 Theoretical Methods
FF2: 73-78
M 9/24 Single Point Energy and Geometry Optimizations
FF3: 87-137; FF4: 141-142; FF6: 267-271; FF7: 277-278
M 10/1 Accuracy
FF2: 81-84
M 10/8 Electron Density, Electron Potential and Reactivity
M 10/15 IR/Raman Spectroscopy and Thermodynamics
M 10/22 UV/Vis and NMR Spectroscopy
W 10/24 Last Day for Withdrawal W Grade
M 10/29 Systems in Solution
FF5: 201-225
M 11/12 Transition States
FF6: 236-249, 255-262, 265-267, 271-274
M 11/19 Chemical Kinetics (GIDES)
M 11/26 QSAR
M 12/3 Project Presentations
Course-Instructor Evaluation*

* The Associate Provost for Faculty Affairs has made in-class administration of Course-Instructor Evaluations mandatory. You must bring your smart phone, laptop, panel or other device capable of communicating with the College website with you to class.

Class Preparation
Each class has a reading assignment as indicated above. Please complete the assigned reading before class—this material will not be covered verbatim in class.

Homework assignments will be made each class period. The assignments are due at the beginning of the next class period. Late assignments—more than a week late—will not be accepted. Depending on the assignment, submission of homework in PC compatible format will be by (a) hard copy (printout of results); (b) on-line files stored in your WebMO account; and/or (c) files (spreadsheet, text document, or screen shots) on a USB2 memory stick (flash drive, etc., the drive will undergo a virus screening each time). You will be issued two memory sticks to use during the semester for the course and you must return these at the end of the semester. Please keep a copy of all submitted work. Please use the envelope provided for the homework submission.

Each student is responsible for their own individual work—although group discussion and/or helping each other is encouraged. Of course, we follow the statement concerning Academic Dishonesty as given in the Student Handbook. Most homework items will be worth 30 points each and the kinetics homework assignment will be worth 120 points. If the quality of the submitted material is such that it requires re-submission, 5 points will be deducted for each re-submission. All previous submissions should accompany the re-submission.

The final project will be to develop and write a complete first-draft handout for a molecular modeling “experiment/exercise” suitable for use in one of our classes. Stay alert for ideas. More later...
Point Distribution

The course grade will be based on homework (750 points possible—see above) and the final project (250 possible points) for a total of 1000 possible points. Anyone earning at least 90% of the total possible points will earn a guaranteed A (likewise, 80% for a B, 70% for a C, and 60% for a D) although these standards may be relaxed slightly at the end of the semester resulting in slightly higher grades. A total under 50% will be considered failing. The assignment of + or - to the letter grade will be at the discretion of the instructor.

Please consult with the instructor concerning any absence as soon as possible. Excessive class absences will not be tolerated and will be reflected in the final grade.

Software

We will be using Gaussian and MOPAC as our main molecular modeling software engines with WebMO as the user interface to these computational engines. WebMO is web-based and may be accessed from most computers. You may access WebMO using a login and password that will be assigned at a later date. Please do not change these codes—I need access to your files for grading homework.

Our molecular modeling calculations will be carried out on a server at the Shodor Education Foundation. We acknowledge the Computational Chemistry for Chemical Educators program at the National Computational Science Institute.

Occasionally, WebMO cannot be accessed because of technical problems. Please report this to me and I will notify the IT people about the problem. So that you can complete the assignment on time, consider doing your calculations within a day or so after class and not wait for the weekend.

Later this semester we will be using Vensim PLE as our icon-based system dynamics modeling package (graphical interfaced differential equation solver, GIDES). Vensim PLE is available for free at http://www.Vensim.com/venple.html for academic use and is supposedly installed on the computers in the labs on the third floor of SSMB.

Disabilities

If there is a student in this class who has a documented disability and has been approved to receive accommodations through SNAP services, please feel free to come and discuss this with me during my office hours.

Catalog Description

CHEM 343 Introduction to Modeling in Chemistry (1)

An introduction to computer modeling of various properties and structures of molecules, thermodynamic properties and structures of simple crystals, and the kinetics of chemical reactions. Prerequisite: CHEM 231.

Student Learning Outcomes

This course is not designed to prepare the student as a “quantum” chemist. It is designed to introduce modeling and, in particular, molecular modeling as another tool that chemists can use along with tools such as IR, Raman, UV-Vis, and NMR spectroscopy in their everyday work.

Upon satisfactory completion of this course, the student would be expected to

1) recognize and understand various types of modeling that are used commonly by chemists
2) evaluate some specific models using VVA
3) gain experience in remote access (cloud) computing on a server or super computer
4) gain experience with a typical molecular modeling user interface for constructing molecular models and for interpreting molecular modeling calculation results
5) understand and choose the appropriate theoretical method(s) and basis set(s) for a given calculation based on desired accuracy and computational “expense”
6) calculate and interpret single point, optimized, and transition structure energies for a molecule
7) calculate and interpret simple molecular properties such as geometry and dipole moment
8) calculate and interpret electron density, electron potential, and reactivity diagrams for molecules
9) calculate and interpret theoretical values of IR, Raman, UV-Vis and NMR spectra and associated thermochemical properties
10) perform and interpret molecular modeling calculations for molecules in solution
11) model simple and complex first order kinetics reaction using GIDES
12) formulate, design, perform the calculations, and interpret the results of a molecular modeling “experiment/exercise” suitable for use in an undergraduate chemistry class