Chemistry
UNIVERSITY OF TORONTO

CHM 223H: Physical Chemistry: The Molecular Viewpoint

Course Syllabus, Winter 2023 (V1.1)

I TEACHING TEAM

INSTRUCTOR

Name: Mark W.B. Wilson (he/him)
Email: mark.w.b.wilson@utoronto.ca
Office: LM241

Online student hours: Mondays, 6:30-7:30pm EST
(See Quercus for Zoom links)

Prof. Wilson leads a research team that uses optical spectroscopy to explore 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 lower-cost infrared imaging. 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. Moungi 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.

TAs

Rees Hughes (he/him) TUT0101A (Surnames A-L) Tuesdays 2-3pm Room: LM155
Rees will also hold online tutorials for our computation assignments (see Quercus.)

Nita Ghosh (she/her) TUT0101B (Surnames M-Z) Tuesdays 2-3pm Room: LM157

Guillermo Lozano Onrubia (he/him) TUT0201 Fridays 11am-noon Room: LM155

Note: In preference to e-mail, we *strongly* recommend posting 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, upvoted by others, and responses are threaded and categorized so that all can benefit from the interaction.

Please also 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 the expected values of measurements on this and other exactly solvable systems.
- Discuss approximate models of the electronic structure of atoms and molecules, including relevant assumptions/qualifications, mathematical formalism, 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 mathematical concepts in integral and differential calculus that are expected background for this course.

READINGS:
Main: Physical Chemistry (LibreTexts) (Oct 6, 2022 edition)
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Physical_Chemistry_(LibreTexts) 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. 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

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 class materials and assignments will be available on Quercus, and all assignments will be submitted via Quercus. Further, *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.

Classes:
Lectures will take place in LM158 on Mondays and Wednesdays from 4-5pm, EST.

Lectures will formally commence at 4:10pm.

Lectures are where concepts are introduced, discussed, and placed in context. Material may be covered in class that is not in the textbook. Until further notice, lectures will *also* be synchronously streamed via Zoom. Prof. Wilson does this on a voluntary basis as an aid to students unable to attend lecture in-person due to reasons that could include (suspected) illness. Please refer to Quercus for relevant information including Zoom links.

Lastly, streamed 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 in real-time, as well as the *strong correlation* 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 an occasional class is missed, and a way to reinforce concepts 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.

All tutorial sections in a given week will address the same core topics, but will not be identical. We do *not* recommend attending more than one section.

One tutorial section (TUT0201) will be recorded in support of student accommodations. Other tutorials will ***not*** be recorded to promote discussion. Students may contact Prof. Wilson by e-mail to obtain access to a particular recording in case of non-routine absence (*e.g.* due to illness), though detailed justifications are unnecessary. Instead, we emphasize that synchronous attendance is a broadly superior strategy for student success.

Discussion Board:
We will be using 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 9th – 30th	Machinery of Quantum Mechanics	Motivation for quantum mechanics. The wavefunction, Schrödinger equation, and particle-in-a-box. Operators and ensemble measurement. Uncertainty. Postulates. **Computational Assignment 1, due Fri, Jan 20th at 6:59pm** **Computational Assignment 2, due Fri, Jan 27th at 6:59pm** **Analytical Assignment 1, due Tues, Jan 31st at 6:59pm** **Test 1 (*Online*), Tues, Feb 7th, 6:30-8:00pm**
Feb 1st– Mar 6th	Vibrations and the H-atom: 'Single-particle' systems	Solutions of the quantum harmonic oscillator and rigid rotor. Applications to molecular vibrations and spectroscopy. Angular momentum. The wavefunctions of the hydrogen atom. Spin. **Comp. Assignment 3, due March 3rd at 6:59pm** **Analytical Assignment 2, due Tues, Mar 7th at 6:59pm** **Test 2 (*In person*), Tues, Mar 14th, 6:30-8:00pm**
Mar 8th– Apr 5th	He-Og & molecules: Multi-particle systems	Multi-electron atoms, and approximate treatments. The spin-statistics theorem. The Born Oppenheimer approximation. Chemical bonding in diatomic molecules. Molecular-orbital theory. **Analytical Assignment 3 due Tues, Apr 4th at 6:59pm.** **Final Exam (*In person*) (During final assessment period)**

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.

IV EVALUATION/GRADING SCHEME

Overview: (See table above for assessment dates.)
Computational Assignments (x3): 9%
Analytical Assignments (x3): 15%
Test 1 (Online): 20%*
Test 2 (In-person): 20%*
Final Exam (In-person): 36%*

*When calculating each student's final grade, students will receive the higher score from two alternative weightings. The standard weighting is listed above. However, if a student's score on the final exam is greater than their average score on the two tests, their final exam will be up-weighted to 46%, and the two tests (each) down-weighted to 15%. Thus, the two tests+exam will still count for 76% in total.

All assignments will be submitted via Quercus and time-stamped. (See below)

Late Policy: The mark for a late analytical or computational problem set will be reduced by 25% of the score earned if submitted (via Quercus) before 6:59pm on the Friday 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 end-of-term (i.e. 6:59pm on Friday, April 7th.)
Also, assignments submitted late may be graded/returned after those submitted on-time.
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*. 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 Quecus. See the relevant Assignment page on Quercus for further details. Assignments submitted in other file formats may incur late penalties if they are not corrected before the relevant due date.
(If you don't have access to a scanner, we note that there are many scanning apps for phones that make this straightforward. You are recommended to find one that works effectively 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.)

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 test and the final exam 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 materials and videos 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 specific 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.

Note that all course material (including assignments) is © the University of Toronto, so the extent of this ban is not limited to the duration of the course.

- 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 course material (including tests) is © the University of Toronto, so the extent of this ban is not limited to the duration of the course.

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, they must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited. Similarly, students may not create personal audio or video recordings of classes or tutorials with the exception of those students requiring accommodation who have sought and received the instructor's written content beforehand. Such consent will not be unreasonably withheld. Students creating unauthorized audio recording of lectures violate an instructor's intellectual property rights and the Canadian Copyright Act. Students violating this agreement will be subject to disciplinary actions under the Code of Student Conduct.

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 *at least one week* **before** the session/assignment date to arrange accommodations (*three weeks* in the case of the final exam), and so are strongly advised to review the course schedule (above) before the start-of-term.

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 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.