SHIV NADAR UNIVERSITY

Prospectus Ph.D. Program Chemistry

Department of Chemistry
School of Natural Sciences
Shiv Nadar University
Post office Shiv Nadar University
Gautam Buddha Nagar
UP-201314

The Ph.D. program in chemistry at SNU consists of a rigorous regimen of both broad-based and in-depth course work, development of project proposals, research and literature seminars, in-depth dissertation research under the supervision of a research advisor, and a public thesis defense.

SNU also offers a comprehensive and unique Master's program in Cheminformatics and Bioinformatics, launched in 2013. Students for this program are drawn from the fields of Chemistry, Biology, Computer Science and Statistics. Foundation courses in the first semester ensure that all students, irrespective of undergraduate specialization, possess the requisite background to complete the course of study and benefit fully from the program. The estimated demand for around 8000 bioinformatics professionals in India indicates good job opportunities for high quality graduates. Both Bioinformatics and Cheminformatics offer good career opportunities, in industry as well as in academia, in developed markets abroad such as the US and Europe - the major employers being: industries from biotechnology, agribiotech, pharmaceutical; IT industries working towards providing solutions to life Sciences, biotechnology and health-care sectors; as well as R&D institutes and academia.

Chemistry Research at SNU

Opportunities for research in chemistry at SNU are available under the guidance of our faculty (from Chemistry and the Center for Informatics) in the following broad areas:

- Bioorganic Chemistry – B. K. Sarma, G. Roy
- Chemical Biology – G. Roy, P. Munshi
- Supramolecular Chemistry – D. Ray
- Chemical & Biological Crystallography – P. Munshi, S. Sukumar
- Chemical Library Design & Screening – S. Sen, B. K. Sarma, N. Sukumar
- Cheminformatics – N. Sukumar, V. K. Jayaraman
- Chemistry of Nanomaterials – B. Lochab
- Diversity Oriented Synthesis – S. Sen, R. Sagar
- Environmental Chemistry – S. Bhandari
- Green Chemistry – B. Lochab, S. Sukumar
- Medicinal Chemistry – R. Sagar, S. Sen, B. K. Sarma, G. Roy
- Organometallic Chemistry – S. Bhandari, D. Ray
- Polymer Chemistry – BimleshLochab

- Quantum Chemistry – N. Sukumar, V. Kumar
- Structural Chemistry – P. Munshi, S. Sukumar
- Synthetic Organic Chemistry – S. Sen, R. Sagar, B. Lochab

Chemistry Post-graduate Course Catalog

CHY501: **Medicinal Chemistry** (3 credits: 2 Lec + 1 Tute) Monsoon

The objectives of the course are to give synthetic chemists, biochemists and pharmacologists a broad and balanced introduction to the background, general principle, concepts and tools of medicinal chemistry. The course will also highlight the new understanding of the factors governing modern drug discovery. Case histories of drug discovery will be explained with particular examples along with their biochemistry, pharmacology and toxicology, drug metabolism and disposition. Modern preclinical drug research is thus the focus of the course, which combines lectures, tutorials and practical work. This course will cover the following main topics:

- Introduction to Medicinal Chemistry
- Biological Mechanisms
- Pharmacokinetics and Drug Metabolism
- Screening of New Compounds
- Molecular Biology in Medicinal Chemistry
- Exploiting a Chemical Lead
- Combinatorial Chemistry and Molecular Diversity
- Case Histories of Drug Discovery
- Toxicology in Drug Discovery
- Pharmaceutical Considerations in Drug Development
- Structure-guided Drug Design
- Diversity oriented synthesis (DOS)
- Fragment based drug design (FBDD)
- Physical Properties and Quantitative Structure-Activity Relationships
- Hints and Tips in Medicinal Chemistry

[Course required of all Organic/Chem/Bioinformatics students]

CHY 502: **Synthetic Organic Chemistry** (3 credits) Monsoon

1) Organic Synthesis and Structure
    a. Mechanism,
    b. Applicability and limitations of the major reactions in organic synthesis.
    c. Stereochemical control in synthesis.
2) New Synthetic Reactions and Catalysts
    a. Recent highlights of new synthetic reactions and catalysts for efficient organic synthesis.
    b. Mechanistic details as well as future possibilities will be discussed.
3) Tactics of Organic Synthesis
    a. A dissection of the most important syntheses of complex natural and unnatural products.
    b. Synthesis, planning and methodology.
    c. The logic of synthesis.
    d. Biogenesis.

[Course required of all Organic/Medicinal/Polymer Chemistry students]

CHY 503: **Chemistry of Glycoconjugates** (3 Credits) Spring

Introduction of glycocongugates, Structure and function of Glycoproteins, proteoglycans and glycosaminoglycans; Glycopeptides. glyco-amino-acids and glycosyl-amino-acids and Peptidoglycans. Inter- and intra-cellular communication and “Glycocode”, The need for homogeneity and pure, well-defined conjugates. Glycocongugate assembly and vaccine development.

CHY512: **Advanced Molecular Spectroscopy** (4 credits: 3 Lec + 3-hr.Lab) Monsoon

This course and the associated lab deal with deal with the foundations and applications of Molecular Spectroscopy.

- Group theory
  - Theorems of linear algebra
  - Time-independent and time-dependent perturbation theory
  - Discrete and Continuous Groups, Group multiplication tables, Generators
  - Symmetry Elements, Symmetry Operations and Point Groups
  - Reducible and Irreducible Representations, Great Orthogonality Theorem and Character Tables
  - Projection Operators and symmetry-adapted linear combinations
  - Selection Rules for Molecular Spectroscopy
  - Electron Density, Structure Factor, Density Matrix, Density Operator and Bloch equations
- Molecular Spectroscopy
  - Microwave spectroscopy
  - IR spectroscopy of organic molecules
  - Raman Spectroscopy
  - Atomic and molecular spectroscopy
  - UV-Vis spectroscopy of organic molecules
  - Detection of functional groups of organic molecules by IR spectroscopy
  - UV-Vis Spectroscopy of various Organic Molecules
  - NMR spectroscopy
  - Mass spectrometry
  - Moessbauer spectroscopy

[Core course required of all Ph.D. students]

CHY522: **Informatics and Drug Discovery** (4 credits: 3 Lec + 3-hr.Lab) Spring

This course and the associated computer lab deal with Bioinformatics and Cheminformatics, applied to the search for new drugs with specific physiological effects (*in silico* Drug Discovery). Students will learn the general principles of structure-activity relationship modeling, docking & scoring, homology modeling, statistical learning methods and advanced data analysis. They will gain familiarity with software for structure-based and ligand-based drug discovery. Some coding and scripting will be required. At the end of the course, students will be expected to present a completed piece of software of significant utility and/or an analysis of experimental data from the published literature. Students will be encouraged to seek avenues for publication of their most significant results. Syllabus:

1. ***Introduction***
   - Drug Discovery in the Information-rich age
   - Introduction to Pattern recognition and Machine Learning
   - Supervised and unsupervised learning paradigms and examples
   - Applications potential of Machine learning in Chem- & Bioinformatics
   - Introduction to Classification and Regression methods, and types of classification and regression: KNN and Linear Discriminant analysis

2. *Representation of Chemical and Biochemical Structures*

- Drug Discovery in the Information-rich age
- Sequence Descriptors
- Text mining
- Representations of Molecular Structures
- Characterizing 2D structures with Descriptors and Fingerprints
- Searching 2D Chemical Databases
- Chemical File Formats and SMARTS
- Topological Indices
- Substructural Descriptors
- Molecular Fingerprints
- Physicochemical Descriptors
- Descriptors from Biological Assays
- Representation and characterization of 3D Molecular Structures
- Calculation of Structure Descriptors
- Pharmacophores
- Molecular Interaction Field Based Models
- Local Molecular Surface Property Descriptors
- Quantum Chemical Descriptors
- Shape Descriptors
- Protein Shape Comparisons
- 3D Motif Models
- Representation of Chemical Reactions and Databases

3. *Analysis and Visualization*

- Molecular Similarity Analysis
- Molecular Quantum Similarity Measures
- Cluster and Diversity analysis
- Network graphs from Molecular Similarity
- 3D visualization tools
- Self-Organized Maps
- Semantic technologies and Linked Data

4. *Mapping Structure to Response: Predictive Modeling*

- Linear Free Energy Relationships
- Quantitative Structure-Activity Relationships (QSAR) Modeling
- Ligand-Based and Structure-Based Virtual High Throughput Screening
- 3D Methods - Pharmacophore Modeling and alignment
- ADMET Models
- Activity Cliffs
- Structure Based Methods, docking and scoring
- Site Similarity Approaches and Chemogenomics
- Model Domain of Applicability assessment

5. ***Data Mining and Statistical Methods***

- Linear and Non-Linear Models
- Feature selection
- Partial Least-Squares Regression
- Introduction to Neural Nets, Bayesian Methods and Kernel Methods
- Support vector machines classification and regression and application to chemo & bioinformatics (*3 lectures*)
- Random forest Principal Component analysis and SVD (*1 lecture*)
- Data preprocessing and different performance measures in Classification & Regression (*1 lecture*)
- Introduction to evolutionary computing (*1 lecture*)
- Data Fusion
- Model Validation
- Interpretation of Statistical Models
- Best Practices in Predictive Cheminformatics

[Course required of all Chem/Bioinformatics students]

CHY 542: **Nano molecular Chemistry** (2 Credits)

This course will deal with the basic understanding of the atomic and electronic structures of different nanomaterials such as clusters and nanoparticles of inorganic materials (metals and semiconductors), fullerenes, nanotubes, nanowires, and two dimensional systems such as graphene. Aspects related to optical, magnetic and vibrational properties of nanomaterials as well as the development of nanomaterials will be covered.

CHY 543: **Supramolecular Chemistry** (2 Credits)

This course will help to understand the basic concept of supramolecular chemistry (non-covalent interactions) and their quantification in molecular recognition process. This course will cover the area of non-covalent interaction, multiple hydrogen bonding (H-B) stems, self-assembly, acyclic receptors for neutral and charged guests, macrocycles and macrobicycle, cryptands and macropolycycles, cyclodextrin.

CHY 545: **Fundamentals of Crystallography**(3 credits: 2 Lec + 2-hr.Lab) Spring
Crystallography in combination with X-ray or neutron diffraction yields a wealth of three-dimensional structural information unobtainable through other methods. The course has been designed to give an overview of crystallography, in general. This basic course will cover the topics such as symmetry in crystallography, crystals systems, Bravais lattices, crystal symmetry, crystallographic point groups and space groups, Miller indices, theory of X-ray diffraction, data collection, data reduction, structure factors and Fourier syntheses, electron density, phase problem, direct methods, Patterson method, crystal structure refinement etc. The course will also highlight the application of single crystal and powder X-ray diffraction techniques and will include hands on training on crystal growth, mounting, structure solution, refinement and analysis. Further, training on the use of database for structural search will also be provided.

- **Introduction**
  Introduction on Crystallography and discussion on course structure
- **Crystallographic Symmetry**

Concept of 1D and 2D symmetry and lattices, notations of symmetry elements, space groups in 2D, 3D lattices, 32 point groups and their notations, stereographic projections, Laue symmetry; glide planes, screw axes and their notations, space groups, equivalent points, space group symmetry diagrams etc. Miller Indices, crystallographic planes and directions, close pack structures, linear density, planar density, Miller-Bravais indices for hexagonal systems.

- **Theory of X-ray diffraction**

  What is X-ray, generation and classification of X-ray, X-ray sources, diffraction of X-rays, Bragg's law, the reciprocal lattice, reciprocal relationship, Bragg's law in reciprocal space, Ewald's sphere, Laue Method, Oscillation, rotation and precession methods.

- **Data reduction**

  L-P corrections, structure factor, scaling, interpretation of intensity data, temperature factor, symmetry from intensity statistics, structure factor and Fourier synthesis, Friedel's law; exponential, vector and general forms of structure factor, determination of systematic absences for various symmetry or lattice centering, FFT, Anomalous scattering.

- **The Phase Problem**

  Definition, Direct Methods, structure invariants and semi invariants, probability methods, Phase determination in practice, Patterson Methods, Patterson Symmetry, completion of structure solution, ΔF synthesis.

- **Refinement of Crystal Structures**

  Refinement by Fourier synthesis, refinement by ΔF synthesis, Refinement by least squares method, weighting functions, Goodness-Of-Fit (GOF) parameter, treatment of non-hydrogen atoms, and treatment of hydrogen atoms.

- **Powder X-ray diffraction (PXRD)**

  Methodology, geometrical basis of powder X-ray diffraction, applications of PXRD (determination of accurate lattice parameters, identification of new/unknown phases, applications in pharmaceutical industry, structure solution from PXRD etc.), Reitveld method for structure refinement, indexing of PXRD, handling of PXRD using DASH.

- **Neutron and Electron Diffraction**

  Basics of neutron, synchrotron and electron diffraction and their applications.

- **Practical**

  Crystal growth, selection, indexing of crystals, data collection, data reduction, space group determination and structure refinement using SHELXS97, SIR and SHELXL97, introduction to International Tables for Crystallography and crystallographic packages (e.g. WinGx, PLATON, OLEX-2), IUCr validation of the structure and use of Cambridge Structural Database for structural search.

[Course required of all Inorganic/Organic Chemistry students]

CHY 551: **Advanced Chemical Biology** (3 Credits)

Mechanistic chemistry and biology, chemical and enzymatic methods for construction of nucleic acids, oligopeptides and proteins. Bimolecular interactions: protein-nucleic acid, protein-small molecule, protein-protein, Nucleic acid and small molecule and their mechanism; Chemical glycomics and biophysical techniques. Carbohydrate and protein signalling in living system, mechanism and their application.

CHY 552: **Polymer Chemistry and its Scope** (3 Credits) Monsoon

How do changing demands in society lead to polymer invention? How are monomers bonded in nature to form our body's building blocks? How do scientists mimic nature in labs? How does the several-fold change in molecular weight from monomer to polymer result in different sets of properties? Most of the polymeric materials around us are synthesized in different ways, depending upon end usage. This course will help the students to understand the need and importance of polymers in today's world. Interesting chemical aspects of synthesis of polymeric architectures from small molecules will be explored. Course Outline:

1. Introduction to Polymers

Nomenclature, Classification, Molecular weight, Physical state, Applications

2. Step Growth Polymerization

Polyamide, Polyesters, Polycarbonates, Phenolic polymers, Epoxy resins, Polyethers, Polyurea, Polyurethanes, Carother's equation

3. Chain Growth Polymerization

Free Radical polymerization: Initiators, Inhibitors and retarders, Mechanism, Kinetics and Thermodynamics, Polymerization processes (Bulk, Solution, Suspension, Emulsion), Copolymers

Ionic polymerization

Cationic and Anionic Polymerization: Mechanism, Ring Opening Polymerization (ROP)

Controlled/Living polymerizations: ATRP (Atom Transfer Radical Polymerization), RAFT (Reversible Addition Fragmentation Chain Transfer), GTP (Group Transfer Polymerization), Ziegler Natta Polymerization, Metathesis

4. Specialty Polymers

Conducting Polymers, Liquid Crystal Polymers, Organometallic Polymers, Green Polymers and their applications

5. Polymer Characterization (Molecular weight determination)

Number average molar mass, End group assay, Colligative Properties of Solutions, Osmometry, Light scattering (Dynamic Light Scattering), Viscometry, Gel Permeation Chromatography, MALDI (Matrix Assisted Laser Desorption/Ionization)

6. Polymers in Life

*Proteins:*Synthesis of amino acids and their reactions, Test reactions, Zwitter ion, Isoelectric point and Electrophoresis. Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides by N-terminal and C–terminal analysis. Synthesis of peptides by N-protection & C-activating groups, Merrifield solid-phase synthesis.

Nucleic acids: Nucleosides and Nucleotides, ATP (energy storage and release), Mechanism of Phosphoryl Transfer Reactions, Composition of nucleic acids. Different types of DNA and RNA, Biosynthesis of DNA, m-RNA and proteins, Determining base sequence of DNA, Lab synthesis of DNA fragments, Polymerase Chain Reaction (PCR).

CHY 553: **Coordination and Bio-Inorganic Chemistry** (2 Credits)

Metals ions play important role in many biological processes. Their function can range from simple structural roles in which they hold a protein in a specific conformation, to more complex roles in which they are involve in multiple electron transfer processes and in bond cleavage and formation. Understanding of the biological functions of metal ions lies at the heart of bio-inorganic chemistry. This course will focus on the biologically important metal ions and their binding sites, and the techniques used to probe these sites (e.g.IR, UV-VIS, NMR, EPR, Mossbauer and CV). A more in-depth look at several key metalloenzymes and the functional role of the metal ions therein will also be taken**.**

CHY 554: **Green chemistry and Sustainability** (3 Credits) Spring

Since a decade, scientific community especially chemistry has been mobilized to develop new chemistries that are less hazardous to human health and the environment. Several steps were taken to protect both the nature and maintain ecological balance. But still such an effort is in nascent stage. Are we really protecting earth? Are we utilizing nature's sources wisely? What are the hazards associated with one wrong step…and with several such steps? We are surrounded by chemistry since we wake up in morning till we sleep in night such as toothpaste, soap, cloth, perfume, medicine, plastic furniture, shoes etc. For those of us who have been given the capacity to understand chemistry and practice it as our day to day life, it is and should be expected that we should use it in a sustainable manner. With knowledge comes the burden of responsibility. We should not enjoy this luxury with ignorance and cannot turn a blind eye to the effects of the science in which we are engaged. We have to work hard and put brain waves together to develop new chemistries that are more benign, and safer to mother earth!!

1. **Green chemistry** Lessons from past for a better future: Need, Limitations and Opportunities. Principles of Green Chemistry and their illustrations with examples: Scales of measurement such as Atom efficiency, E factors etc., homo vs. heterocatalysis, reaction efficiency, toxicity reduction etc.
2. **Green reactions:** Green alternatives of starting materials, non-risky reagents, benign solvents (Aqueous medium, Ionic liquids, Supercritical fluids, Solvent free reactions, Flourous phase reactions), and reaction conditions (*Nonconventional energy sources***:** Microwave assisted reaction, Ultrasound assisted reactions, Photochemical reactions), catalysis (heterogeneous catalysis, biocatalysis, phase-transfer catalysis), Replacement of Non-Green reactions with Green reactions (Real/Award cases)
3. **Safety for sustainable environment:** Hazards assessment and mitigation in chemical industry
4. **Future trends in Green Chemistry:** Green analytical methods, Redox reagents, Green catalysts; Green nano-synthesis, Green polymer chemistry, Exploring nature, Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solvent-less reactions; Non-covalent derivatization, Biomass conversion, emission control.

CHY 555: **Synthetic Biology** (2 Credits) [cross-listed with Life Sciences]

Introduction to Synthetic Biology; Synthetic Biology for Biosynthetic Chemistry; Synthetic Biology work, *e.g*. Artemisinin production; A practical approach of biological devices; Synthetic Biology of stem cells; Advanced System and Synthetic Biology;

CHY 557: **Intelligent Materials for Medicine** (3 credits)Spring

Recent advances in field of medicine have resulted in designing and development of large number of novel synthetic architectures for target drug delivery in order to revolutionize the treatment and prevention of disease. Advanced drug delivery and targeting can offer significant advantages to conventional drugs, such as increased efficiency, safety for drug delivery, convenience. However, such potential is severely compromised by significant obstacles to delivery of these drugs in vivo. These obstacles are often so great that effective drug delivery and targeting is now recognized as the key to effective development of many therapeutics. This course will provide a comprehensive introduction to the vehicles for drug delivery, principles of advanced drug delivery and targeting, their current applications and potential future developments.

CHY 600: **Research Methodology** (3 credits) Monsoon

1. **Quantitative Methods:**
   This module will deal with Data handling and Data Analysis, the elements of Quantitative Logic, including Hypothesis testing, Weight of Evidence, and Domain of Applicability estimation.

2. **Research Literature and Seminar:**
This part of the course will be conducted as a Journal Club. Each week one student will be expected to read and summarize a research paper from the recent literature in an area outside their immediate domain of research. The student will familiarize himself/herself with the background necessary to understand the research paper, and will be expected to critically analyze the work and to answer questions from other students and from the faculty moderator(s). Also covered: the research process - meaning of research, objectives, motivation, types; method vs. methodology, scientific and research method, and detailed description of the research process.

3. **Grantsmanship:**
This module will deal with identification of a research problem, formulation of a testable hypothesis and design of experiments to address the question. Strategies for writing a fundable research proposal will be discussed, with particular emphasis on the Specific Aims, and succinctly conveying the significance of the problem to both technical and non-technical readership. Students will refine both writing and presentation skills during this module. Experts will be invited from funding agencies like DBT, DST, ICMR and Wellcome Trust/DBT Alliance to provide recent updates and guidelines for grant submission (as part of an yearly mini-symposium).

[Core course required of all Ph.D. students]

CHY 615: **Graduate Seminar** (1 credit)

Faculty members from the department (and possibly beyond) present seminars about their areas of interest, the proposed research in their respective groups and the experimental (or computational) techniques used in their field. Students will be expected to participate actively in these seminars by asking questions. This module serves to introduce new students to the possibilities for research, preparatory to selection of their research advisors.

CHY 622: **Computational Chemistry** (3 credits: 2 Lec + 2-hr.Lab) Spring

- Classical Force Field Methods; Molecular Mechanics
- Postulates of Quantum Mechanics and measurement
- The Born-Oppenheimer approximation and the Molecular Hamiltonian
- The Concept of the Potential Energy Surface
- Semiempirical and *ab initio* Quantum Mechanics
- Variation and Perturbation Theory
- Independent-Particle Models: the Hartree method
- Spin and statistics in non-relativistic quantum mechanics
- The Hartree-Fock Self-Consistent Field equations
- Basis Sets and Relativistic Pseudopotentials
- Geometry Optimization Techniques
- Valence Bond Methods
- Electron Correlation Methods
- Density Functional Theory
- Configuration Interaction
- Density Matrices and Natural Orbitals
- Diagrammatic Methods: Coupled Cluster Theory
- Wave Function Analysis
- Computation of Molecular Properties
- Periodic systems and theory of Insulators
- Basis Set Superposition Error and the Counterpoise method

- Introduction to Classical Statistical Mechanics
- Continuum (Implicit) solvent and Explicit solvent methods
- Protein Simulations
- QM/MM and ONIOM methods

[Course required of all Physical Chemistry students]