Course title: Physical Chemistry Laboratory I (2 credit hours)
Experiments in computational physical chemistry.
One three-hour laboratory and a single one-hour lecture a week.
Prerequisites: Chemistry 481, (Chemistry 482)

Instructor: Carribeth Bliem
Office: Kenan 147B, 962-6194
Office hours: M 1-3 pm (in MH 213) and by appointment
Email: cbliem@unc.edu
I try to respond to email questions within 24 hours, and I will post questions that might be useful to others on Blackboard’s discussion board.

Class meetings: Recitation, T, 12:30 pm, Chapman 125
Lab, one day/week, hours TBA, Morehead 213

Course mission
The purpose of this course is to provide students with opportunities to use computers to solve numerical problems in chemistry that would be too onerous to approach by hand. We will solve problems in thermodynamics and quantum mechanics.
To that end, we will use:
  • Virtual Substance, a molecular dynamics simulation program that allows one to set parameters of a system and watch the dynamics unfold;
  • Excel or another spreadsheet software;
  • Mathcad, a mathematical software that enables general calculations (or another mathematical software program that evaluates integrals); and
  • Spartan Student Edition, a molecule building program.

Course structure
Lab time will be run as a help center. Each lab day, TAs will be available to assist students as they work to complete the lab protocol and think about the lab write-up. Students are welcome to attend lab any day that TAs are available; a schedule will be posted early in the semester, and it will evolve for the first few weeks in an effort to meet student needs.

Lab write-ups will be due Tuesdays at noon, with specific dates given with each lab module (typically one week after the module is introduced in recitation).

Tuesday recitations will allow for general discussion of concepts, both chemical and computational.

Final Exam
The final exam, worth the equivalent of one lab write-up, will be held on Friday, December 18, at noon, in CH 125 (unless we can find a date earlier in the exam period to which everyone agrees).

Course materials
  • Mathcad 14 or another mathematical software (required – individual disks provided by Chemistry Department – available at first recitation)
  • Spartan Student Edition (required – purchase details to follow)
  • Virtual Substance (required – download instructions to follow)
  • Physical Chemistry, by Peter Atkins, or other pchem textbook (recommended)
Blackboard
This class will use the Blackboard e-Education platform (http://blackboard.unc.edu) to post announcements, assignments, and suggested readings. Please check Blackboard often because I will send class emails, post questions/answers, announcements, and assignments during the semester. Lab reports will be uploaded to Blackboard, and scores will be available in the gradebook.

Course evaluation
Weekly lab write-ups (25 points each)  12 weeks x 25 points = 300 points
Final exam (25 points) = 25 points
Total 335 points

Total number points will be converted to a percentage score, and letter grades will be assigned as follows:

A: 90-100%
B: 80-89%
C: 70-79%
D: 60-69%
F: < 60%

If you miss a lab period due to illness or other difficulty, you should contact me to schedule a make-up opportunity. Only under the most dire circumstances will lab write-ups be excused.

Course calendar
All lab weeks begin on Tuesday and end on Friday. Weekly lab write-ups are due at noon on Tuesdays one week after the module is introduced in recitation; specific due dates are listed on each lab module.

<table>
<thead>
<tr>
<th>Week</th>
<th>Lab Module</th>
<th>Due</th>
</tr>
</thead>
<tbody>
<tr>
<td>8/25</td>
<td>Quantum Mechanics</td>
<td></td>
</tr>
<tr>
<td>9/1</td>
<td>(1) Using mathematical software</td>
<td>9/8</td>
</tr>
<tr>
<td>9/8</td>
<td>(2) Molecular Orbital treatment of H₂⁺</td>
<td>9/15</td>
</tr>
<tr>
<td>9/15</td>
<td>(3) Using Spartan – exploring basis sets</td>
<td>9/22</td>
</tr>
<tr>
<td>9/22</td>
<td>(4) Potential energy curve for H₂⁺</td>
<td>9/29</td>
</tr>
<tr>
<td>9/29</td>
<td>(5) Vibrational levels of H₂⁺</td>
<td>10/6</td>
</tr>
<tr>
<td>10/6</td>
<td>(6) Inversion bend of NH₃</td>
<td>10/13</td>
</tr>
<tr>
<td>10/13</td>
<td>Thermodynamics</td>
<td></td>
</tr>
<tr>
<td>10/20</td>
<td>No recitation – Fall Break</td>
<td></td>
</tr>
<tr>
<td>10/27</td>
<td>(8) Maxwell Distribution</td>
<td>11/3</td>
</tr>
<tr>
<td>11/3</td>
<td>(9) Thermodynamic properties of gases</td>
<td>11/10</td>
</tr>
<tr>
<td>11/10</td>
<td>(10) Properties of real gases</td>
<td>11/17</td>
</tr>
<tr>
<td>11/17</td>
<td>(11) Structure of polymer chains</td>
<td>11/24</td>
</tr>
<tr>
<td>11/24</td>
<td>No recitation – Thanksgiving</td>
<td></td>
</tr>
<tr>
<td>12/1</td>
<td>(12) Structure of solids and liquids</td>
<td>12/8</td>
</tr>
</tbody>
</table>
Lab reports:
Each week's lab will address a set of research questions. Your report should include the following:

- first, describe the research problem that frames the research questions; that is, explain why the research questions (found on each protocol) are worth answering. Also state the research questions in your own words. (4 pts)
- describe experimental protocols used to analyze the question. Provide enough detail that someone could use your report to replicate your experiments. (6 pts)
- discuss relevant findings. (8 pts)
- provide a conclusion section that answers the specific research questions you posed in the introduction. (3 pts)

The text in weekly lab write-ups must be limited to three pages (single-spaced, 11 or 12 point font, 1 inch margins); not included in the page-limit are any pertinent embedded graphs or mathcad equations and output.

In the write-up, content is key but presentation matters as well. Therefore, you should use complete sentences, coherent arguments, and graphs as necessary to substantiate your claims. However, you should be succinct and only include remarks that pertain to the research questions.

Following the three-page write-up (in the same document), you should include the following (4 pts):

- answers to applicable pre-lab questions, post-lab questions, derivations & sample calculations.

Specifics relating to quantum lab report:
Since each quantum module will require a Mathcad (or other mathematical software) worksheet full of equations and their output, this worksheet can serve as the basis of your report ... if it is annotated to include:

- at the beginning, the research problem that frames the research questions, and then the questions in your own words (4 pts);
- a conclusion that answers the specific research questions (3 pts).
- answers to post-lab questions (4 pts).

Because the "experimental and findings" sections are, in effect, the worksheet equations and output, when grading the quantum reports, we combine the experimental steps used to analyze the question and relevant findings (including your comments, explanations and plots) into a single section worth 14 pts.

Alternatively, some students prefer to write the body of the report in a Word document and import equations and output from Mathcad as needed to describe the experiment and findings.

Each worksheet write-up should be submitted in a format that is readable in Word or pdf. Mathcad, for example, allows users to save worksheets in .rtf format for this purpose.

NOTE: Students are not required to use Mathcad to complete the Quantum modules; some students choose to use mathematica or matlab (or other software) because they are already fluent in those programs. However, TAs may be able to offer support in Mathcad only.

Specifics relating to thermo lab reports:
Here, it is easier to disentangle the experiments from the subsequent findings. Please plan, however, to attach documented spreadsheets from Excel that show data and analysis.
Computer upkeep
It is your responsibility to make sure that your laptop is running smoothly. Both Mathcad and Virtual Substance CAN run on the four-year old CCI computers you may have, but the laptops must be in good working order to have success. So, if your computer crashes regularly or if weird windows and errors pop up, take your laptop to the IT Response Center, located in the lower level of the R.B.House Undergrad Library (next to the Pit), for 24-hour technical support via phone (962-HELP). Walk-in support is offered Monday-Thursday, 7:30 am – midnight, Friday 7:30 am – 5:00 pm, and Sunday 3:00 pm – midnight.

Late lab policy
This semester, lab reports will be accepted electronically via Blackboard. Each lab is due at noon on the Tuesday after it is assigned. Late labs must be emailed to me at cbliem@unc.edu with “Chem 481L Lab X” in the subject line. Labs received between 12:01 PM Tuesday and 12:00 PM (noon) Friday will be penalized 20%. Labs submitted after 12:00 PM (noon) Friday WILL NOT BE GRADED. Students will receive a zero for that lab.

Honor Code
Policy adopted by the faculty of the Department of Chemistry on September 9, 1977:

“Since all graded work (including homework to be collected, quizzes, papers, mid-term examinations, final examinations, research proposals, laboratory results and reports, etc.) may be used in the determination of academic progress, no collaboration on this work is permitted unless the instructor explicitly indicates that some specific degree of collaboration is allowed. This statement is not intended to discourage students from studying together or working together on assignments which are not to be collected.”

When you type up the weekly reports, you must do your own work. The exercises required for this class are intended so that your understanding at the end of the course will be proportional to the effort you put into it.

Unless explicitly stated in the lab procedure, students MAY NOT share data.

First class
The first recitation meeting will be held Tuesday, September 1, in Chapman 125. We will review the course syllabus, talk about the role of computers in physical chemistry research, and introduce the first lab.

First lab
Lab sessions begin the week of September 1. Students can attend TA hours (TBA) in Morehead 213. Lab Module #1 – Using mathematical software.

Students will find that working through the Mathcad tutorials (available on Blackboard) before they begin Lab #1 will ease their workload. Mathcad disks will be handed out at the first recitation, although students may stop by Kenan 143 or 147 on Monday, August 31, between 9:30 and 11:30 to pick up their disk if they are eager to begin.

Acknowledgements
The authors of the individual Mathcad documents are indicated on those units. As lab modules for this course continue to evolve, specific faculty authors are listed where appropriate.