Graduate Courses – Spring 2014 - Chemistry

523    Dennis Liotta       TT        11:30-12:45
Advanced Organic Chemistry III
This course is designed to complete the four semester graduate organic chemistry sequence which also includes Chem 521, 522 and 524. The material covered in this course requires a thorough knowledge of physical organic chemistry, basic structural theory, organic reactions, stereochemistry, and spectroscopy. The course focuses on modern concepts and strategies for the synthesis of a broad range of organic compounds including natural and non-natural products.

524    Lanny Liebeskind    MW        8:30-9:45
Spectroscopy in Organic Chemistry
Chemistry 524 is a problem-solving course in spectroscopic and spectrometric techniques used for the structural characterization of organic compounds. Methods to be studied include nuclear magnetic resonance spectroscopy (1H, 13C, 2D), infrared spectroscopy, ultraviolet / visible spectroscopy, and mass spectrometry. A major part of the course will be focused on problem-solving techniques, including the integrated application of spectroscopic and spectrometry techniques to determine structures of polyfunctionalized organic compounds.
Prerequisites: Chem 221 and 222 or equivalent (one full year of introductory organic chemistry); Chem 521 is highly recommended.
Recent textbook used: Organic Structure Analysis, 2nd edition, by Crews, Rodriguez, Jaspars

532    Francesco Evangelista TT        10:00-11:15
Advanced Physical Chemistry II (Modern Techniques in Computational and Theoretical Chemistry)
This course will familiarize students with a variety of methods for current applications of quantum and classical mechanics to problems in chemistry and chemical physics. A significant portion of the course will focus on the numerical methods and software used in real applications and topics will range from electronic structure of "small molecules" to the molecular dynamics and vibrations of biomolecules using empirical force fields.

534    Susanna Widicus Weaver MW        10:00-11:15
Advanced Physical Chemistry IV (Molecular Spectroscopy)
This course will examine the principles that govern the interactions of atoms and molecules with electromagnetic radiation. The topics covered will include rotational, vibrational and electronic spectroscopy. For each sub-topic we will examine the quantum mechanical energy level structures associated with the atoms or molecules, and the spectra that arise from transitions between stationary states. Familiarity with basic quantum mechanics and perturbation theory is assumed. This course will be of value to students working in both experimental and theoretical research areas.
Chemistry 536 covers the statistical theory that underlies thermodynamics, and how that statistical theory can be applied in simulating of systems of molecules at thermal equilibrium. Through computer simulation exercises, students will gain basic skills in using molecular simulation software.

Textbook:
Understanding Molecular Simulation, Second Edition: From Algorithms to Applications by Daan Frenkel and Berend Smit

Advanced Inorganic Chemistry II: Physical Methods
Content: The central goal of bioinorganic chemistry is to elucidate the structures and reactivities of metal centers within biomolecules. The physical methods used to explore the nature of the metal environment within a biomolecule have been critical to progress in this field. This course will explore the fundamentals of physical methods and their specific applications to problems in bioinorganic chemistry, including electronic absorbance and emission, infrared, Raman, CD, MCD, EPR and X-Ray absorption spectroscopies. Students will be evaluated on the basis of problem sets, examinations and a class presentation.

Text: Physical Methods in Bioinorganic Chemistry (Que), University Science Books; in addition, suggested background texts include: Spectroscopic Methods in Bioinorganic Chemistry (Solomon) and Biological Inorganic Chemistry (Bertini, Gray, Stiefel, Valentine).

Advanced Inorganic Chemistry III: Kinetics and Mechanism
This course focuses on the mechanisms of inorganic and organometallic reactions. The course provides both intellectual background and practical methods required for effective research in this area and in condensed phase reaction mechanisms in general. The methods to be covered include kinetics, product distribution, pertinent spectroscopic studies and the use of modern software for data processing. The subjects to be covered include determination of association stoichiometry and binding constants, rate laws, activation parameters and other features of complex mechanisms. The convergence of experimental and theoretical mechanisms and pitfalls in the study of reactions will be addressed.

Advanced Biophysical Chemistry
This course covers advanced topics in biophysical chemistry that focus on structural analysis of native and synthetic biomolecular assemblies.
Directed Study Library Course
This course is required for all first year graduate students and BS/MS students in the Chemistry Department. It is designed to provide the new students with the information and skills needed to function efficiently and effectively in the use of library services and resources during the pursuit of their graduate program of study and research at Emory. It will be offered as a series of seminars at the beginning of Fall and Spring Semesters. During Spring Semester the ACS Style Guide, peer review, and instructor-led consultations will be used to facilitate and provide guidelines in scientific writing of a faculty sponsored research topic paper. Students will receive one credit for the course; a grade of pass/fail will be issued at the end of second semester.

599R: Thesis Research

752: John Bacsa
Structure Determination
The course will cover theoretical crystallography: symmetry elements, crystallographic point groups, the unit cell, Bravais lattices and space groups. The theory of crystal diffraction. The course will also cover the practical methods of the determination of crystal structures from X-ray data including growing crystals, the experimental techniques involved in collecting X-ray data and using software to process the data. Solving and refining a crystal structure with background theory: structure factors, the phase problem and electron densities. Powder diffraction will also be covered. Dealing with and treating twinned crystals. Technical details of X-ray instruments: X-ray generators and the 3-circle goniometer. Discussion of applied interests in different aspects of crystallography and solid state chemistry with an emphasis on structure-property relationships, chemical bonding, shapes of molecules and inorganic structures.

791R: BioMolecular Seminar
792R: Inorganic Seminar
793R: Organic Seminar
794R: Physical Seminar
799R: Advanced Research