The University *of* Western Ontario
Department of Chemistry

Chemistry 2284B

PHYSICAL CHEMISTRY II: QUANTUM THEORY

Winter 2025

Course Information

Instructor: [redacted]

Lectures and Tutorials: [redacted]

Office hours (for administrative matters): by appointment

Course web site: `https://westernu.brightspace.com`

Prerequisite(s): Chemistry 1301A/B, Chemistry 1302A/B, 0.5 course from Calculus 1000 A/B, Calculus 1500A/B, Numerical and Mathematical Methods 1412A/B, and any other 0.5 course at the 1000-level from Calculus, Applied Mathematics, Mathematics, or Numerical and Mathematical Methods. Integrated Science 1001X may be used as a substitute for the combination of Chemistry 1302A/B and Calculus 1301A/B.

Antirequisite(s): Chemistry 2214A/B, Chemistry 3374A, the former Chemistry 2384B.

Brief Description: Foundations of the quantum theory of chemical structure and bonding. Topics include chemically relevant model problems of quantum mechanics, elements of atomic and molecular spectroscopy, relationship between classical and statistical thermodynamics.

Recommended texts:

1. A. J. Thakkar, *Quantum Chemistry: A Concise Introduction for Students of Physics, Chemistry, Biochemistry and Materials Science*, 3rd ed. (IOP Publishing, Bristol, UK). The 2nd edition is available in electronic form (PDF) from Western Libraries. Cost: Free for UWO students
2. P. Atkins, J. de Paula, and R. Friedman, *Physical Chemistry: Quanta, Matter, and Change*, 2nd ed. (W. H. Freeman & Co., NY, 2014). Cost: ∼$165 on Amazon.ca
3. D. J. Griffiths and D. F. Schroeter, *Introduction to Quantum Mechanics*, 3rd ed., Cambridge University Press, 2018. Cost: ∼$86 on Amazon.ca. Highly recommended for advanced learning.

Learning Outcomes

1. Scientific principles: Recognition that quantum mechanics provides a theoretical basis for all of chemistry, materials science, and spectroscopy.
2. Theoretical knowledge: Understanding of the key ideas and principle of quantum mechanics such as wave-particle duality, operators, wavefunctions, uncertainty principle, orbitals, etc.
3. Practical knowledge: Problem-solving skills in applying the key principles of quantum mechanics to simple problems in chemistry and spectroscopy.
4. Awareness of the limitations of the discipline: Recognize the limitations of the models and assumptions used in quantum mechanics as applied to chemistry, being able to illustrate these limitations with specific examples.
5. Autonomy and impact: Develop the ability to work productively, being able to illustrate the relevance of the discipline to chemical research.

Course Topics

1. Wave-particle duality of matter. The wavefunction and its interpretation.
2. The Schrödinger equation for the wavefunction. The formalism of quantum mechanics: operators, eigenfunctions and eigenvalues.
3. Conceptually important model problems of quantum mechanics: particles in potential wells of various shapes. Quantum tunneling.
4. Quantum-mechanical description of translational, rotational, and vibrational motion.
5. Elements of statistical mechanics. The Boltzmann distribution, molecular partition functions, calculations of thermodynamic state functions from partition functions.
6. Atomic orbitals, orbital energies, quantum numbers. Many-electron atoms. How quantum mechanics describes the electronic structure of molecules and solids.
7. Applications of quantum theory to molecular spectroscopy: Selection rules, lasers, elements of photochemistry.

Evaluation

Assessment	*Date*	*Format*	*Total Weight*
Tests	Test 1: Friday, January 24 Test 2: Wednesday, February 12 Test 3: Friday, March 14	In class, open book	40%
Final Exam	TBA	3 hours, closed book	60%

Assignments. Assignments will be posted throughout the course but will not be collected or marked. The open-book tests will consist of problems that are analogous to those of the assignments. You are encouraged to use your worked-out assignments on the tests.

Policies

Fair evaluation. All students will be treated equally and evaluated using the same criteria described in this course outline. Private requests for reweighting of marks, additional assessments, special arrangements, etc. will be left without response.

Missed tests and built-in assessment flexibility. Should you miss a test for any reason, there is no need to request academic consideration, provide documentation of any kind, or even contact the instructor. The weight of the first missed test will be automatically transferred to the other tests. The weight of each subsequently missed test (20%) will be transferred to the final exam. Students who write all three tests will receive a **bonus**: only the best 2 of the 3 test marks will be counted toward the course grade, at 20% each. There are no make-up tests.

Missed final exam. When a student misses the Final Exam and their Academic Consideration has been granted, they will be allowed to write the Special Examination. See the Academic Calendar for details (under Special Examinations).

Use of electronic devices. During tests and exams, only basic electronic calculators are allowed; all other devices (cell phones, tablets, cameras, or iPod, etc.) are prohibited.

Accommodation policies. Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. Link

Scholastic offences. Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence. Link