Room:  BSB-424 or SCI-329 (below), Wed 2:40 PM – 5:30 PM.
Instructor: Dr. Alexander Samokhvalov, SCI-306C, x6282, alexsam@camden.rutgers.edu, 
http://crab.rutgers.edu/~alexsam/. Office Hours: Wed 1:20 PM - 2:20 PM, BSB-424
(Section 1) or SCI-306C (Section 2).
Chemistry: A Laboratory Textbook”, by Arthur Halpern and George McBane, WH

Course Outline and Goals

Physical Chemistry I course 50:160:347 is designed to introduce you to the following
laboratory techniques: 1) the basics of computational Quantum Chemistry and 2) experimental
Molecular Spectroscopy. Therefore, this Course consists of two Sections: 1) Computational
Quantum Chemistry Labs and 2) Experimental Molecular Spectroscopy instrumental wet
chemistry Labs.
The specific goals of this course are to:
1. learn the structure, major physical properties of molecules and changes in their structure and
   properties, using modern tools of quantum chemical computations and molecular modeling;
2. convey the enjoyment of Computational and Experimental Physical Chemistry, and the
   satisfaction to be obtained from doing quality work in Chemistry;
3. understand how molecules are built, and deliver practical hands-on working experience in
   major experimental methods and equipment used in Spectroscopy;
4. provide training on computer-assisted acquisition of the data generated during the
   physicochemical experiment;
5. teach the methods of data collection, modern instrumentation, processing of raw
   experimental data, and error analysis;
6. teach the basics of data presentation;
7. provide opportunities to exercise and improve scientific writing via computations and experiments–based Lab Reports and computational Term Paper;
8. teach the basics of the topic-specific literature search in the web databases of scientific data (e.g. molecular constants, molecular spectra) and research papers;
9. foster critical analytic thinking and logical reasoning skills that are of a great value in the advanced courses, graduate or medical school, industrial laboratory or business profession.

Access to Course Materials
A Sakai course site 50:160:347:01 F13 has been created for this course, and the course materials will be uploaded as needed. All students must have a Rutgers email address (RU Net ID) in order to access Sakai at https://sakai.rutgers.edu. New email accounts may require 24-48 hours before Sakai courses are activated. Location of each Lab (BSB-424 or SCI-329) will be specified on Sakai site, under the Schedule menu of the given Lab, in the Event Location section. Remote access to computing resources needed for the Quantum Chemistry Labs is available via https://apps.camden.rutgers.edu and https://apps.camden.rutgers.edu/novnc/. Students are expected to be able to retrieve the additional information as needed from the Internet sources, texts of the other online Physical Chemistry courses, and from the library.

Attendance
Attendance is strictly required to both Quantum Chemistry and Molecular Spectroscopy Labs. I will grant permission to have a make-up Labs if the absence is due to any of the following documented reasons: (1) serious illness with the written note from the doctor; (2) an order from the U.S. Military; (3) an order from the U.S. Court/jury duty; (4) officially representing the College; (5) death in the immediate family. The Instructor needs to be notified of the excused absence due to any of those reasons before the Lab to be missed, and the proper documentation must be provided in a timely fashion, before the make-up Lab is to take place. No make-up Labs will be provided in case of the non-attendance of the Labs for any other reason, and such non-attendance will result in zero grade for the Lab Report of that missed Lab. No separate make-up Labs will be arranged, other than on the available Wednesdays during the given Section (Computational or Experimental) this semester. An officially announced Rutgers Severe Weather will supersede those requirements.
Reading
Except the first Intro Lab, students are expected to have reviewed the content of the coming Lab prior to the start of the Lab. Content of each Lab is to be posted to Sakai site (under the Schedule menu) the day prior to the day of the Lab. For experimental wet chemistry Labs (Section II), students are expected to have read the posted Lab Protocol before they start doing that Lab. If nobody in the given Lab Group knows how to do the scheduled experiment (or “where to start”) at the beginning of the Lab, the group is considered not prepared, and will not be allowed to start this experiment. Please understand that this policy has to do not just with the organization matters, but also with the safety in chemical lab. Then, the group is allowed to make-up the lab next Wed, but such re-scheduling will be made only once. If the whole group is not ready for the experiment for the second time, zero grade will be given to everybody in that group for that Lab, and no further make-up Lab will be allowed.

Work Groups and Rotating Schedule
For Experimental Labs (Section II), students will be divided into the work groups of 2-4 on the first day of Experimental section of this course (in mid-October). These groups will remain until the end of the semester. Each group will be conducting the same experiment. Rotating schedule of the experiments will be established during the first Experimental lab (Section II) of the semester. The rotating schedule will be posted in SCI-329 during each experimental Lab. Rotation schedule needs to be updated by the Groups as and if needed.

No experiments may be performed without supervision by the instructor, and no other experiments other than those on rotating schedule are allowed. If the instrument does not work as needed, please promptly notify the Instructor. If an experiment fails for “technical reasons”, the Lab Report should not be written; instead, the group needs to notify the Instructor and repeat the lab the next Wed, when/if the technical problem is fixed. In such a case, the Rotation Schedule will need to be updated accordingly.

Good Lab Practices and Academic Integrity
When in doubt about any particular detail of the experiment or data processing, please ask the Instructor. While students from the same group will work together, the individual Lab Notebooks and individual typed Lab Reports (in the MS Word 2003, *.doc file) will be
required. That is, those Lab Notebooks and Lab Reports need to be **different and unique for each student**: each student needs to keep his/her own notebook records, and the Lab Reports need to be different as well. If two (or more) Lab Reports of the members of the same or different Groups, or major parts of those Reports are identical, this is a *copy-paste plagiarism* that will not be tolerated. *Zero grade* will be given to all students with *verbatim copy-pasted materials* in the Lab Reports or the computational Term Paper. Scientific and academic misconduct e.g. *fabrication of data* or *copying the old data from members of another group or from students who have taken this course earlier* is a serious offence that will not be tolerated. If you have any questions related to this point, please contact the Instructor as soon as possible. The instances of *copy-pasted plagiarism* or other *academic misconduct* will be treated according to the Rutgers university academic integrity policy [http://academicintegrity.rutgers.edu/integrity.shtml](http://academicintegrity.rutgers.edu/integrity.shtml).

Please understand that the high quality scientific writing is one of the major goals of the Higher Education in Sciences, and your scientific writing is one of the major assets you will carry with you when graduating from the University.

**Work Schedule this semester**

The first half of the semester is scheduled for Quantum Chemistry Labs (Section I, COMP in Table 1 below). Quantum Chemistry Labs will be conducted in the computer labs of the Business Science Building, rooms BSB-424 and BSB-134. Those rooms have Linux workstations with the necessary software and Smart Classroom equipment. Homework can be done remotely via remote login at [https://apps.camden.rutgers.edu](https://apps.camden.rutgers.edu) and [https://apps.camden.rutgers.edu/novnc/](https://apps.camden.rutgers.edu/novnc/). In addition, Linux workstations with necessary software are in the Paul Robeson Library.

Quantum Chemistry Labs are math intensive, and this course will utilize the Rutgers University computing resources. Students will be required to learn and utilize Linux-based workstations, Open Office programs (equivalents of MS Word, Power Point and Notepad), GaussView and Gaussian computational software. Quantum chemistry Labs will consist of several computer based projects. One graded Quantum chemistry Lab will be conducted (Table 1).

The second half of semester is scheduled for the Experimental wet Chemistry Labs (Section II, EXP in Table 1 below) that will be conducted in SCI-329. The recommended book for this part of the semester is: “Experimental Physical Chemistry”, 3-rd Ed., by McBane, Halpern. However,
all necessary Lab Descriptions will be posted on Sakai. During Experimental labs, questions on quantum chemistry labs can be answered by the instructor using internet access of the PCs in SCI-329, if time permits.
<table>
<thead>
<tr>
<th>#</th>
<th>Date</th>
<th>Rm.</th>
<th>Lab</th>
<th>Title/List of Topics</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>10-16-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>Introduction. Lab Protocols. <strong>Preparing for Wet Lab next Wed.</strong> Data manipulation: raw vs. ASCII data. MS Excel, data plotting and fitting. MS Excel and SDAS plugin for non-linear curve fitting.</td>
</tr>
<tr>
<td>8</td>
<td>10-23-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>Labs I and II on rotating schedule. Lab I: rotovibrational spectrum of HCl. Lab II: particle in box by absorption spectra of dyes</td>
</tr>
<tr>
<td>9</td>
<td>10-30-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>Labs I and II on rotating schedule. Lab I: rotovibrational spectrum of HCl. Lab II: particle in box by absorption spectra of dyes</td>
</tr>
<tr>
<td>10</td>
<td>11-06-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>Labs I and II on rotating schedule. Lab I: rotovibrational spectrum of HCl. Lab II: particle in box by absorption spectra of dyes</td>
</tr>
<tr>
<td>11</td>
<td>11-13-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>As needed: Make-up Labs / Labs not done yet / writing Lab Reports/ questions about Term Paper.</td>
</tr>
<tr>
<td>12</td>
<td>11-20-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>As needed: Make-up Labs / Labs not done yet / writing Lab Reports/ questions about Term Paper. <strong>Deadline for the Draft of Computational Term Paper.</strong></td>
</tr>
<tr>
<td>13</td>
<td>11-27-13</td>
<td>No Lab</td>
<td></td>
<td>Friday schedule</td>
</tr>
<tr>
<td>14</td>
<td>12-04-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>Final deadline for any make-up Lab Reports. <strong>Deadline for the Final Computational Term Paper.</strong></td>
</tr>
<tr>
<td></td>
<td>12-11-13</td>
<td>SCI-329</td>
<td>EXP</td>
<td>Last day of the semester, reserved for any unforeseen circumstances.</td>
</tr>
</tbody>
</table>
Software Requirements
Computational labs will require the students to learn and utilize Linux-based workstations, Open Office programs (equivalents of MS Word, Power Point and Notepad), GaussView 5.0 and Gaussian 09 computational software. For processing data and preparation of the typed Lab Reports, you will also be expected to be able to use MS Word, MS Excel, ChemDraw and Scientific Data Analysis Software (SDAS). The student version of ChemDraw can be downloaded and installed after logging into https://software.rutgers.edu/. The Scientific Data Analysis Software (SDAS) is the plugin to MS Excel that allows linear or non-linear curve fitting, digital differentiation and integration of the curves, and other math functions to be performed on the data in Excel worksheet. The SDAS is installed as the plugin for MS Excel on every PC in the lab room SCI-329. The installation .exe file of SDAS program and .pdf file with Instructions are posted on sakai, under the Schedule of the first wet chemistry Lab.

Typed Lab Reports
The typed individual Lab Reports will be required from each student for each Experimental Lab and one graded computational Lab. There is no length requirement on the Report, but the Report should be more than two and less than 5 pages. The detailed Format for the typed Lab Reports is posted on sakai as Word file. These Reports are due two weeks after the experiment is successfully completed. Please contact the instructor with your questions before that deadline. No extension of the deadline will be provided, and zero grade will be given for the Lab Report turned in past due.

Lab Reports are accepted as hardcopies (preferred) or by email. When emailing the Lab Report to the instructor, please make sure that you save that email (with Lab Report as word .doc file attachment) in the Sent-Mail folder of your email software. To deliver the hardcopies:
1. hand it to the Instructor during the Lab, Class or the office hours;
2. place it into the mailbox of the Instructor in the secretary’s office (1-st floor of Science bldg.) with the signature of the secretary and the date of submission.

This is the responsibility of the student to ensure that the secretary’s office is open, when the submission of Lab Report needs to be done. Although this office is normally open during normal business days and hours, the Instructor has no control over whether the secretary’s office is open or closed. Ultimately, the best way to ensure that everything is furnished to the Instructor by the
deadline is *not to postpone the submission until that deadline day*, but rather submit the materials few days before that deadline: the earlier, the better.

**Lab Notebooks**

Each student has to have the own Lab Notebook that is the standard composition notebook with at least 200 pages. Those notebooks are strongly recommended for the Computational Labs (Section I) and required for the Experimental Labs (Section II). The Lab Notebook contains the critical information of the experiment performed that will need to be used when performing data processing and writing the Lab Report. The standard laboratory notebook keeping techniques should be followed that are outlined in the document “Good Laboratory Practices” that is posted on sakai, and in the Appendix at the end of this Syllabus. Please become familiar with those recommendations. Specifically, the pages must be numbered, and pages should never be removed from the notebook. This is an upper level course, and the students are supposed to be familiar with the good record keeping practices. If unsure, please see me.

**Computational Term Paper**

The detailed Format for the typed Computational Term Paper is to be posted on sakai. Calculations for the chosen topic of Term Paper can be done entirely online at [https://apps.camden.rutgers.edu](https://apps.camden.rutgers.edu) and [https://apps.camden.rutgers.edu/novnc/](https://apps.camden.rutgers.edu/novnc/). Therefore, students working on the individual Term Paper during the second half of the semester (when wet labs and the instructor are in SCI-329) are not required to attend SCI-329. The BSB-424 and BSB-134 are normally open during the PChem I labs this semester, and the necessary computers and hardware are also available in the Robeson library. During Experimental labs, questions on quantum chemistry can be answered using internet access of the PCs in wet chemical lab SCI-329, provided that those computers are not used by students doing Experimental labs. At least two computers in SCI-329 are not designed for Experimental labs, and are available for the internet access to computational resources.

*Pre-submission* of the draft of the computational Term Paper is **required** for every student by the end of **Wednesday, November 20, 2013**. This activity is intended to ensure that all students keep working on the computational Term Paper throughout the second half of the Semester, following the regular pattern. There is no requirement on the length of the Draft. However, the draft should have all major parts of the full Term Paper, including References and the Output.
code of Gaussian program. The draft will not be graded; however, if the draft of the Term Paper is not received by the deadline above, grading points for the Final Term Paper (below) are automatically reduced by half. The Draft can be delivered to the instructor in the same ways as the Lab Reports above. When emailing the Draft to the instructor, please make sure that you save that email (with Draft as word .doc file attachment) in the Sent-Mail folder of your email software.

Final submission of the final form of computational Term Paper is on Wednesday, December 4, 2013. No extension of the deadline for submission of the final Term Paper will be granted. Submission past deadline will not be accepted and zero points will be given for the whole Term Paper. When emailing the Final Term Paper to the instructor, please make sure that you save that email (with Term Paper as word .doc file attachment) in the Sent-Mail folder of your email software.

Grading
Quantum Chemistry graded lab (one): 20 pts.
Molecular Spectroscopy Labs (two): 2 x 20 pts. = 40 pts.
Quantum Chemistry Term Paper: 40 pts.
Total: 100 pts.

Work/Study Ethics and Professional Behavior
Work/Study Ethics and Professional Behavior http://studentconduct.rutgers.edu/university-code-of-student-conduct are essential for success of your learning and your future professional career. Disruptive behavior of the students during Classes will not be tolerated. Disruptive behavior includes, but not limited to, patterns as on Rutgers website http://studentaffairs.camden.rutgers.edu/classroomdisruption.html. The repeated lack of professional attitudes and/or disruptive behavior of the student in the group work setting will result in the loss of up to 20 % of the earned points for the whole Lab Course. Rutgers academic integrity policy: http://academicintegrity.rutgers.edu/integrity.shtml will be enforced.

Disabilities
If you have a disability that may require some modification of seating, testing, or other class or lab procedures, please see me after the Class/Lab or during my office hours to discuss the
appropriate modifications. You should also contact the Disabled Student Services of Rutgers Camden, http://campuscenter.camden.rutgers.edu/disabled_services.html

Appendix: Guidelines for keeping Laboratory Notebook

A laboratory notebook should provide a complete description of everything that has been done by a researcher or the student in the laboratory. In a research environment (both academic and corporate), it is essentially a legal document that clearly indicates what a given single investigator has done. Records in the lab notebook should be complete enough to permit anyone with proper training in the same scientific discipline to repeat the work. The following is required in this course, and should serve as a guide to maintain a laboratory notebook:

1. The notebook should be a bound notebook. Loose leaf binders and spiral notebooks are not permitted. The pages should be permanently bound, and page numbers should be printed (by manufacturer or by the owner using ink) on each page. Pages should never be removed from a notebook. If a page is not to be used, a line should be drawn across the page and an explanation should be written at the bottom explaining the problem.

2. All entries in the lab notebook should be made in ink. Mistakes should not be erased; instead, a single line should be drawn through the error, and the correction placed adjacent to the error. An explanation should be provided on the same page why the change was made.

3. The first few pages of the notebook should be used for a Table of Contents. Start the first experiment entry on page 5 or so. Fill in the Table of Contents as you do the experiments.

4. Major sections of the records in the lab notebook should be as follows: 1) Title, 2) Date, 3) Name of the student and lab partners; 4) Purpose of the lab; 5) safety considerations for this specific lab; 6) short Background on the topic (several sentences); 7) detailed description of experimental procedures performed, sketches of any apparatuses used, raw data collected or the folder paths to digital files with data; 8) Calculations; 9) Processed data; 10) Discussion; 11) Conclusions; 12) References; 13) optional Appendix. Appendix may include printouts.

5. Provide a brief summary of the Purpose of an experiment on the first page of each day's work. If you are doing two or more different experiments on the same day, do not interleave entries for them on the same page. Instead, keep the two experiments on separate pages. Make sure there is no ambiguity. Use sketches to describe experimental setups used.

6. The notebook should be complete, neat, and well organized. Details may be perfectly clear to you at the moment, but a few months later you may have trouble recalling what exactly and
how exactly was done. If in doubt, write more details. Write down everything relevant or significant you observe in the experiment. If an instrument is drifting or behaving in an unusual way, make a note of it with an explanation, if any.

7. Each entry page for an experiment should have the day’s date at the top right corner. Write on one side of a page. As additional pages are used for an experiment, always place the date at the top right corner. Always start a new page for each experiment and each day. Do not crowd too much information onto a page.

8. All information relevant to the experiment should be recorded in the notebook. Loose paper and notes (e.g. from a weighing) should not be used. Take your notebook with you to the balance and record the exact weight immediately. Any information that you think should be on a scrap piece of paper or a paper towel should be entered directly in the lab notebook. All calculations should be clearly written. The notebook is a detailed record of everything you have done. For example, if you have to make up a new solution in the middle of an experiment, make sure this is perfectly clear and there is no ambiguity when this was made.

9. All “raw data” should be entered directly into the notebook when practical. Alternatively, the file names and folder paths should be specified for each set of digital data acquired, and those need to be referenced to the experiment conducted. Plots of the data should be entered or sketched in the notebook as the data is being collected. This can help in detecting problems with experimental design. It is normally not a good idea to do an experiment "blind", i.e. without looking at what data is being obtained. Instead, look at the data as it is being collected; you must also be careful that such information does not bias your observations.

10. Computer data such as graphs should be printed out if possible and attached with tape or staples on the appropriate page of the notebook. Clearly, this is not possible with large data files containing hundreds or many thousands of data points. The computer file names and the storage location (e.g. hard drive, CD, or DVD name) must be clearly indicated instead. A printout of spectra and scans should be attached whenever possible for clarity.