



CHM 223H: Physical Chemistry: The Molecular Viewpoint
Course Syllabus, Winter 2022 (V1.0)

I TEACHING TEAM

INSTRUCTOR



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(See Quercus for Zoom links)

Prof. Wilson leads a [research team](#) that uses optical spectroscopy to explore, understand, and develop excitonic and nanostructured materials for optoelectronic devices. Our present research focus is to better understand the synthesis, structure, and photophysics of colloidal quantum dots (and functionalized architectures) to advance nanocrystal-sensitized triplet-fusion photon upconversion for use in additive manufacturing, biomedicine, and low-cost imaging in the short-wave infrared.

Proudly hailing from Port Colborne, Ontario, he studied at Queen's University, receiving a B.Sc. (2006, Engineering Physics), a B.A. (2008, History), and an M.Sc. (2008, Eng. Phys.) under the supervision of Prof. James Fraser. He next earned a PhD in Physics (2012) from the University of Cambridge for his studies of singlet exciton fission under the supervision of Prof. Sir Richard Friend. Then, as a member of the Centre for Excitonics at the Massachusetts Institute of Technology, he pursued postdoctoral studies (2012-2016) into triplet energy transfer between organic molecules and semiconductor nanocrystals with Prof. Mounqi Bawendi (Chemistry) and Prof. Marc Baldo (Electrical Engineering), before starting his independent career.

When not doing science, Mark can be found cooking, canoe tripping, swing dancing, and trying to make the world a better place for his son.

TA(s)

Name: Margarita Gladkikh TUT0101A (Surnames A-L)

Name: Phillip Jensen TUT0101B (Surnames M-Z)

Name: Sumner Alperin-Lea TUT0201

Name: Kelly-Marie Yokuda, Computational Tutorials

Note: In preference to e-mail, we *strongly* emphasize that it is much better to post most course-related questions on the Ed discussion board (see below). Here, they can be answered by a peer, the first-available TA, or Prof. Wilson. Posts can be made anonymous to other students if desired, recommended/upvoted by others, and responses are threaded and categorized so that all can benefit from the interaction.

Please consult the [FAQ page on Quercus](#) before e-mailing Prof. Wilson. Particularly, email is *not* the mechanism to receive explanations of course material. Instead, please ask such questions during your tutorial, during Prof. Wilson's online student hours, or in a post on the course discussion board.

When e-mailing Prof. Wilson, please include your full name, student number, and identify yourself as a CHM223 student. Most emails will receive a reply within 24 hours during the work-week, but expectations should be kept reasonable as to the degree of detail that an email reply to your enquiry can realistically provide.

Note that teaching assistants (TAs) are not expected to provide assistance via email.

II COURSE OVERVIEW

COURSE DESCRIPTION:

CHM223 introduces key concepts and mathematical approaches that underly fundamental quantum mechanical models of atoms and molecules. Connections are drawn between these microscopic models and macroscopic properties of systems in physical chemistry—both how experimental observations shaped the chosen structure of the models, and how these models can now successfully predict the results of experiments, especially spectroscopies.

STUDENT LEARNING OUTCOMES:

By the end of this course, students will be able to:

- Explain some compelling experimental observations that show that a quantum mechanics is necessary to understand aspects of the physical world
- Use quantum mechanical concepts, and associated models of atoms and molecules, to predict some physical behaviours of chemical materials.
- Defend the interplay of theory and experiment in the scientific method.
- Communicate quantum mechanical concepts quantitatively using appropriate formalism
- Employ conventional methods to determine the allowed wavefunctions of a 'particle in a box', and use the tools of quantum mechanics to describe measurements on these and other exactly solvable systems.
- Discuss approximate models of atomic and molecular structure, including relevant assumptions/qualifications, mathematical structure, and physical significance.
- Solve relevant quantitative problems by applying concepts from class, planning a strategy that allows the answer to be calculated, and interpreting the result obtained.
- Write basic scripts (in Python) to perform calculations and visualize wavefunctions.

PREREQUISITE COURSE(S):

CHM222, or CHM220 (with a minimum grade of B, or instructor's permission)

RECOMMENDED COURSES: MAT235/237 introduce critical mathematical concepts in integral and differential calculus that are expected background for this course.

READINGS:

Main: Physical Chemistry (LibreTexts) (September 26, 2021 edition)

<https://chem.libretexts.org/@go/page/9054> Chapters 1–10

Alternate:

Ira N. Levine, Physical Chemistry (6th Ed.), Chapters 17–20

Atkins' Physical Chemistry (11th Ed.) Foci 7–9, 11

These textbooks can be useful resources to strengthen your understanding of key topics, give additional context/extensions, and to provide more sample problems. We will not cover all the content in the highlighted chapters in any of these textbooks, and our sequence will differ to an extent from each. However, Prof. Wilson will identify in-class the key sections in the LibreText that are associated with lecture topics and are suitable subjects for questions on assessments. This book is [freely available online](#) (either as a live website, or as a downloadable pdf.)

III COURSE ORGANIZATION

QUERCUS:

This course will primarily 'live' on [Quercus](#). As a result, please ensure that you can access the site, and contact the [Quercus Helpdesk](#) or Prof. Wilson promptly (as appropriate) if you encounter issues. For instance, all announcements will be made via Quercus. As a result, it is your responsibility to either check the site regularly, or, ensure that you are able to receive announcements as e-mails at an account that you monitor.

For instance, all class materials and assignments will be available on Quercus, and all assignments and assessments will be submitted via Quercus.

CLASSES:

Until further notice, classes will be held synchronously via Zoom on Mondays and Wednesdays from 4-5pm, EST. Lectures will formally commence at 4:10pm.

Refer to Quercus for relevant information including Zoom links.

Lectures are where concepts are introduced, discussed, and placed in context. Material may be covered in class that is not in the textbook. Lectures will be recorded, and links posted to Quercus. (Please allow up to 72 hours for this process to complete for a particular lecture.)

Students are *strongly* advised to attend class synchronously: for anecdotal reasons that include the ability to interact/ask questions in real-time, as well as the *strong correlation* often observed between synchronous attendance and superior student experience and achievement. (E.g. [Martins-Roballino et al., Proc. CEEA-ACEG 2021](#)) In this light, it is best to view the lecture recordings as a 'back-up' in case a class must be missed, as well as a way to permit concepts to be reinforced by review.

TUTORIALS:

Tutorials are a key part of CHM223, and students are *strongly* advised to attend each week. Time will be dedicated to direct discussion of problems from the analytical assignments, and TAs can also respond to student questions on these exercises and general course content.

Additional instructive problems will be solved by the TA in this smaller, synchronous setting to facilitate student participation and discussion. These problems will complement, reinforce, and extend topics addressed in lecture, and aid in preparing for tests.

Students must register for a tutorial section via ACORN/ROSI. Two sections will run simultaneously on Tuesdays from 2-3pm, and one will run Fridays from 1-2pm.

Tutorials will be held via Zoom until further notice. See Quercus for links.

One tutorial section (TUT0101A) will be recorded and made available via Quercus as a back-up resource in case of unavoidable absence, and to permit post-facto review. We emphasize that synchronous attendance is a broadly superior strategy for students success. Other tutorials will *not* be recorded to promote discussion. All tutorials will address the same core topics, but will not be identical. We do not recommend attending more than one section.

Discussion Board:

We will be using the Ed Discussion, a free platform that facilitates threaded online Q&A's. Information on how to join Ed can be found in Quercus. As stated above, we *highly* encourage you to ask your content questions on Ed where all students can collaborate on and benefit from response. The teaching team will monitor the discussion, validate strong student answers (you folks are usually faster!), and provide input as needed.

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

DATES	UNIT	TOPICS
Jan 6–28	Machinery of Quantum Mechanics	Motivation for quantum mechanics. The wavefunction, Schrödinger equation, and postulates. Operators and measurement. Computational Assignment 1, due Fri, Jan 21th at 6:59pm Computational Assignment 2, due Fri, Jan 28th at 6:59pm Analytical Assignment 1, due Tues, Feb 1st at 6:59pm Test 1, Tues, Feb 8th, 6-7:30pm
Jan 31 st – Mar 4 th	Electronic Structure of Atoms	Solutions of the quantum harmonic oscillator. Applications to molecular vibrations and spectroscopy. Angular momentum. The wavefunctions of the hydrogen atom. Spin, multi-electron atoms, and approximate treatments. Comp. Assignment 3, due Fri, Feb 18th at 6:59pm Analytical Assignment 2, due Tues, Mar 8th at 6:59pm Test 2, Tues, Mar 15th, 6-7:30pm
Mar 7 th – Apr 8 th	Molecular Orbitals and Chemical Bonds	The Born Oppenheimer approximation. Chemical bonding in diatomic molecules. Molecular-orbital theory. Analytical Assignment 3 due Tues, Apr 5th at 6.59pm. Test 3 (During final assessment period, date TBD)

Note: All times [EST/EDT](#) as appropriate. The 'Dates' column refers to the approximate days during which the associated topics will be discussed in lectures.

If you will be in a time zone that makes it challenging to write a test at the chosen time, you will be given the opportunity to write at an alternative time. Contact Prof. Wilson by e-mail as soon as possible if this will apply to you so that arrangements can be made.

IV EVALUATION/GRADING SCHEME

OVERVIEW:

Computational Assignments (x3):	10%
Analytical Assignments (x3):	15%
Test 1: Tues, Feb 8 th , 6-7:30pm	25%*
Test 2: Tues, Mar 15 th , 6-7:30pm	25%*
Test 3: (Date TBD, see above)	25%*

*When calculating each student's final grade, the lowest of their three individual test scores will be only weighted at 20%, and the highest will be boosted to 30%. Thus, the three tests will still count for 75% in total.

All assignments will be submitted via Quercus and time-stamped.

The mark for a late analytical or computational problem set will be reduced by 25% if submitted (via Quercus) before 4pm on the Monday that follows the due date, and by 50% if handed in afterwards. However, no marks will be awarded for any problem sets submitted after the beginning of our final class (i.e. 4pm) on Wednesday, April 6th.

Computational assignments will be submitted by file upload via Quercus. See [the instructions on Quercus](#) for details.

Analytical assignments must be hand-written, scanned/photographed clearly, and assembled into a single PDF file. (We emphasize that there are many scanning apps for phones that make this straightforward. You are recommended to find one that works well for you. A fall-back solution is to manually import photos to pages in e.g. Google Docs/Slides, Microsoft Word/Powerpoint, or a similar program, and then export the result as a pdf. Many free (if sketchy) websites can also be effective.) Please include your name and student number on the first page of the assignment. You will then be able to upload the single PDF via Quercus. See the relevant Assignment page on Quercus for further details.

For a student missing one test for a valid reason, the missed test grade will be replaced by an extrapolation involving the average of that student's performance on the other two tests relative to the respective class averages. Situations where a student misses multiple tests for valid reasons will be addressed on a case-by-case basis, likely via a cumulative oral or written exam during the final assessment period. In the absence of a valid reason, failure to complete a test will generally result in a mark of zero.

IMPORTANT: if an unexpected technical issue occurs with a *university* system (e.g., Quercus services, network outage) that affects availability or functionality, it may be necessary to revise the timing or weighting of the quizzes/term tests.

V COURSE POLICIES

Each member of this course is expected to maintain a:

- (i) professional and respectful attitude during all course activities, including classes, laboratories, tutorials and online activity.
- (ii) personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
- (iii) collection of notes recorded independently based on concepts covered in course activities (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation)
- (iv) familiarity with the university policy on Academic Integrity (overleaf)

The University of Toronto is committed to equity, human rights, and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. As a Course Instructor, I will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment, and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our Equity Offices.

Aspects of this course, including your participation, will be recorded on video and will be available to students in the course for viewing remotely and after each session.

Course videos and materials belong to your instructor, the University, and/or other sources depending on the specific facts of each situation, and are protected by copyright. Do not

download, copy, or share any course or student materials or videos without the explicit permission of the instructor. For questions about the recording and use of videos in which you appear please contact your instructor.

VI TECHNOLOGY REQUIREMENTS

Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here: <https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/>

Advice for students more broadly regarding online learning is available here: <https://onlinelearning.utoronto.ca/getting-ready-for-online/>

This course requires the use of computers, and technical issues are possible. When working on a course activity, students are responsible for scheduling enough time to allow for reasonable delays due to technical difficulties to be overcome, so such issues will not generally be acceptable grounds for deadline extension. Particularly, maintaining an up-to-date, independent backup copy of your work is *strongly* recommended to guard against hard-drive failures, corrupted files, lost computers, etc.

VII INSTITUTIONAL POLICIES & SUPPORT

ACADEMIC INTEGRITY

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University's Code of Behaviour on Academic Matters (governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In assignments:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Obtaining or providing unauthorized assistance on any assignment.
 - **Please note that the use of external platforms (including websites, chegg.com, discord servers, etc.) to post assignment materials/questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters.** Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.
 - You are welcome to use the course discussion board to discuss any tutorial questions (and their answers) that are not graded. You are also welcome to ask for clarification regarding the *graded* questions on assignments on the discussion board, and TAs and Prof. Wilson may respond. However, ***it is not acceptable to post (or access) answers to graded questions on the discussion board.*** Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student

Academic Integrity office.

On tests:

1. Looking at someone else's answers or collaborating/discussing during a test.
2. Misrepresenting your identity.
3. Using or possessing unauthorized aids. **Please note that the use of any platforms (including social media, chegg.com, or the course discussion board) to post test questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.** Accordingly, student access to the course discussion board may be suspended during our three tests.

Note that all assessment material is © the University of Toronto, so the extent of this ban is not limited to the duration of the course. Prof. Wilson will hold 'debrief' sessions after the first two tests to discuss commonly-made errors.

In general academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see www.academicintegrity.utoronto.ca/).

COPYRIGHT

If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited. More information regarding this is available here: <https://teaching.utoronto.ca/ed-tech/audio-video/copyright-considerations/>

ACCESSIBILITY NEEDS

Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact [Accessibility Services](#) as soon as possible. Particularly, accommodations involving assessment will only be made on the advice of Accessibility Services. Accordingly, students are encouraged to be proactive in making appropriate arrangements.

ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor a reasonable amount of time **before** the session/assignment date to arrange accommodations.

ADDITIONAL SERVICES & SUPPORT

The following are some important links to help you with academic and/or technical service and support:

- General student services and resources at [Student Life](#)
- Full library service through [University of Toronto Libraries](#)
- Resources on conducting online research through [University Libraries Research](#)
- Resources on academic support from the [Academic Success Centre](#)
- Learner support at the [Writing Centre](#)
- Information for [Technical Support/Quercus Support](#)

ACKNOWLEDGEMENT OF TRADITIONAL LANDS

The University of Toronto wishes to acknowledge this land on which it operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and members of the university are grateful to have the opportunity to work on this land.