A. DESCRIPTION

Physical chemistry is the study of the physical principles governing the properties and behavior of chemical processes. It is sub-divided into four principal areas: quantum mechanics, statistical mechanics, thermodynamics, and kinetics. Quantum mechanics examines the motions of electrons and nuclei of molecules to determine molecular properties; thermodynamics investigates the properties and changes in properties of physical and chemical processes at equilibrium; kinetics involves examining rate changes in physical and chemical systems; and statistical mechanics deduces thermodynamic and kinetic properties from molecular properties. Physical chemistry thus allows a fundamental understanding and description of the principles underlying all of chemistry.

Physical chemistry relies heavily on applied mathematics. In order to succeed in physical chemistry, students must have a good grounding in applied mathematics. It is common for chemistry and biochemistry majors to have had limited exposure to the mathematical and computational methods needed for a fundamental comprehension of physical chemistry. To remedy this situation CHEM 4161 is not a laboratory course. It instead focuses on developing students’ skill in mathematical and computational methods. The major goal of this course is to teach students the necessary computational skills they need for the CHEM 4361/4362 physical chemistry lecture courses.

B. ORGANIZATION

CHEM 4161 is a computer workshop course in which topics are first presented by the instructor followed by in-class computer exercises in order to reinforce the material just covered. Material for the presentation is primarily based on several references (see list below) and the instructor’s research work. Course assessment is based on in-class quizzes and computational/programming projects.
PRE-REQUISITE COURSES

The pre-requisite lecture courses for CHEM 4161 are Calculus I and II (MATH 1431/1432) or their equivalents. Other courses (not pre-requisite) that will benefit students taking CHEM 4161 are as follows:

1. Differential Equations I (MATH 2343)
2. Differential Equations II (MATH 3343)
3. Introduction to Partial Differential Equations (MATH 4343)
4. Linear Algebra I (MATH 3334)
5. Linear Algebra II (MATH 4341)
6. Mathematics for Engineering I with MATLAB Applications (MATH 2344)
7. Mathematics for Engineering II with MATLAB Applications (MATH 3354)
8. Mathematical Methods in Engineering (MATH 3344)
9. Introduction to Technical Computing (MATH 2338)

C. COMPUTATIONAL SOFTWARE

The computer is a standard tool in any modern scientific, engineering, computational, or mathematical discipline. As such, students in CHEM 4161 are required to fully utilize computer technology whenever necessary to solve numerical problems. This course will require the use of MATLAB, a powerful technical computing platform. The concurrent lecture course, CHEM 4361, will provide many opportunities for students to solve problems using the MATLAB techniques covered in CHEM 4161. Students have access to MATLAB on any university computer on campus. Students may also purchase a personal copy of MATLAB at a discounted, student rate. Personal purchases can be made at the following site:

http://www.mathworks.com/academia/student_version/

D. TEXTBOOK

There is no required textbook for this course. Reference textbooks that either supplement or expand on the material covered in the lecture presentations are listed below. For those of you who plan to do graduate-level work in theoretical physics, physical chemistry, chemical physics or transition into chemical engineering, I highly recommend the books labeled with three asterisks.

Mathematical Methods and MATLAB

Mathematical Handbooks


E. GRADING PLAN

The grading scheme and breakdown for the course is as follows:

<table>
<thead>
<tr>
<th>Component</th>
<th>Frequency</th>
<th>Unit Value</th>
<th>Total</th>
<th>% of Grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class Quiz</td>
<td>10</td>
<td>50</td>
<td>500</td>
<td>50</td>
</tr>
<tr>
<td>MATLAB Project</td>
<td>2</td>
<td>125</td>
<td>250</td>
<td>25</td>
</tr>
<tr>
<td>Gaussian Project</td>
<td>2</td>
<td>125</td>
<td>250</td>
<td>25</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>1000</strong></td>
<td></td>
<td><strong>100</strong></td>
<td></td>
</tr>
</tbody>
</table>

Grading Scale

Your final grade for the course will be determined by the following percentage scale:

- A    100–93
- A-   92–90
- B+   89–87
- B    86–83
- B-   82–80
- C+   79–77
- C    76–73
- C-   72–70
- D+   69–67
- D    66–60
- F    <60

Class Assessments

Your grade for this course will be based on the following: (a) ten 30-minute class quizzes; (b) two MATLAB programming projects; and (c) two computational chemistry projects.

Important Notice

Academic honesty is expected. Any questionable conduct will be treated as dishonest behavior. Please see the current undergraduate catalogue for details concerning the University’s policy on academic dishonesty.

F. CLASSROOM RULES OF CONDUCT

1. Silence or disable cell phones
2. Class attendance is required
3. Desk computer is for class work only; use of desk computer for social activities is not permitted
G. IDEAS, EVALUATIONS, ETC.

Your ideas, comments, suggestions, questions, current progress, etc. are welcome. Your discretion in these matters is expected, however. No part of your grade will be based on anything other than your coursework. You are encouraged to take advantage of instructor office hours for help with coursework or anything else connected with the course, your progress, career decisions, or anything regarding chemistry or science in general.

H. HOW TO TAKE THIS COURSE

This is a very mathematically challenging and demanding course, but if you are well prepared you will succeed. The key to success is organization:

- Review the material you have covered in your calculus courses. Once you know the basics, then it is just a matter of applying the basics to new concepts, definitions, etc.
- Attend classes.
- Follow the slide presentation on your computer or in print, annotating it with the important notes that are mentioned in class. The slide presentations will be posted on Blackboard a day before presentation.
- Avoid rewriting everything on the slide presentation onto paper. You will easily miss the tips and hints and other important notes that are mentioned.
- For in-class example problems with MATLAB, follow the solution procedure step-by-step using MATLAB on the class computers.
- Work through the example problems as they are presented in class. After class, work through them again.
- Do, understand and know how to solve all suggested problems.
- Use computer algebra systems (Maple, MathCad, Mathematica, etc.) to check your work. However, do not use these technologies to do the work for you. These systems will not be available to you in exam situations.
- Some students find it effective to work in study groups. This is highly encouraged and recommended. But remember: do not copy other people’s work; you will not learn anything.
- See me if you are unsure about anything. I keep an open-door policy.

I. ACCOMMODATIONS AND DISABILITY

Any student with a documented disability requiring accommodations in this course is encouraged to contact me after class or during office hours. Additionally, students will need to contact Counseling and Disability Services in Crooker Center. This office can be reached at (713) 525–6953/3162.

J. ABOUT YOUR PROFESSOR

I am an associate professor of chemistry. My research interest is centered on fuel science and technology, with a particular focus on pyrolysis and combustion of fuels. I teach general chemistry and physical chemistry courses. My interests outside of academia are landscape and nature photography, camping and hiking, classical Latin and Greek, Baroque music, slide rules and mathematical tables, and the performing arts in the city of Houston.
## K. TENTATIVE SCHEDULE

<table>
<thead>
<tr>
<th>Date</th>
<th>Topic</th>
<th>Assessment</th>
</tr>
</thead>
<tbody>
<tr>
<td>SEP 01</td>
<td>MATLAB: Elementary Programming</td>
<td></td>
</tr>
<tr>
<td></td>
<td>08  MATLAB: Functions, M-Files, Root Finding and Integration</td>
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<tr>
<td></td>
<td>15  MATLAB: Arrays and 2D Plots</td>
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<td>22  MATLAB: Data Analysis</td>
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<td>29  MATLAB: Iterations and Decisions</td>
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<tr>
<td>OCT 06</td>
<td>Gaussian: Introduction to Computational Chemistry</td>
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<tr>
<td></td>
<td>20  Gaussian: Geometry Optimization</td>
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<tr>
<td></td>
<td>27  Gaussian: Frequency Calculations</td>
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</tr>
<tr>
<td>NOV 03</td>
<td>Gaussian: Enthalpies of Reaction</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10  Gaussian: Studying Chemical Reactions</td>
<td></td>
</tr>
<tr>
<td></td>
<td>17  Gaussian: Studying Chemical Reactions</td>
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</tr>
</tbody>
</table>

This schedule is tentative and subject to change at the discretion of the instructor.