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, 2-3:30, location TBA
Email: cbliem@unc.edu
I am usually able to respond to email questions within 24 hours.

Class meetings: Recitation, T, 12:30 pm, Chapman Hall 125
TA-run help center, WHF, ML 213, hours TBA

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:
• Mathcad (required – free courtesy of the Chemistry Department);
• Virtual Substance, a molecular dynamics simulation program that allows one to set parameters of a system and watch the dynamics unfold (required – download instructions to follow);
• Excel or another spreadsheet software for statistical analysis;
• Physical Chemistry, by Peter Atkins, or other pchem textbook (recommended).

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 exercises. Students are welcome to attend lab any day/time that TAs are available.

Lab exercises 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.

Sakai
This class will use Sakai (sakai.unc.edu) to post announcements, assignments, and suggested readings. Please check Sakai often because I will send class emails, post questions/answers, announcements, and assignments during the semester.

Lab reports will be uploaded to Sakai via the Upload Assignments tool, and scores will be available in the Gradebook.
Course evaluation
Assessment will take several forms:

1) Weekly lab exercises: a series of questions will be assigned with each lab. The exercises get at the process of the lab; they would be the findings and discussion sections of a formal report. A document providing answers to these exercises (not a formal report) is due one week after the lab is introduced in recitation. Each exercise is worth 10 points.

2) Some weeks will have a 3-5 page report instead of the exercises. Reports should include an Introduction, Experimental section, Findings, Discussion, and Conclusions. They should incorporate themes from previous labs as appropriate (for instance, while Report #1 delas primarily with Lab 4, it will also draw on work in Labs 2 & 3.) Each report is worth 20 points.

3) Final exam: one-hour written exam worth 20 points.

Weekly lab exercises (10 points each) 8 weeks x 10 points = 80 points
Lab reports (20 points each) 3 weeks x 20 points = 60
Final exam (20 pts) 20 points
Total 160 points

Total 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 emergent difficulty, you should contact me. Only under the most dire circumstances will lab exercises or reports be excused.

Late lab policy
This semester, lab exercises and reports will be accepted electronically via Sakai using the “Upload Report” link.
Late exercises must be emailed to me at cbliem@unc.edu with “Chem 481L Lab X” in the subject line. Exercises received between 12:01 PM Tuesday and 12:00 PM (noon) Friday will be penalized 30%. Exercises submitted after 12:00 PM (noon) Friday WILL NOT BE GRADED; any such labs will earn a zero.

First class/lab week
The first recitation meeting will be held Tuesday, August 19, in Chapman 125. We will review the course syllabus, talk about the role of computers in chemistry research, and introduce the first lab. Lab sessions begin the week of August 19. Students can attend TA hours in Morehead Labs 213 any afternoon that help is available.

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 prevent problems. 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 or call (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.

Mac users note: ITS will install, free of charge, BootCamp, a program that partitions your hard drive and enables it to run MS Windows.
Course calendar
All lab weeks begin on Tuesday and end on Friday. Weekly lab exercises 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>Report type</th>
<th>Due Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>8/19</td>
<td>(1) Using mathematical software</td>
<td>Exercises</td>
<td>8/26</td>
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<tr>
<td>8/26</td>
<td>(2) Shapes of orbitals</td>
<td>Exercises</td>
<td>9/9</td>
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<tr>
<td>9/2</td>
<td>(3) Molecular orbital treatment of H₂⁺</td>
<td>Exercises</td>
<td>9/9</td>
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<tr>
<td>9/9</td>
<td>(4) Vibrational levels of H₂⁺</td>
<td>Report</td>
<td>9/23</td>
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<tr>
<td>9/16</td>
<td>No new lab</td>
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<tr>
<td>9/23</td>
<td>(5) Vibrational levels of NH₃ bend</td>
<td>Exercises</td>
<td>9/30</td>
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<tr>
<th>Week</th>
<th>Lab Module</th>
<th>Report type</th>
<th>Due Date</th>
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<tbody>
<tr>
<td>9/30</td>
<td>(6) Introduction to molecular dynamics</td>
<td>Exercises</td>
<td>10/7</td>
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<tr>
<td>10/7</td>
<td>(7) Maxwell distribution of speeds</td>
<td>Exercises</td>
<td>10/14</td>
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<td>10/14</td>
<td>Fall Break</td>
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<td>10/21</td>
<td>(8) Real gases at high density</td>
<td>Exercises</td>
<td>10/28</td>
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<tr>
<td>10/28</td>
<td>(9) Thermodynamic properties of real gases</td>
<td>Report</td>
<td>11/11</td>
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<td>11/4</td>
<td>No new lab</td>
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<tr>
<td>11/11</td>
<td>(10) Structure of polymer chains</td>
<td>Exercises</td>
<td>11/18</td>
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<tr>
<td>11/18</td>
<td>(11) Small-group Project</td>
<td>Report</td>
<td>12/2</td>
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<td>11/25</td>
<td>No new lab</td>
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<tr>
<td>12/2</td>
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<tr>
<td>12/9</td>
<td>One-hour Final exam, noon</td>
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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 exercises/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.

Behavior in this course is governed by the University of North Carolina’s Honor System and the codes contained therein. The entire code, and information pertaining to the code, can be found at: http://studentconduct.unc.edu/ The guiding principle of academic integrity is that the work submitted by a student must be that student’s own work.

When writing up your lab report there is no collaborative work. You must write your own report, answer your own questions, and work up your own data. If you are having difficulties or have
questions you need to see a TA for help. Collaboration on lab reports is a violation of the University Honor Code and will be treated as such.

A second area where misunderstandings of academic integrity arise is with regards to when you should reference external sources in your lab report. The submission of any material that is substantially the same as some other written document or source (i.e., a journal article, a textbook, a lab manual, a book) that is not properly referenced constitutes a violation of academic integrity. Using someone else’s words or ideas without giving credit for their work is called plagiarism. Furthermore, simply rearranging the words from a source to make them seem like your own words is also plagiarism.

The following situations below will be treated as honor code violations.

- Unauthorized collaboration. NOTE: Unauthorized collaboration is defined differently for each lab course. Please read carefully. All lab reports must be written independently. In this course, unless explicitly stated in the lab procedure, students MAY NOT share data.
- Plagiarism. The ideas presented in your report must be your own. If you present someone else’s ideas or work (from books, old lab reports, the Web, the lab manual) as your own, this is plagiarism. You can present facts from an outside source, as long as you properly reference the source.
- Allowing students to use your work as their own. Do not allow your partner or other students to have access to your lab reports. You may share data if you collected the data together, but everything else (calculations, graphs, tables) must be done alone.
- Using old lab reports, even if you just want to glance over them, is an honor code violation.
- Do not rearrange a paragraph or some other piece of work that is not yours in the hope of disguising the work as your own.
- Using an old lab manual from a previous semester.

Established by the Undergraduate Labs Committee
April 2014