UNIVERSITY OF CALGARY
FACULTY OF SCIENCE

**Department of Chemistry**
Science B 605
403 220-5385
chem.info@ucalgary.ca

# COURSE OUTLINE

1. **Course:** CHEM 373, Physical Chemistry: Quantum Chemistry - Fall 2021

   Lecture 01: TR 12:30 - 13:45 in MFH 160

| Instructor | Email | Phone | Office | Hours |
|---|---|---|---|---|
| Dr. Syeda Asghar | syedafarina.asghar@ucalgary.ca | | TBA | TBA |

**In Person Delivery Details:**

**Lectures:** Lectures starts in the week of September 07, 2021.

Lectures will be in-person and class sessions will include graded work (mid-terms) that will be completed during the scheduled class time. Lectures will not be recorded, but any materials (e.g. handouts) will be posted to D2L. Midterm examinations will be held in-person during the class time and the in-person final exam will be 2 hours long, scheduled dates mentioned in section 3.

**Tutorials:** Tutorial will starts in the week of September 20, 2021.

Tutorials will occur in-person. Students will complete lecture-based practice problems along with discussions facilitated by an instructor or teaching assistant. Students will be graded through short tutorial quizzes (20 minutes each). See Section 3 for more details.

**Note: Students must attend their own scheduled Tutorial session.** See Section 4 for what to do if you miss your scheduled tutorial due to unexpected or extenuating circumstances.

**Re-Entry Protocol for Labs and Classrooms:**

To limit the spread of COVID-19 on campus, the University of Calgary has implemented safety measures to ensure the campus is a safe and welcoming space for students, faculty and staff. The most current safety information for campus can be found here. **Online Delivery Details:**

This course is being offered online in real-time via scheduled meeting times, you are required to be online at the same time.

To help ensure Zoom sessions are private, do not share the Zoom link or password with others, or on any social media platforms. Zoom links and passwords are only intended for students registered in the course. Zoom recordings and materials presented in Zoom, including any teaching materials, must not be shared, distributed or published without the instructor's permission.

**Laboratories:** Laboratories will starts in the week of September 13, 2021.

Labs (Synchronous) will be online in live zoom sessions (Zoom meeting details will be posted on D2L) students will be asked during the live sessions to watch videos and perform simulations using Microsoft Excel available through the University of Calgary d2l learnings. An evaluation in the form of Quizzes (synchronous, dates will be provided before the quiz commencement and quiz will be of 20 minutes long ) during the live lab sessions and assignments (submission Asynchronous) on dues dates will be graded for each laboratory activity see section 3.

**Note: Students must attend their own scheduled Lab zoom sessions.** See Section 4 for what to do if you miss your scheduled Zoom session due to unexpected or extenuating circumstances.

**Course Site:**

D2L: CHEM 373 L01-(Fall 2021)-Physical Chemistry: Quantum Chemistry

**Note:** Students must use their U of C account for all course correspondence.

2. **Requisites:**

   See section 3.5.C in the Faculty of Science section of the online Calendar.

**Prerequisite(s):**
Chemistry 201 or 211; and 203 or 213; Physics 223 or 355; Mathematics 267 or 277.

3. **Grading:**

The University policy on grading and related matters is described in F.1 and F.2 of the online University Calendar.

In determining the overall grade in the course the following weights will be used:

| Component(s) | Weighting % | Format & Date(s) |
|---|---|---|
| Online Laboratories Assignments (4 of 6) | 20 | Asynchronous: Various Dates-- See schedule below |
| Online Lab Quizzes(4 of 6) | 10 | Synchronous, during lab: weekly starting Sep 13 |
| Tutorial Quizzes/Assignments (6 of 8) | 10 | In-person, during tutorial; weekly starting Sep 20th |
| Midterm 1 | 15 | In-person, Oct 14th, during class time |
| Midterm 2 | 15 | In-person, Nov 16th, during class time |
| Final Examination | 30 | In-person, dateTBA, Scheduled by the Registrar |

**For tutorials**, the best 6 out of 8 quizzes/assignments grades will be considered towards your final grade.

**For the laboratories**, there will be 6 different Quizzes (synchronous, best 4 quizzes will be considered for the final grade) and 6 assignments (submission asynchronous, best 4 assignments will be considered for the final grade) (Info on specific dates is provided in section 3 grading) overall 4 quizzes+4 assignments will be considered for the final grade in Laboratories activities. Lab assignments submissions will not be accepted after 11:59 PM on the due date.

**Laboratory assignment schedule**

| # | Title | Due Date |
|---|---|---|
| 1 | Excel Introduction ( use formula, create custom functions, make and interpret graphs) | 2021-09-22 |
| 2 | The Uncertainty Principle (Building a Wave packet - Simulation) | 2021-10-07 |
| 3 | The Absorption of Linear Polyene Dyes (particle in a box) | 2021-10-14 |
| 4 | The Harmonic Oscillator (Simulation) | 2021-10-28 |
| 5 | Molecular Symmetry, Point Groups and Character Tables – Part I | 2021-11-18 |
| 6 | Character Tables and its applications (acetone) – Part II | 2021-11-25 |

Each piece of work (reports, assignments, quizzes, midterm exam(s) or final examination) submitted by the student will be assigned a grade. The student's grade for each component listed above will be combined with the indicated weights to produce an overall percentage for the course, which will be used to determine the course letter grade.

The conversion between a percentage grade and letter grade is as follows.

| | A+ | A | A- | B+ | B | B- | C+ | C | C- | D+ | D |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Minimum % Required** | 95 % | 90 % | 85 % | 80% | 75% | 70 % | 65 % | 60% | 55% | 50 % | 45 % |

This course will have a final exam that will be scheduled by the Registrar. The Final Examination Schedule will be published by the Registrar's Office approximately one month after the start of the term. The final exam for this course will be designed to be completed within 2 hours.

The University of Calgary offers a flexible grade option, Credit Granted (CG) to support student's breadth of learning and student wellness. Faculty units may have additional requirements or restrictions for the use of the CG grade at the faculty, degree or program level. To see the full list of Faculty of Science courses where CG is not eligible, please visit the following website: https://science.ucalgary.ca/current-students/undergraduate/program-advising/flexible-grading-option-cg-grade

4. **Missed Components Of Term Work:**

The university has suspended the requirement for students to provide evidence for absences. Please do not attend medical clinics for medical notes or Commissioners for Oaths for statutory declarations.

In the event that a student legitimately fails to submit any online assessment on time (e.g. due to illness etc...), please contact the course coordinator, or the course instructor if this course does not have a coordinator to

arrange for a re-adjustment of a submission date. Absences not reported within 48 hours will not be accommodated. If an excused absence is approved, one possible arrangement is that the percentage weight of the legitimately missed assignment could also be pro-rated among the components of the course. This option is at the discretion of the coordinator and may not be a viable option based on the design of this course.

A student who will miss a midterm, a quiz or deadline of due dates of assignments submissions due to exceptional circumstances (e.g. disease, etc.) the student should contact Dr. Syeda Farina Asghar within 24-hour and accommodations for students will be granted on a case by-case basis under the university protocols section 4. However, if a student fails to contact Dr. Syeda within 48-hour, accommodations will be automatically denied.

If a student misses a mid term without extenuating circumstance, that will automatically score a zero. If a student misses a midterm due to exceptional circumstances (e.g. disease, etc.) students will be graded to the other class performance which includes all; laboratories, tutorials, other midterm and final term exam.

5. **Scheduled Out-of-Class Activities:**

   There are no scheduled out of class activities for this course.

6. **Course Materials:**

   Recommended Textbook(s):

   Thomas Engel & Phillip Reid, *Physical Chemistry*: Pearson.

   In order to successfully engage in their learning experiences at the University of Calgary, students taking online, remote and blended courses are required to have reliable access to the following technology:

   - A computer with a supported operating system, as well as the latest security, and malware updates;
   - A current and updated web browser;
   - Webcam/Camera (built-in or external);
   - Microphone and speaker (built-in or external), or headset with microphone;
   - Current antivirus and/or firewall software enabled;
   - Stable internet connection.

   For more information please refer to the UofC ELearning online website.

7. **Examination Policy:**

   **Note:** Exams must be completed individually, following details should be considered for different exam categories;

   **In-person quizzes and exams (Tutorial quizzes, midterms and final exam):** Closed-book exams will be commenced, during the exams scientific calculator will be allowed. No other resources or aids will be allowed.

   **Online quizzes (lab quizzes):** Open book exam will be commenced; notes and course resources will be allowed during the online quizzes.

   Students should also read the Calendar, Section G, on Examinations.

8. **Approved Mandatory And Optional Course Supplemental Fees:**

   There are no mandatory or optional course supplemental fees for this course.

9. **Writing Across The Curriculum Statement:**

   For all components of the course, in any written work, the quality of the student's writing (language, spelling, grammar, presentation etc.) can be a factor in the evaluation of the work. See also Section E.2 of the University Calendar.

10. **Human Studies Statement:**

    Students will not participate as subjects or researchers in human studies.

    See also Section E.5 of the University Calendar.

11. **Reappraisal Of Grades:**

    A student wishing a reappraisal, should first attempt to review the graded work with the Course coordinator/instructor or department offering the course. Students with sufficient academic grounds may request

a reappraisal. Non-academic grounds are not relevant for grade reappraisals. Students should be aware that the grade being reappraised may be raised, lowered or remain the same. See Section I.3 of the University Calendar.

a. **Term Work:** The student should present their rationale as effectively and as fully as possible to the Course coordinator/instructor within **ten business days** of either being notified about the mark, or of the item's return to the class. If the student is not satisfied with the outcome, the student shall submit the Reappraisal of Graded Term work form to the department in which the course is offered within 2 business days of receiving the decision from the instructor. The Department will arrange for a reappraisal of the work within the next ten business days. The reappraisal will only be considered if the student provides a detailed rationale that outlines where and for what reason an error is suspected. See sections I.1 and I.2 of the University Calendar

b. **Final Exam:**The student shall submit the request to Enrolment Services. See Section I.3 of the University Calendar.

12. **Other Important Information For Students:**

a. **Mental Health** The University of Calgary recognizes the pivotal role that student mental health plays in physical health, social connectedness and academic success, and aspires to create a caring and supportive campus community where individuals can freely talk about mental health and receive supports when needed. We encourage you to explore the mental health resources available throughout the university community, such as counselling, self-help resources, peer support or skills-building available through the SU Wellness Centre (Room 370, MacEwan Student Centre, Mental Health Services Website) and the Campus Mental Health Strategy website (Mental Health).

b. **SU Wellness Services:** For more information, see www.ucalgary.ca/wellnesscentre or call 403-210-9355.

c. **Sexual Violence:** The Sexual Violence Support Advocate, Carla Bertsch, can provide confidential support and information regarding sexual violence to all members of the university community. Carla can be reached by email (svsa@ucalgary.ca) or phone at 403-220-2208. The complete University of Calgary policy on sexual violence can be viewed at (https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Sexual-and-Gender-Based-Violence-Policy.pdf)

d. **Misconduct:** Academic integrity is the foundation of the development and acquisition of knowledge and is based on values of honesty, trust, responsibility, and respect. We expect members of our community to act with integrity. Research integrity, ethics, and principles of conduct are key to academic integrity. Members of our campus community are required to abide by our institutional Code of Conduct and promote academic integrity in upholding the University of Calgary's reputation of excellence. Some examples of academic misconduct include but are not limited to: posting course material to online platforms or file sharing without the course instructor's consent; submitting or presenting work as if it were the student's own work; submitting or presenting work in one course which has also been submitted in another course without the instructor's permission; borrowing experimental values from others without the instructor's approval; falsification/fabrication of experimental values in a report. Please read the following to inform yourself more on academic integrity:

Student Handbook on Academic Integrity
Student Academic Misconduct Policy and Procedure
Research Integrity Policy

Additional information is available on the Student Success Centre Academic Integrity page

e. **Academic Accommodation Policy:**

It is the student's responsibility to request academic accommodations according to the University policies and procedures listed below. The student accommodation policy can be found at: https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Student-Accommodation-Policy.pdf

Students needing an accommodation because of a disability or medical condition should communicate this need to Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities: https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Accommodation-for-Students-with-Disabilities-Procedure.pdf.

Students needing an accommodation in relation to their coursework or to fulfil requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, by filling out the Request for Academic Accommodation Form and sending it to Dr. Yuen-Ying Carpenter by email yyscarpe@ucalgary.ca preferably 10 business days before the due date of an assessment or scheduled absence.

f. **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). Students should identify themselves on all written work by placing their name on the front page and their ID number on each subsequent page. For more information, see Legal Services website.

g. **Student Union Information:** VP Academic, Phone: 403-220-3911 Email: suvpaca@ucalgary.ca. SU Faculty Rep., Phone: 403-220-3913 Email: sciencerep@su.ucalgary.ca. Student Ombudsman, Email: ombuds@ucalgary.ca.

h. **Surveys:** At the University of Calgary, feedback through the Universal Student Ratings of Instruction (USRI) survey and the Faculty of Science Teaching Feedback form provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses. Your responses make a difference - please participate in these surveys.

i. **Copyright of Course Materials:** All course materials (including those posted on the course D2L site, a course website, or used in any teaching activity such as (but not limited to) examinations, quizzes, assignments, laboratory manuals, lecture slides or lecture materials and other course notes) are protected by law. These materials are for the sole use of students registered in this course and must not be redistributed. Sharing these materials with anyone else would be a breach of the terms and conditions governing student access to D2L, as well as a violation of the copyright in these materials, and may be pursued as a case of student academic or non-academic misconduct, in addition to any other remedies available at law.

**13. Lab exemptions.**

Students repeating the course within the last three years can be exempted from the Laboratory Component of the course if a grade of 75% or higher was obtained. Students choosing to exempt from the lab should be aware that,

- current online labs being may be significantly different from in-person labs from Fall 2019 or prior;
- the material covered in labs may be integrated into non-lab-based course assessments; and,
- the lab grade achieved on the previous attempt will be carried forward.

Students will still be evaluated on other course components, including any tutorials.

Prior to applying for an exemption, students are encouraged to connect with their course instructor or coordinator to better understand the risks and benefits in their specific course, particularly if these labs are not in the same format (online or in-person) this semester. Instructors can tell you what access you will have (or not have) to lab materials as an exempt student, and how the lab materials may be integrated.

Applications for lab exemptions must be emailed to the Undergraduate Science Center (science.advising@ucalgary.ca) before Monday September 13th, 2021.

**Course Outcomes:**

- recognize the limitations of classical mechanics at molecular length scales
- identify the differences between classical and quantum mechanics
- illustrate the connection of quantum mechanical operators to observables
- evaluate probabilities, amplitudes, averages, expectation values, and observables
- explain the quantum mechanical nature of the chemical bond.
- practice how molecular phenomena can be related to model problems
- predict structure, bonding of molecules with the help of qualitative molecular orbital and valence bond theory

Electronically Approved - Sep 09 2021 15:13

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**Department Approval**

Electronically Approved - Sep 09 2021 15:30

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**Associate Dean's Approval**