Physical Chemistry and Theoretical Chemistry

CHM1441H *Mathematical Methods*
The aim of this course is to introduce mathematical techniques that are commonly encountered in Physical Chemistry. Topics discussed include complex variables, Fourier transforms, and applications to electronic and optical spectroscopies. Physical concepts in electronics and optics will be introduced as necessary and will be illustrated using homeworks and hands-on exercises. **Instructor:** Al-Amin Dhirani

CHM1443H *Open Quantum Systems*
The course will cover central methodologies in the area of open quantum systems, along with the introduction of relevant mathematical tools and the discussion of applications. The course will begin with a detailed analysis of quantum relaxation processes: particle decay and vibrational relaxation. Continuing with the Liouville von Neumann equation, the course will cover the derivation of the quantum master equation, Nakajima Zwanzig equation, Quantum Langevin equation and Feynman's path integral representation of time evolution. Methods will be discussed in light of various applications, including charge transfer in condensed phases (Marcus theory), pure decoherence, exciton and vibrational energy transfer, and chemical reaction dynamics. Computer codes will supplement the theoretical material.

Prerequisite: Core course in quantum mechanics and basic knowledge in programming

CHM1444: *Statistical Mechanics of Condensed Phases*
The course will cover various topics relating to the structure and dynamics of systems in condensed phases. Possible subjects of study include phase transitions and critical phenomena, stochastic and microscopic descriptions of the dynamics in condensed phases both in and out of equilibrium, and recent progress in the development of fundamental principles in non-equilibrium systems. The course assumes an elementary knowledge of equilibrium and non-equilbrium statistical mechanics.

Prerequisite: Core course in statistical mechanics

CHM1445H *Coherent Control of Molecular Processes*
Quantum interference effects and their role in the control of atomic and molecular processes; Theoretical formulation and discussion of experimental implementation. **Prerequisite:** Graduate level quantum mechanics.

CHM1446H *Quantum Computation and Information Theory*
This course will be a comprehensive introduction to the emerging new field of quantum information processing, with particular emphasis on quantum computation and the theory of quantum information. The course will be at a level appropriate to an advanced graduate student in chemistry or physics who has taken graduate level quantum mechanics. Topics to be covered include superdense coding and teleportation, the abstract properties of quantum computers (qubits, universal computation), quantum algorithms (factoring, database search, simulating physical systems), physical realizations of quantum computers (trapped ions, NMR, quantum dots, cavity QED, trapped atoms), the theory of open quantum systems (decoherence, Lindblad equation), quantum error correction (stabilizer codes, decoherence-free subspaces, symmetrization), formal aspects of quantum information theory (measures of entanglement, quantum communication complexity). **Recommended Text:** M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information.

CHM1447H *Biophysical Chemistry*
The course will review protein and polynucleotide structure and electronic levels. This will be followed by a detailed discussion of Levinthal's paradox with respect to the mapping problem onto active structures. This discussion will be based on recent progress on identifying a very limited class of topologically distinct domains for the plethora of macromolecules studied to date. This issue will be addressed within the context of proteomics and the search for gene sequenced activity. This subject mater will be complemented by a treatment of energy transduction in biological systems, from energy transport involved in photosynthesis, ATP interconversion and coupling to reaction coordinates, and motor protein driven conformational feedback loops. Other topics to be covered in the context of recent research advances.

CHM1448H *Modelling of Biochemical Systems*

An introduction to mathematical modelling of complex biological systems. The primary focus will be on sets of chemical reactions arising in biological contexts (for example, in gene regulation). Such sets of coupled reactions give rise to mathematical models that display nonlinear and stochastic behaviour. The course will provide a survey and practical introduction to the mathematical techniques used in modelling, simulating, and analyzing such systems, including nonlinear dynamics as well as Monte Carlo and other simulation techniques for stochastic systems. Although examples will be drawn mainly from biochemical systems, the techniques discussed will be applicable to many systems in physics, chemistry, and biology. The course will be presented in a self-contained and pragmatic manner aimed at providing an applied introduction to these mathematical techniques to a potentially interdisciplinary audience.

CHM1450H ***Nanoscale Characterization with Scan Probe Microscopy***
This course provides an introduction to scan probe microscopy (SPM). Scanning tunneling microscopy, molecular (atomic) force and near-field scanning optical microscopy will be covered. The course will cover a broad range of topics, including theory behind tunneling from metals and through organic layers, contact mechanics, the molecular basis of adhesion, single molecule mechanics, basic principles of nanophotonics, experimental considerations in implementing and using SPM, and applications to imaging and spectroscopy. Applications to both synthetic and biological materials will be considered.

CHM1455H ***NMR Spectroscopy I: Introduction to Theory and Application***

CHM1456H ***NMR Spectroscopy II: Advanced Theory and Application***
Advanced theoretical description of NMR spectroscopy, including multi-dimensional experiments and the development of density matrix and operator descriptions of leading edge magnetic resonance experiments.

CHM1464H ***Topics in Statistical Mechanics***

CHM1478H ***Quantum Mechanics for Physical Chemists***
This core course in Quantum Mechanics covers the basic Hilbert space formulation of Quantum Mechanics as well as operator algebra, representations, the Heisenberg and Schrodinger pictures, angular momentum coupling, and the von-Neumann equation for open quantum systems. Specific applications will be chosen from a range of topics in chemical physics.

CHM1478H: ***Quantum Mechanics for Physical Chemists***
This core course in quantum mechanics covers the basic Hilbert space formulation of quantum mechanics as well as operator algebra, representations, the Heisenberg and Schrodinger pictures, symmetry, and the von-Neumann equation for open quantum systems. Specific applications will be chosen from a range of topics in chemical physics.

CHM1480H ***Basic Statistical Mechanics***
(Cross-listed undergrad CHM427H)

CHM1481H ***Reaction Kinetics and Dynamics***
Chemical kinetics is an important aspect of chemistry, not only from a fundamental perspective, but also in understanding and predicting the rates of any chemical reaction. This course will begin with a review of the principles of kinetics, and cover theoretical and experimental approaches to studying unimolecular (including photochemical), bi- and ter-molecular and surface reactions in gas and condensed phases. Approximately 1/3 of the course will be devoted to special topics, which will be determined by the interests of the participants.

CHM1482H ***Laser Spectroscopy and Photophysics***

CHM1485H ***Molecular Dynamics and Chemical Dynamics in Liquids***

CHM1486H ***Modern Molecular Spectroscopy***
The course will cover the theory and application of a selection of modern methods in molecular spectroscopy, with an emphasis on time-domain measurements. The theoretical basis for understanding and analyzing the measurements will be covered in detail. It will be assumed that students are well-grounded in basic quantum mechanics and statistical mechanics. Topics will include lasers, time-resolved fluorescence,

pump-probe spectroscopies, nonlinear spectroscopy, anisotropy and rotational averaging. Applications to FRET and reaction dynamics will be discussed.

CHM1488H *Current Directions in Experimental Physical Chemistry*

IOS1500 *Selected Topics in Optics Research*
This course gives an introduction to topics of current research in optics, both at the University of Toronto and in other research institutions. Students will attend a number of guest lectures, complemented by other seminars. Credit or no credit is assigned for this course based on attendance.

CHM1490Y *Physical Chemistry Seminar*