## **CHEM 401-0 Principles of Organic Chemistry**

An accelerated one quarter course in organic chemistry (without laboratory) intended for graduate students in chemistry and related fields needing a working knowledge of the principles of organic chemistry. Topics include structure and reactions of organic molecules and an introduction to the strategy of organic synthesis. These topics approximately parallel those covered in Chemistry 212-1,2. This course may also be appropriate for graduate students or advanced undergraduates in other fields of science and engineering having little or no prior course work in organic chemistry. This course is not appropriate for Northwestern undergraduates who have completed Chemistry 210-1,2 or 212-1,2. Registration by Chemistry Department placement or by permission of the instructor only.

# **CHEM 402** Principles of Inorganic Chemistry

This course covers basic concepts in Inorganic Chemistry and is intended for first-year graduate students. It is designed to introduce students in key subjects which are used over and over again in chemistry and uses inorganic chemistry systems to illustrate the concepts. The course covers the donor-acceptor concept, hard-soft acids-bases, advanced concepts of basicity and acidity and acid-base view of salvation phenomena. The course also delves into introductory solid state chemistry including unit cells and the structure of simple solids, structure types and electronic structure and Band Theory (with the aim of understanding properties). A certain fraction of the time is also devoted to descriptive chemistry which utilizes the concepts learned in the first part of the course and the focus is generally on main group chemistry. This includes the chemistry of hydrogen and the chemistry of the elements of Group 12, 13, 14, 15 and 16. Registration by Chemistry Department placement or by permission of the instructor only.

### **CHEM 403-0 Principles of Physical Chemistry**

This course is a brief survey of the main topics in physical chemistry, quantum mechanics, thermodynamics, statistical thermodynamics, and kinetics. The course is intended for first-year graduate students in Chemistry. Consent of the instructor is required for undergraduate students and graduate students in other departments. Registration by Chemistry Department placement or by permission of the instructor only.

### **CHEM 405-0 Chemistry of Life Processes**

In this topics class we will cover the chemistry involved in various biological processes. Topics may include intracellular signaling and signaling pathways, ligand-receptor interactions, post-translational modifications, molecular probe design for biological targets, glycobiology, molecular imaging techniques and translation science. In the second half of the class, students will learn how to prepare, present and evaluate NIH R01 style research proposals.

### **CHEM 406-0 Environmental Chemistry**

This course covers advanced concepts in physical chemistry of the climate system and geochemical environments, emphasizes critical reading of the current subject literature, and focuses on formulating scientific hypotheses and proposals that are then evaluated and ranked in peer-to-peer based mock grant review panels following NSF merit review criteria.

#### **CHEM 407-0 Materials and Nanochemistry**

This course introduces first year graduate students and seniors in chemistry to the field of materials and nanotechnology focusing on synthetic methods to create materials and nanostructures with specific functions. Following an introduction that defines "materials" and "nanoscience", the course covers specific synthetic strategies and methodologies. The first topic covered is polymerization chemistry, starting with basic principles followed by the most advanced methods known to synthesize polymers such as living free radical reactions, ring opening methathesis polymerization, recombinant DNA synthesis of polymers, and supramolecular noncovalent polymers. This is followed by topics in self-assembly of materials and nanostructures including liquid crystals, gels, self-assembly of amphiphiles, self-assembling monolayers, layer-by-layer assemblies, and colloidal crystals. The last third of the course covers chemical synthesis of ceramics, and synthesis of nanomaterials such as quantum dots, metal nanoparticles, graphene, and carbon nanotubes.

## CHEM 408-0 Design, Synthesis, and Applications of Nanomaterials

Approaches to the rationale, physical and chemical synthesis, assembly and characterization of controlled dimensionality materials including metals, semiconductors, oxides, polymers, and mesoporous scaffolds. Topics will include interfacial phenomena and particle stability, nano-forms of carbon, and applications-driven material design.

## **CHEM 410-0 Physical Organic Chemistry**

This course will focus on modern topics in physical organic chemistry, while emphasizing the relationship between structure and reactivity. Topics to be covered are molecular orbital theory, orbital symmetry and reactivity, stereoelectronic effects, transition state theory, electron transfer, free energy relationships, nucleophilic and electrophilic reactivity, kinetic isotope effects, and basic photochemistry.

### CHEM 411-0 Organic Spectroscopy

### NO DESCRIPTION AVAILABLE

### **CHEM 412-0 Organic Reaction Mechanisms**

Elucidation of organic and organometallic reaction mechanisms: experiment, theory, and selected case studies.

### **CHEM 413-0 Organic Reactions**

Strategies and tactics involved in complex target synthesis. Modern reaction classes as applied to chemical synthesis, coupled to in-depth discussion of the underlying key principles of synthesis design and execution, are covered in the class. Students will gain experience in problem solving, creative thinking, structural analysis and writing techniques.

### CHEM 415-0 Medicinal Chemistry: the Organic Chemistry of Drug Design and Action

This is a survey course designed to show how organic chemistry plays a major role in the design, development, and action of drugs. Although concepts of biology, biochemistry, pharmacy, physiology, and pharmacology will be discussed, it is principally an organic chemistry course with the emphasis on physical interactions and chemical reactions and their mechanisms as applied to biological systems. We will see how drugs are discovered and developed; how they get to their site of action; what happens when they reach the site of action in their interaction with receptors, enzymes, and DNA; how resistance occurs; how the body gets rid of drugs, and what a medicinal chemist can do to avoid having the body eliminate them before they have produced their desired effect. The approaches discussed are those used in the pharmaceutical industry and elsewhere for the discovery of new drugs.

## CHEM 415-0 Bio-Organic Chemistry

The aim of this course is to make students familiar with the recent developments in the field of chemical biology. This is a relatively new field of science that transcends the areas of chemistry, biology, and drug discovery. The major dogma in this field is to use principles of chemistry to provide answers to fundamental questions in biology and human medicine. Particular emphasis in this field is placed on designing drug-like molecules (precursors to FDA drugs) and chemical reaction and use those molecules/reactions to study basic biological processes. These approaches are particularly powerful in the cases when standard biological techniques such as gene-knock out and RNAi to study biology do not work. The knowledge obtained during these studies is then directly translated into the drug discovery process, to produce new human medicines. The course introduces students into a wide variety of experimental techniques and control experiments using in the area of chemical biology. This course is suited for graduate students, as well as undergraduate students majoring in chemistry, chemical and biological engineering, biomedical engineering, and biology.

### CHEM 415-0 Advanced Organic Chemistry

The emergence of the mechanical bond during the past 25 years is giving chemistry a fillip in more ways than one. While its arrival on the scene is already impacting materials science and molecular nanotechnology, it is also providing a new lease of life to chemical synthesis where mechanical bond formation occurs as a consequence of the all-important templation orchestrated by molecular recognition and self-assembly processes. The way in which covalent bond formation activates noncovalent bonding interactions, switching on molecular recognition that leads to self-assembly and the template-directed synthesis of mechanically interlocked molecules of which the so-called catenanes and rotaxanes may be regarded as the prototypeshas introduced a level of integration into chemical synthesis that has not previously been attained. The challenge now is to carry this level of integration beyond relatively small molecules into the realms of precisely functionalized extended molecular structures and aggregated superstructures that perform functions in a collective manner as the key sources of instruction, activation and performance in multi-component integrated devices. In this course I will propose the adoption of the term mechanostereochemistry to describe the rapidly emerging area of chemical science where components of molecules and extended structures are mechanically interlocked or sterically encumbered in such a manner that the components interact dynamically with one another as a result of a panoply of weak noncovalent bonds and/or as a consequence of dynamic coordinative or covalent bonds. Mechanostereochemistry is the stereochemistry of molecules with mechanical bonds. The practice of mechanostereochemistry can be seen to have both a creative aspect (molecular recognition, self-assembly, templation, etc.) and a functional role (relative movements of

components, switching, self-energizing, etc.) associated with its territory. Both the creative aspect and the functional role are dynamic in nature and ultimately molecular in context. The conundrum facing the wider chemical community at present is to unravel how to get from relatively small, yet highly programmable molecules to contraptions and gadgets that do something useful in the real world. Suggested Reading : "Big and Little Meccano" Tetrahedron 2008, 64, 8231-8263.

# CHEM 416-0 Practical Training in Chemical Biology Methods and Experimental Design

By the end of this course you will expected to have obtained a general understanding of many commonly used measurement techniques available to augment research at Northwestern. It features two weeks of classroom-based instruction on experimental design and analysis; supplemented by NIH Rigor And Reproducibility Training Modules. This overview will be followed by a combination of lectures and labs addressing a broad range of analytical techniques and imaging methods. These lessons will then be applied to inquiry-based learning in Northwestern's advanced instrumentation cores. In addition to lecture, students are expected to devise two Mini-Research Projects and will work on one of these with senior staff to apply specific services and protocols utilizing instrumentation available within Research Cores and University Centers. Students will design specific experiments in selected areas of their interest, and learn new sample preparation methods and instrumentation within one of the following areas: mass spectrometry; proteomics, in vivo and molecular imaging, small molecule synthesis and purification; high-throughput screening, x-ray crystallography, and analysis of bioelements. Material generated in the class counts for course credit will be usable in research group settings.

## CHEM 419-0 Advanced Organic Synthesis - Concepts and Applications

The design of synthetic routes to natural products and other medicinally relevant organic compounds will be covered in detail. Retrosynthetic analysis, substructure keying, and pattern recognition, along with other methods for synthetic planning will be discussed within the context of specific case studies. Classic and modern organic reactions, including asymmetric synthesis and catalysis, will be introduced and their application in synthetic planning examined. Case studies will include the synthesis of terpenes, alkaloids, polyketides, steroids, proteins and pharmaceuticals. The end result should be that students are familiar with the important issues associated with synthesis and gain intimate knowledge of a wide variety of chemical reactions. Ultimately, when presented with a given molecule, students should be able to develop a reasonable synthesis plan based on firm ideas and reliable transformations.

### CHEM 432-0 X-Ray Crystallography

This class focuses on structure determination by X-Ray Crystallography. The course will include lectures on crystallographic theory and practice as well as hands-on experience with instrumentation and structure solution and refinement software. Students will be asked to provide single-crystal samples from their own research or from their research groups for in-class analysis.

### CHEM 433-0 Structural Inorganic Chemistry

Chemical applications of group theory and the determination of inorganic and organic molecular and extended structures by modern physical techniques.

## **CHEM 434-0 Inorganic Chemistry**

This course will be focused on magnetism and electronic structure of transition metal complexes. By the end of the course students will learn how to acquire and interpret magnetic data for transition metal complexes. The primary focus of the course will be molecular species.

## CHEM 435-0 Advanced Inorganic Chemistry: Chemical Structure and Bonding

This purpose of this course is to present a number of topics that highlight the influence of electronic structure in coordination compounds on determining molecular and solid-state structure, bonding, reactivity, and magnetic behavior. Of particular focus are topics not commonly covered in upper-division undergraduate inorganic courses, especially those relevant to areas of active chemical research. Much of the content and examples will be taken directly from the primary chemistry literature. The first approximately 60% of the course will be comprised of lectures, with the remainder involving short critical literature review student presentations.

# CHEM 435-0 Advanced Inorganic Chemistry: Chemistry of Alternate Energy (co-listed as) CHEM 445-0 Advanced Physical Chemistry: Chemistry of Alternate Energy

The course will cover fundamental aspects of light-to-electrical energy conversion, light-to-chemical energy conversion, molecular hydrogen as a potentially renewable fuel source, carbon dioxide capture and transformation, and related concepts, chiefly from a chemistry and materials perspective. Emphasis will be placed on promising emerging science and technology, including that associated with organic photovoltaics, solid-state dye cells, and photo-catalytic and electro-catalytic materials for water splitting. Depending on interest, other topics such as thermoelectrics, thermal-solar water splitting, biofuels, or redox flow batteries and other electrical energy storage technologies may be discussed. The course will be taught at the beginning-graduate-student/upper-level-undergraduate-student level.

# CHEM 442-1 Quantum Chemistry

Preliminaries

Motivation

Concepts:

Measurement & the uncertainly principle

- The superposition principle
- The dual wave/particle nature of matter and light
- Waves in classical mechanics
- A physically motivated introduction to the Schrodinger approach
- <u>Quantum Theory</u> Postulates of the quantum theory Operator algebra The time-independent Schrodinger equation Time-dependent superposition states Dirac's approach
- <u>Applications</u>
   Tunneling through a barrier
   Field ionization of atoms
   Scanning tunneling microscopy

Tunneling in chemistry **Diatomic molecules** Separation of the center-of-mass and internal modes Rotations in a 2D world Rotor on a surface: STM-induced rotation in DCCD/Cu Rotations in 3D & Angular momentum within the Schrodinger picture Molecular vibrations The harmonic oscillator model (within Dirac's approach) Anharmonic vibrations Time-independent perturbation theory Numerical solution of eigenvalue problems The correspondence principle in the context of the harmonic oscillator Vibrational wavepackets Pump-probe experiments in vibrational wavepackets Vibrational dephasing, vibrational revivals A brief introduction to polyatomic molecules **One-electron atoms** The Schrodinger equation, eigenstates and frequency-resolved spectra (a brief review) Electronic wavepackets and the classical limit Two-electron atoms Variational methods Angular momentum within Dirac's approach The electron spin The Stern-Gerlach experiment Current Directions and Open Questions Schroedinger's cat The Einstein-Podolsky-Rosen Paradox Bell's Theorem Quantum Erasure

\*\*Review of relevant topics in mathematics will be provided in the first few of weekly exercises.

### CHEM 442-2 Quantum Chemistry

This course covers time dependent quantum mechanics and its application to the interaction of radiation and matter, to scattering theory and to time-dependent spectroscopy.

### **CHEM 443-0 Kinetics**

This course will be focused on a practical approach to chemical kinetics and dynamics. It begins with basic rate laws and moves to rate laws for complex reactions, temperature dependence of reaction rates, a discussion of potential energy surfaces for reaction, models for reactions in the gas phase and solution and a development of the theory of unimolecular reactions, and finally partition functions and transition state theory. If time allows we will also cover catalytic reactions.

#### **CHEM 444-0 Elementary Statistical Mechanics**

Topics: (1) Thermodynamics, Fundamentals (2) Foundations: Microcanonical, canonical, and generalized ensembles (3) Theory of Phase Transitions (4) Equilibrium and Stability (5) Non-interacting systems (6) Ising Model (7) Fluctuation Dissipation

#### **CHEM 445-0 Analytical Chemistry**

Principles and applications of analytical methods, with emphasis on advanced separation science, dynamic electrochemistry, and advanced mass spectrometry.

### CHEM 445-0 Advanced Physical Chemistry: Modern Spectroscopy

#### NO DESCRIPTION AVAILABLE

#### **CHEM 448-0 Computational Chemistry**

The aim of this course is to study the application of modern computer technology, in combination with theoretical chemistry methods, to molecular problems. Each student is expected to complete a series of seven assignments that require the use of electronic structure, molecular mechanics and molecular dynamics methods. There is no final exam but rather a final project (on a topic of the student's choice) that is reported in the form of a short oral presentation to the class and a written summary.