Ph.D. in CHEMISTRY
Program code: 0420

INTRODUCTION

The Department of Chemistry (College of Science) offers a Ph.D. program in **Chemistry.** A graduate successfully completing this program will be expected to have an in-depth knowledge in specific areas of Chemistry. In addition, he/she would be trained to become an independent thinker, planner and executor of specific ideas relevant to Chemistry. A major part of the program is the dissertation, which requires high quality research in a specific area of Chemistry.

PROGRAM REQUIREMENTS

15 TOTAL COURSE CREDITS

9 COMPULSORY (3 credits each)

0420-620 Advanced Topics in Physical Chemistry
0420-641 Selected Topics in Advanced Inorganic and Analytical Chemistry
0420-651 Advanced Organic Chemistry -II

6 ELECTIVES* (3 Credits each)

0420-611 Catalytic Chemistry
0420-621 Thermo Chemistry of Solids
0420-622 Colloid and Surface Chemistry
0420-623 Photo-Electrochemistry & Solar Energy Conversion
0420-625 Structure and Bonding
0420-626 Molecular Modeling
0420-627 Corrosion and Protection of Metallic Materials
0420-628 Surfactant Science
0420-642 Bio-Inorganic Chemistry
0420-643 Advanced Chemistry of Coordination Compounds and Homogeneous Catalysis
0420-644 Physical Methods and Data Analysis in Inorganic Chemistry
0420-652 Non-Thermal Reactions in Organic Chemistry
0420-653 Advances in Organic Synthesis

* Students may substitute up to 3 credit hours from the (500 level) graduate courses offered by the Department of Chemistry and which has not been previously studied by the student.

NC COMPULSORY

0420-697 Dissertation (0)
0420-698 Dissertation (0)
0420-699 Dissertation (0)

COURSE DESCRIPTION

0420-611: CATALYTIC CHEMISTRY
CR: 3

Catalysis in solution: Acid-base catalysis by electron transfer, organometallic catalysis, catalysis by macromolecules, phase transfer catalysis, and catalysis by micelles.

Catalysis by enzymes: Composition and structure of enzymes, reactions catalyzed by enzymes, nature of catalytic sites, and supported enzyme catalysts.

Catalysis by polymers: The nature of polymers, catalysis by polymer gels, kinetics of polymer-catalyzed reactions, bi-functional and multi-functional catalysis, porous polymers and surface catalysis, and applications of polymer catalysts.

Catalysis in molecular-scale cavities: Structure of crystalline solids, structure of zeolites, families of zeolites, adsorption and diffusion in zeolites, the solvent-like nature of zeolite pores, catalysis by zeolites. Catalysis on surfaces: surface structure, adsorption, surface catalysis, industrial catalysis, and catalytic surfaces.

0420-620: ADVANCED TOPICS IN PHYSICAL CHEMISTRY
CR: 3

Chemical Kenetics, quantum Chemistry, electrochemistry, colloid and surface chemistry, molecular spectroscopy, macromolecular chemistry, nanoparticles and nanotechnology, and other topics.

0420-621: THERMOCHEMISTRY OF SOLIDS
CR: 3

Heterogeneous equilibria: Generalization of equilibrium conditions, thermodynamic properties of substances, energy balance, thermodynamics of phase changes and chemical reactions, and thermodynamics of interfaces. Study of equilibrium states by methods of thermal analysis: Calorimetric measurements, measurements of other thermo-physical properties, direct investigations of equilibria (condensed state, solid-gas equilibra, solid-liquid equilibra), and calculation of standard enthalphy changes of phase transitions from phase diagrams. Theory of kinetics and mechanism of solid state heterogeneous processes: Types of processes, activated state concept, homogeneous-like descriptions of heterogeneous processes, physico-geometrical description of heterogeneous processes, and molecular description of heterogeneous processes Study of kinetics under non-isothermal conditions: Fundamental problems, methods of kinetic data evaluation, study cases, kinetic parameters by differential thermal measurements.

0420-622: COLLOID AND SURFACE CHEMISTRY
CR: 3

1. The Colloidal State: Classification of colloidal systems, structural characteristics, preparation and purification of colloidal systems.
2. Kinetic properties: Brownian motion, osmotic pressure.
3. Optical Properties: Optical and electron microscope, light scattering.
4. Surfaces and interfaces: General concepts: surface free energy, the molecular nature of interfacial region, the Gibbs surface energy, adsorption, the Gibbs adsorption equation.
5. Liquid-gas and liquid-liquid interfaces: Surface and interfacial tension. orientation at interfaces, surfactant and the reduction of surface tension, micelle formation, spreading, mono-molecular films.
6. Charged interfaces: The electric double layer, electro-kinetic phenomena and electro-kinetic theory.
7. Colloidal stability: DLVO theory, reversible flocculation and secondary minimum, kinetic of coagulation, steric stabilization. depletion flocculation,. solvent effects in steric stabilization.
8. Rheology: Viscosity, non-Newtonian flow viscoelasticity.
9. Emulsions: Formation and stability, surfactants, emulsion type. The Hydrophilic-Lipophilic Balance (HLB),. multiple emulsions, microemulsion.
10. Foams

11. Industrial importance of colloids: Medical and pharmaceutical. applications in food industry, cosmetic emulsion.

0420-623: PHOTO-ELECTROCHEMISTRY & SOLAR ENERGY CONVERSION
CR: 3

Introduction: The sun: ultimate origin of most of the energy available, heat energy wind-hydroelectric power. fossil fuels, radioactivity, sun model.

Semiconductors: Origin of semi-conductivity, types of semiconductors, mechanism of excitation, temperature effects. Photo effects, examples and problems.

Photovoltaic effects: The p-n junction, current transport phenomena, forward current, reverse saturation current, the junction photovoltatic, electronic model, mechanism of energy conversion.

Schottky barrier solar cells: SIS, SIM cells, SnO solar cells, principle of operation, current transport, improvement of the characteristics for practical applications.

Spectral responsivity of the photocurrent: Maximum theoretical efficiency of a solar cell, solar arrays and systems, examples and problems.

Semiconductor electrochemistry: Semiconductor/electrolyte interface, energy barrier and redox potentials, principle of photoelectrochemical energy conversion.

Photoelectrochemical cells: Different types, applications.

Photoelectrochemical semiconductors: Advantages and disadvantages of photoelectrochemical cells, corrosion of semiconductors, stabilization of semiconductors, applied systems.

0420-625: STRUCTURE AND BONDING
CR: 3

Introduction to atomic structure and molecular properties and Valence bond theory; the molecular orbital theory of electronic structures and the spectroscopic properties of diatomic molecule; electronic structures; photoelectronic spectroscopy and frontier molecular orbital theory of reactions of polyatomic molecules; bonding in solids and liquids; correlation diagram; walsh diagram (triatomics); Polyatomic molecules: Huckel theory, Woodward-Hoffman rules, Bond theory of solids; insulators and semiconductors.

0420-626: MOLECULAR MODELING
CR: 3

Building and Visualizing molecules; building small and large molecules and coordination complexes; Molecular geometry and properties; bond length and angles; electron affinity; structure stability relationship; molecular orbitals and bonding; formation of MO; Walsh diagram; Jahn-Teller Effect; conformational analysis; small and large conformation analysis; inversion barrier in ammonia; thermodynamics; heat of formation; combustion; hydrogen bonding; steric effects tautomerism; resonance energy; charge distribution; dipole moment, charge transfer and excited states; spectroscopy, UV, vibrational spectra; solvent effects n spectra; molecular dynamics; stability or carbocations; conformation searches; stimulated annealing; langevin dynamics and intramolecular vibration.

0420-627: CORROSION AND PROTECTION OF METALLIC MATERIALS
CR: 3

Electrochemical equilibria, free energy calculations, phase diagrams, grain boundaries, inclusion, crystal structure, diffusion in solids, electrical double layer, thermodynamics and kinetics of electrode reactions.

0420-628: SURFACTANT SCIENCE
CR: 3

Micellization and surfactants absorption at interfaces; liquid crystals, emulsion and microemulsions; thin films and foams; Rheology of surfactant solutions; Self-assemblies as templates for nanoparticles and porous materials; characterization of self-assembles systems; Industrial applications; relevant legislation.

0420-641: SELECTED TOPICS IN ADVANCED INORGANIC AND ANALYTICAL CHEMISTRY
CR: 3

Part (I) Inorganic Chemistry

1. Solid state chemistry
2. Mechanism of inorganic reactions.
3. Chemical crystallography
4. Organometallic Chemistry
5. Advanced inorganic spectroscopy
6. Advanced magnetochemistry

Part (II) Analytical Chemistry

1. Analytical spectroscopy
2. Electrochemical methods
3. Separation methods

0420-642: BIO-INORGANIC CHEMISTRY
CR: 3

1. The identification of the functions of metal ions and main groups compounds in biological systems. The chemistry of model and isolated biological compounds.
2. Study of metalloproteins and other metal-containing biological molecules.
3. The tradition metals in biological redox reactions.
4. Nitrogen fixation.
5. The biochemistry of iron.
6. Metal ions and chelating agents in medicine

0420-643: ADVANCED CHEMISTRY OF COORDINATION COMPOUNDS AND HOMOGENEOUS CATALYSIS
CR: 3

Part (I)

1. Review of the chemistry of transition and inner transition elements.
2. Theories of bonding.
3. Structure and reactivity
4. Coordination compounds in biological systems.

Part (II)

1. Theories
2. Homogeneous and heterogeneous catalysis
3. Recent developments

0420-644: PHYSICAL METHODS AND DATA ANALYSIS IN INORGANIC CHEMISTRY
CR: 3

Part (I)

1. Physical methods in inorganic chemistry.
2. Nuclear magnetic renounce. Mossbauer effect, optical rotary dispersion and circular dichorism, electron paramagnetic resonance, nuclear quadruple resonance and photoelectron spectroscopy.
3. Theoretical principles and applications of physical methods relevant to characterization and organomaetallic compounds.

Part (II)

The application of mathematical and statistical techniques to chemical measurements. These applications include the theory of single detection, filtering and smoothing, curve fitting, uni-and multi-component calibration and analysis.

0420-651: ADVANCED ORGANIC CHEMISTRY - II
CR: 3

Specific and general acid and base catalysis. Enzyme mimics and catalysis. Stereoelectronic effects. Treatment of steric effects. T.S. recognition and molecular recognition processes. Physical organic chemistry of macromolecular systems and supermolecular assemblies. Structure/reactivity correlation analysis with emphasis on LFER. Interpretation of isotope effects. Non-catalytic thermal gas-phase free radical and molecular processes. Organic reactions involving carbocations. carbanions, and radical cations and anions; tautomerism; resonance energy; charge; charge distribution.

0420-652: NON-THERMAL REACTIONS IN ORGANIC CHEMISTRY
CR: 3

1. Photochemistry
2. Sonochemistry
3. Biotransformations

0420-653: ADVANCES IN ORGANIC SYNTHESIS
CR: 3

1. Organometallics in Synthesis
2. Free radicals in organic chemistry
3. Asymmetric synthesis
4. Classical and modern natural products total synthesis.
5. Computer assisted routes to organic synthesis

0420-697: DISSERTATION
CR: 0

0420-698: DISSERTATION
CR: 0

0420-699: DISSERTATION
CR: 0