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 homework and hands-on exercises.

CHM1443H *Intermediate Quantum Mechanics*
Elements of group theory and its applications to quantum mechanics, potential scattering, formal scattering theory, and second quantization. **Prerequisite:** Core course in quantum mechanics.

CHM1444H *Advanced Topics in Chemical Physics*
Selected topics of current research interest in Chemical Physics not covered in the core curriculum.

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, symmetrisation), 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.

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.

CHM1449H *Machine Learning and Physics Based View on Chemical Compound Space*
This is an advanced, continuously updated research-oriented course for students with interests in computational and theoretical chemistry/physics/materials typically attend). Prerequisites include undergraduate knowledge in terms of:
-statistical mechanics
-computer programming
-quantum mechanics
-applied math (linear algebra, differential equations)
-atomistic simulation

The typical outline is
-Introduction to chemical compound space
-First principles view on chemical compound space
-Machine learning in chemical compound space
-Optimization in chemical compound space
-Examples

CHM1450H *Nanoscale Characterization with Scan Probe Microscopy*
This course introduces 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.

CHM1453H *Density Functional Theory*
The goal of this course is to introduce the basics of computational quantum chemistry, specifically the density functional theory (DFT), and high-performance computing to students with primarily experimental background. It aims to provide students with the necessary computational background and hands-on experience in running DFT calculations to complement their ongoing lab-based research projects. The course will cover organic molecules and periodic inorganic systems, calculations for geometry relaxation, formation energies, and electronic structure, and will cover the tools to run and analyze the results. It will discuss the main numerical methods used, as well as the capabilities and limitations of DFT.

CHM1455H *NMR Spectroscopy I: Basic Theory & Applications for Biological Chemists*
Fundamentals of Nuclear Magnetic Resonance (NMR) spectroscopy including classical and quantum descriptions, NMR parameters and relaxation times, product operators, multi-dimensional NMR, and solid-state techniques. On successful completion of the course, students will be able to:
1. Understand fundamental concepts in NMR spectroscopy.
2. Describe spin dynamics using both classical and quantum descriptions.
3. Gain experience in data processing and analysis using software packages.
4. Understand theoretical and practical aspects of multidimensional NMR.
5. Describe fundamentals mechanisms of spin relaxation and molecular dynamics.
6. Appreciate and describe modern methods and applications of NMR spectroscopy

CHM1464H *Topics in Statistical Mechanics*
This course covers the basic principles involved in simulating chemical and physical systems in the condensed phase. Simulations are a means to evaluate equilibrium properties such free energies as well as dynamical properties such as transport coefficients and reaction rates. In addition, simulations allow one to gain insight into molecular mechanisms. After presenting the theoretical basis of Monte Carlo and molecular dynamics simulations, particular attention is given to recent developments in this field. These include the hybrid Monte Carlo method, parallel tempering, and symplectic and other integration schemes for rigid, constrained, and unconstrained systems. Time permitting, techniques for simulating quantum systems and mixed quantum-classical systems are also discussed.

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, and the von-Neumann equation for density matrix. The list of other topics is as follows.
•Basic formalism of quantum mechanics: time-independent and time-dependent pictures
•Variational, perturbational, and semi-classical approaches
•Symmetry, representation theory
•Identical particles, second quantization
•Different boundary conditions: open and periodic systems

CHM1480H *Basic Statistical Mechanics*
(Cross-listed undergrad CHM427H)
Equilibrium statistical mechanics with applications to molecular dynamics; an introduction to nonequilibrium statistical mechanics. Knowledge of the foundations of statistical mechanics and its application to gas phase and liquid phase; familiarity with computer molecular dynamics simulations; understanding the integration of statistical mechanics with classical thermodynamics and quantum mechanics; communication of scientific ideas and results; basic scientific programming

CHM1481H *Reaction Kinetics and Dynamics*
(Cross-listed undergrad CHM421H)

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*
A tailored course for advanced students with an interest in Experimental Physical Chemistry here in the department. To support your broader research ambitions, we will jointly pursue three aims: 1) develop and demonstrate your knowledge of the fundamentals of optics & light-matter interactions 2) build, or extend, your familiarity with scientific writing and computational data analysis 3) introduce you to selected topics in nonlinear, near-field, ultrafast, and quantum optics as they relate to experimental spectroscopy.

CHM1485H *Selected Topics in Chemical Physics*
Selected topics of current research interest in Chemical Physics not covered in the core curriculum.

CHM1488H *Advanced Experimental Methods*
This course will provide a hands-on introduction to this subject using a combined guided and open-ended approach. In particular, the course will:
1) Discuss important fundamental principles and techniques commonly used in experimental physical chemistry/chemical physics;
2) Provide practice exercises (take-home kits with fundamental electro-optical components, an Arduino microcontroller, and an introduction to programming and data acquisition); and
3) Provide guidance and an opportunity to design and conduct your own experiment. The course content will be split 50:50 between electronics and optics/experimental design, combining physical principles and experimental methods + apparatus to solve interesting and useful problems.

CHM1490Y *Physical Chemistry Seminar*