CHEM 3374A: Quantum Chemistry and Spectroscopy
Fall 2020 Course Outline

Lecture and Instructor Information

<table>
<thead>
<tr>
<th>Section</th>
<th>Time</th>
<th>Room</th>
<th>Instructor</th>
<th>Office</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td>Course</td>
<td>M-W-F</td>
<td>9:30–10:30pm</td>
<td>NCB101</td>
<td>Prof. François Lagugné-Labarthe</td>
<td>MSA0202</td>
</tr>
<tr>
<td>Tutorial</td>
<td>Thursday</td>
<td>11:30–12:30 pm</td>
<td>NCB101</td>
<td>Prof. François Lagugné-Labarthe</td>
<td>MSA0202</td>
</tr>
<tr>
<td>Office</td>
<td>Hours</td>
<td>Zoom Meetings by appointment</td>
<td>online</td>
<td>Prof. François Lagugné-Labarthe</td>
<td>MSA0202</td>
</tr>
</tbody>
</table>

Prerequisite Requirements

Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you may be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites. The prerequisite for this class is CHEM 2384B or the former 2284B. Anti-requisite is Physics 3200A/B.

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Course Materials

Textbooks
Any of the following textbooks is optional:

All books are on reserve at the Taylor library for a two-hour loan. The primary material of the course consists of: your lecture notes, material that is worked-out on the board, material distributed in the class and posted on the OWL website of the course and your work on the assignments and quizzes. References to parallel material in various books available in the library may also be made.

Learning Expectations Outcomes

Course-Specific Expectations
- Recognize the importance of quantum chemistry and of its application.
- Think critically about, explain, integrate, and apply physical models to describe material and energy levels associated with atoms.
- Learn a variety of physical principles and to solve models.
- Solve a variety of novel problems, both qualitative and quantitative.
- Draw scientific conclusions from experimental results or data.

Soft-Skill Expectations
- Analyze and critically assess problems, and take a systematic approach to solve them.
- Execute mathematical calculations accurately.
- Communicate thoughts, ideas, and observations verbally and in writing.

Course Materials

-All courses materials will be available on OWL.

-In Class will be using powerpoint slides. We recommend to print the slides before each class ( 2 slides per page) and take notes on the slides.

-Each course and tutorials will be recorded and made available online.

Brief Course Description: The course builds a background in quantum chemistry/mechanics needed to understand the physical and chemical behavior of matter on the atomic scale. Quantum-mechanical concepts are developed and applied to four model systems: a particle in a box, the harmonic oscillator, the rigid rotor, and the hydrogen atom. The results are used to explain the principles of electronic, vibrational and rotational spectroscopy, atomic electronic structure, and chemical bonding.
Lecture Topics:


7. The structure and spectra of hydrogenic atoms. The Schrödinger equation for hydrogenic atoms. Energy levels, eigenfunctions (atomic orbitals) and probability densities for hydrogenic atoms. Complex and real orbitals. Radial distribution functions. Orbital angular momentum and electron spin.

Upon successful completion of this course, the student will be able to:

- Solve basic differential equations used to model electron energy and wavefunction
- Understand energies associated with electron transitions between energy levels.
- Calculate wavefunctions associated with orbitals
- Understand the concepts of electron density probabilities and represent them.
- Perform quantum mechanics common problems such as particles in 1D and 3D box.
- Understand the intimate relation between electron, energy and spectroscopy.
Students should check OWL (http://owl.uwo.ca) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class. Students are responsible for checking OWL on a regular basis.

All course material will be posted to OWL: http://owl.uwo.ca.

If students need assistance, they can seek support on the OWL Help page. Alternatively, they can contact the Western Technology Services Helpdesk. They can be contacted by phone at 519-661-3800 or ext. 83800.

**Important dates 2020**

- September 9th, Classes begin
- October 12th, Thanksgiving Monday
- November 2-8, fall reading week.
- **October 29th, 10:30-12:30 pm, mid-term.** Room to be confirmed
- Dec. 9th, Last day of class
- Dec 11-22, Mid-year Examination Period
- Final Exam: TBA, 3 hours.

Notes.
- No courses on:
- Friday 26th of September.

**Technical Requirements**

Course is scheduled to be in person. In the eventuality where we change to virtual course, the course will be virtual Asynchronous. Requirements are a computer with working microphone and webcam as web a stable internet connection. These requirements are needed for students who cannot come in class.

**Evaluation Components**

The overall course grade, out of 100, will be calculated as listed below. Listed next to the respective components are their maximum contributions toward the course grade.

<table>
<thead>
<tr>
<th>Component</th>
<th>Notes</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quizzes</td>
<td>4 best Quizzes (15-20min)</td>
<td>20%</td>
</tr>
<tr>
<td>Midterm</td>
<td>2 hoursTest</td>
<td>40%</td>
</tr>
<tr>
<td>Final Exam</td>
<td>Scheduled by the Registrar</td>
<td>40%</td>
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</table>
**Midterm exam**: Two hours exam on Oct 29th 2019- 10:30-12:30 pm Room to be announced. The format of the exam will be problems and short answers.

**Final exam**: Three-hour exam. The date is decided by the registrar’s Office. The final exam will be cumulative, with emphasis on the materials that was not examined in the midterm exam. The format of the exam will be problems and short answers.

**Assignments and quizzes**: Every two weeks, an assignment will be posted on the course website (see the schedule below). Hints and short answers will be made available on the due date. The assignments will not be collected nor marked. However, on the day following the due date there will be a quiz asking you to solve a problem that is similar to one of the problems of the assignment. During the quiz, you will be allowed to use your hand written solutions prepared at home, but not any other materials (no tablet or PC, calculator are ok) . Students writing the quizzes remotely will be monitored using Zoom. The quizzes will be collected and marked by the instructor. Detailed solutions to the problems will be released after the quiz. You are required to take at least 4 out of the total of 5 quizzes. If and only if you take all the 5 quizzes, you will earn a bonus: the quiz for which you received the lowest score will not be counted toward your final course grade. A table with the dates of quizzes and assignments is included below. The quizzes will take place on a Friday and will last for 15 to 20 minutes.

<table>
<thead>
<tr>
<th># Quiz</th>
<th>Assignment posted on</th>
<th>Due Wednesdays</th>
<th>Quiz on Thursdays (tutorial days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sept 16th</td>
<td>Sept 23rd</td>
<td>Sept 24th</td>
</tr>
<tr>
<td>2</td>
<td>Sept 30th</td>
<td>Oct 7th</td>
<td>Oct 8th</td>
</tr>
<tr>
<td>3</td>
<td>Oct 14th</td>
<td>Oct 21st</td>
<td>Oct 22th</td>
</tr>
<tr>
<td>4</td>
<td>Nov11 th</td>
<td>Nov18th</td>
<td>Nov 19th</td>
</tr>
<tr>
<td>5</td>
<td>Nov 25th</td>
<td>Dec 2nd</td>
<td>Dec 3rd</td>
</tr>
</tbody>
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Mid term: 2 hours, scheduled Thursday October 29th, 10:30-12:30, room TBA.

**To pass the course**, you must obtain a minimum of 50% in the average of quizzes, midterm and final. One should write the midterm and final exam to pass the course. Obtaining a good average grade in the quizzes and midterm is not sufficient to pass the course.

**Accommodation and Accessibility**

**Accommodation Policies**
Students with disabilities work with Accessible Education (formerly SSD) which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. The Academic Accommodation for Students with Disabilities policy can be found at: [https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf](https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf)

**Academic Consideration for Student Absence**
Students will have up to two (2) opportunities during the regular academic year to use an on-line portal to self-report an absence during the semester, provided the following conditions are met: the absence is no more than 48 hours in duration, and the assessment for which consideration is being sought is worth 30% or less of the student’s final grade. Students are expected to contact their instructors within
24 hours of the end of the period of the self-reported absence, unless noted on the syllabus. Students are not able to use the self-reporting option in the following circumstances:

- for exams scheduled by the Office of the Registrar (e.g., December and April exams)
- absence of a duration greater than 48 hours,
- assessments worth more than 30% of the student’s final grade,
- if a student has already used the self-reporting portal twice during the academic year

If the conditions for a Self-Reported Absence are not met, students will need to provide a Student Medical Certificate if the absence is medical, or provide appropriate documentation if there are compassionate grounds for the absence in question. Students are encouraged to contact their Faculty academic counselling office to obtain more information about the relevant documentation.

Students should also note that individual instructors are not permitted to receive documentation directly from a student, whether in support of an application for consideration on medical grounds, or for other reasons. All documentation required for absences that are not covered by the Self-Reported Absence Policy must be submitted to the Academic Counselling office of a student's Home Faculty.

For policy on Academic Consideration for Student Absences - Undergraduate Students in First Entry Programs, see: https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Consideration_for_absences.pdf
and for the Student Medical Certificate (SMC), see: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/medicalform.pdf

**Religious Accommodation**

Students should consult the University’s list of recognized religious holidays, and should give reasonable notice in writing, prior to the holiday, to the Instructor and an Academic Counsellor if their course requirements will be affected by a religious observance. Additional information is given in the Western Multicultural Calendar: https://multiculturalcalendar.com/ecal/index.php?s=c-unico

You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation” (see http://www.registrar.uwo.ca/examinations/exam_schedule.html).

[optional] If a student fails to write a scheduled Special Examination, the date of the next Special Examination (if granted) normally will be the scheduled date for the final exam the next time this course is offered. The maximum course load for that term will be reduced by the credit of the course(s) for which the final examination has been deferred. See Academic Calendar for details (under Special Examinations).

**Academic Policies**

The website for Registrarial Services is http://www.registrar.uwo.ca.
In accordance with policy, http://www.uwo.ca/its/identity/activatenonstudent.html, the centrally administered e-mail account provided to students will be considered the individual’s official university e-mail address. It is the responsibility of the account holder to ensure that e-mail received from the University at his/her official university address is attended to in a timely manner.

**Contingency plan for an in-person class pivoting to 100% online learning**

In the event of a COVID-19 resurgence during the course that necessitates the course delivery moving away from face-to-face interaction, all remaining course content will be delivered entirely online, either synchronously (i.e., at the times indicated in the timetable) or asynchronously (e.g., posted on OWL for students to view at their convenience). The grading scheme will **not** change. Any remaining assessments will also be conducted online as determined by the course instructor.

**All of the remote learning sessions for this course will be recorded.** The data captured during these recordings may include your image, voice recordings, chat logs and personal identifiers (name displayed on the screen). The recordings will be used for educational purposes related to this course, including evaluations. The recordings may be disclosed to other individuals participating in the course for their private or group study purposes. Please contact the instructor if you have any concerns related to session recordings.

Participants in this course are not permitted to record the sessions, except where recording is an approved accommodation, or the participant has the prior written permission of the instructor.

**Scholastic offences** are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site:

Tests and examinations in this course will be conducted using Zoom. You will be required to keep your camera on for the entire session, hold up your student card for identification purposes, and share your screen with the invigilator if asked to do so at any time during the exam. The exam session will **not** be recorded.*

More information about the use of Zoom for exam invigilation is available in the Online Proctoring Guidelines at the following link:
https://www.uwo.ca/univsec/pdf/onlineproctorguidelines.pdf

Completion of this course will require you to have a reliable internet connection and a device that meets the system requirements for Zoom. Information about the system requirements are available at the following link:
https://support.zoom.us/hc/en-us

* Please note that Zoom servers are located outside Canada. If you would prefer to use only your first name or a nickname to login to Zoom, please provide this information to the instructor in advance of the test or examination.
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Completion of this course will require you to have a reliable internet connection and a device that meets the system and technical requirements for Zoom
https://support.zoom.us/hc/en-us

* Please note that Zoom servers are located outside Canada. If you would prefer to use only your first name or a nickname to login to Zoom, please provide this information to the instructor in advance of the test or examination.

**Support Services**

Please visit the Science & Basic Medical Sciences Academic Counselling webpage for information on add/drop courses, academic considerations for absences, appeals, exam conflicts, and many other academic related matters: https://www.uwo.ca/sci/counselling/

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Student Accessibility Services (SAS) at (519) 661-2147 if you have any questions regarding accommodations.

Western University is committed to a thriving campus as we deliver our courses in the mixed model of both virtual and face-to-face formats. We encourage you to check out the Digital Student Experience website to manage your academics and well-being: https://www.uwo.ca/se/digital/.

Learning-skills counsellors at the Student Development Centre (http://www.sdc.uwo.ca) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Students who are in emotional/mental distress should refer to Mental Health@Western (http://www.health.uwo.ca/mental_health) for a complete list of options about how to obtain help.

Additional student-run support services are offered by the USC, http://westernusc.ca/services.