TIFR HYDERABAD
CHEMISTRY SUBJECT BOARD – Course work for Integrated M.Sc. – Ph.D.

CORE COURSES		
Course Code	**Name of the Course**	**Credits**
CHM-101.7	Mathematical Methods (for Chemistry)	4
CHM-104.7	Quantum Mechanics – I	4
CHM-111.7	Organic Chemistry	4
CHM-115.7	Chemistry of Main group elements and organometallic Chemistry	4
CHM-120.7	Biochemistry	4

ELECTIVE COURSES		
Course Code	**Name of the Course**	**Credits**
CHM-110.7	Statistical Mechanics – I	4
CHM-113.7	Spectroscopy of atoms and molecules	4
CHM-114.7	Basic Chemistry of Transition and Lanthanide Metal Ions	4
CHM-116.7	Numerical Methods and Algorithms in Chemistry Physics	4
CHM-118.7	Biophysics	4
CHM-200.7	Principles of NMR Spectroscopy	4
CHM-210.7	Physics and Chemistry of materials: Bulk to Nano	4
CHM-214.7	Advanced Topics in Organic Chemistry and Inorganic Chemistry	4
CHM-215.7	Molecular and nonlinear dynamics	4
CHM-216.7	Protein structure and synthesis	4
CHM-217.7	Solid State NMR	4
CHM-219.7	Advanced Mathematics	4
CHM-220.7	Electronic structure theory of matters	4
CHM-222.7	Molecular Dynamics Simulation and application in chemical physics	4
CHM-224.7	Chemistry of Materials Based on p-Block Elements	4
CHM-225.7	Organic and Perovskite materials	4
CHM-253.7	NMR Instrumentation	2
CHM-255.7	Introduction to Data Science	2
CHM-211.7 / PHY-206.7	Advanced Quantum Mechanics / Quantum Mechanics – II	4
CHM-212.7 / BIO-101.7	Basic Cell Biology	4
CHM-213.7 / BIO-202.7	Fluorescence Methods in Cellular Biophysics	4
CHM-223.7 / PHY-325.7	Polymer Physics & Soft Matter	4
CHM-119.7 / BIO-205.7	Biological Thermodynamics	4
CHM-218.7 / BIO-203.7	Mechanobiology	4
CHM-121.7 / BIO-208.7	Chemical Biology I	4
CHM-221.7 / PHY-417.7	Magnetism	4
CHM-300.7 / PHY-418.7	Quantum Thermodynamics	4
PHY-215.7	Error Analysis and Statistical Inference in Experiments	2
CHM-254.7 / PHY-201.7	Computer Programming using Python language	2

TIFR HYDERABAD
CHEMISTRY SUBJECT BOARD – Course work for Ph.D.

CORE COURSES		
Course Code	**Name of the Course**	**Credits**
CHM-101.7	Mathematical Methods (for Chemistry)	4
CHM-104.7	Quantum Mechanics – I	4

ELECTIVE COURSES		
Course Code	**Name of the Course**	**Credits**
CHM-110.7	Statistical Mechanics – I	4
CHM-111.7	Organic Chemistry	4
CHM-112.7	Inorganic Chemistry	4
CHM-113.7	Spectroscopy of atoms and molecules	4
CHM-114.7	Basic Chemistry of Transition and Lanthanide Metal Ions	4
CHM-115.7	Chemistry of Main group elements and organometallic Chemistry	4
CHM-116.7	Numerical Methods and Algorithms in Chemistry Physics	4
CHM-118.7	Biophysics	4
CHM-200.7	Principles of NMR Spectroscopy	4
CHM-210.7	Physics and Chemistry of materials: Bulk to Nano	4
CHM-214.7	Advanced Topics in Organic Chemistry and Inorganic Chemistry	4
CHM-215.7	Molecular and nonlinear dynamics	4
CHM-216.7	Protein structure and synthesis	4
CHM-217.7	Solid State NMR	4
CHM-219.7	Advanced Mathematics	4
CHM-220.7	Electronic structure theory of matters	4
CHM-222.7	Molecular Dynamics Simulation and application in chemical physics	4
CHM-224.7	Chemistry of Materials Based on p-Block Elements	4
CHM-225.7	Organic and Perovskite materials	4
CHM-253.7	NMR Instrumentation	2
CHM-255.7	Introduction to Data Science	2
CHM-211.7 / PHY-206.7	Advanced Quantum Mechanics / Quantum Mechanics – II	4
CHM-212.7 / BIO-101.7	Basic Cell Biology	4
CHM-213.7 / BIO-202.7	Fluorescence Methods in Cellular Biophysics	4
CHM-223.7 / PHY-325.7	Polymer Physics & Soft Matter	4
CHM-119.7 / BIO-205.7	Biological Thermodynamics	4
CHM-218.7 / BIO-203.7	Mechanobiology	4
CHM-120.7 / BIO-107.7	Biochemistry	4
CHM-121.7 / BIO-208.7	Chemical Biology I	4
CHM-221.7 / PHY-417.7	Magnetism	4
CHM-300.7 / PHY-418.7	Quantum Thermodynamics	4
PHY-215.7	Error Analysis and Statistical Inference in Experiments	2
CHM-254.7 / PHY-201.7	Computer Programming using Python language	2

Compulsory Course:

Course Code	Name of the Course	Credits
CHM-100.7	Research Methodology	4

CHM-101.7: Mathematical Methods (for Chemistry))

Syllabus:

- *Determinants and Matrix Algebra*

  Properties of determinants and matrices, Linear transformation, Eigenvector-Eigenvalue problems, Similarity and unitary transformations

- *Differential Equations*

  Separable, Exact, and First-order homogeneous linear differential equations, Sturm-Liouville eigenvalue problem, Legendre polynomials and properties, Spherical harmonics, Bessel equations and properties

- *Vector Algebra*

  Gradient, Divergence, Curl, Gauss and Stokes theorem, Curvilinear coordinates, Tensor analysis

- *Complex Analysis*

  Cauchy-Riemann conditions, Analytic functions, Contour integrals, Taylor and Laurent series, Singularities, Residue theorem, Gamma and Beta function, Method of steepest descent, Stirling series, Asymptotic series, Convergence tests

- *Integral Transforms*

  Fourier series, Fourier transform, Laplace transform, Solution of initial boundary-value problem, Convolution

- *Error Analysis*

Primary Text / Reference Books:

1. Arfken and Weber: Mathematical methods for physicists
2. Mary L Boas: Mathematical methods in physical sciences
3. E. Kreyszig: Advanced engineering mathematics

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):
50% assignments, 25% mid-term exam, 25% end-term exam

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Understand determinants and matrix theory and their applications.
CO 2	Obtain a knowledge of eigenvalue-eigenvector problems and applications.
CO 3	Get insight into rotations and angular momentum operators.
CO 4	Solve first-order and second-order ordinary differential equations.
CO 5	Familiarise with special functions, such as Legendre, Bessel, and Gamma.
CO 6	Work out Fourier series and transforms, Laplace transforms, and some applications.

CO 7	Comprehend complex analysis and solve contour integrals.
CO 8	Work our problems related to error analysis and relevant distributions.

<u>CHM-104.7: Quantum Mechanics-I</u>

Syllabus:

1) Origins: Wave-particle duality: Blackbody radiation, Compton Effect, de Broglie's hypothesis; Heisen-berg's uncertainty principle; Atom models; Waves

2) Representation of states and operators: Linear vector space and Hilbert space; Operators: Her-mitian adjoint, projection, functions of operators, unitary operators, eigenvalues and eigenvectors of an operators; Discrete basis; Continuous basis; Matrix-vs-wave mechanics

3) Postulates of QM: Probability density; Observables; Measurement; Time-evolution; Symmetries; Connection to classical mechanics

4) 1D problems: 1D Schroedinger equation; Free particle; Potential step; Potential barrier and well; Infi-nite square well; Finite square well; Harmonic oscillator; Numerical solution

5) Angular momentum: Orbital angular momentum; Spin angular momentum; Eigenfunctions and ei-genvalues

6) 3D problems: Variable separation; 3D: free particle, box, harmonic oscillators; Spherical coordinates: Central potential, spherical well, isotropic harmonic oscillators, hydrogen atom, effect of magnetic field on central potentials

7) Rotation and addition of angular momentum: Rotations; Addition of angular momentum; Clebsch Gordon coefficients; Tensor operators; Wigner-Eckart theorem

8) Identical particles: Many-particle systems: Permutation symmetry; Identical particles: Exchange de-generacy, symmetrisation, anti-symmetrisation; Pauli-exclusion principle

9) Approximation methods: Time-independent perturbation theory: Degenerate and non-degenerate versions; Variational method; WKB method

10) Introduction to advanced topics: Time-dependent perturbation theory; Scattering theory; Relativistic quantum mechanics: Dirac equation

Required Text 1. *Quantum Mechanics Concepts and Applications,* Nouredine Zettili, Wiley (Edition-2, 2009).

Evaluation Method: Assignment (6x5=30%), closed-book mid-term exam (30%), closed-book final exam (40%).

Course Outcome:

Sr. No.	**On completing the course, the student will be able to:**
CO 1	Understand the foundational aspects of quantum mechanics.
CO 2	Thorough knowledge of Schrodinger and Heisenberg pictures of QM.
CO 3	Comprehend basic spin dynamics and Hamiltonian analysis.
CO 4	Analytically solve various potential-related problems of relevance to molecules.
CO 5	Obtain an insight into perturbation theory and use of that in model calculations.
CO 6	Familiarise with angular momentum and symmetry problems and applications.
CO 7	Tackle various problems that have relevance to Physics and Chemistry research.
CO 8	Get an idea on advanced topics, such as DFT calculations.

CHM-111.7: Organic Chemistry

1. Introduction to organic chemistry: Chemical bonding and molecular structure
   - Why study organic chemistry
   - Localized chemical bonding
     - Hybridization index; Field effect; Inductive effect; Atomic and molecular polarizability; Molecular dipoles and quadrupoles
   - Delocalized chemical bonding
     - Cross conjugation; Homoconjugation; Hyperconjugation; Baker-Nathan effect, Mesomeric effect
   - Aromaticity
     - Hückel 4*n*+2 rule; Biard's rule; Homoaromaticity; Möbius aromaticity; Spherical aromaticity; Annulenes; Azulenes; Fullerenes

2. Conformation and stereochemistry
   - Rotation & rigidity
     - Rotation barriers; Syn-pentane interactions; 1,3-Diaxial interactions; Allylic strain; Baeyer strain; Pitzer strain; Bredt's rule; Anomeric effect
   - Optical activity, symmetry & chirality
     - Origin of optical activity; Symmetry arguments of chirality; Chiral molecules having no asymmetric atom; Chirality due to helical shape; Prochirality
   - Stereoisomers
     - Enantiomers, diastereomers & meso-compounds; Racemic mixture & resolution; Atropisomers; Ansa compounds
     - Topicity
     - Stereochemical descriptors
     - Stereo selectivity & stereo specificity
   - The importance of being asymmetric

3. Organic reactions
   - Elimination and substitution reactions (Reaction rates and activation energy, α-eliminations, β-elimations, S_N1, S_N2 reactions)
   - Addition reactions
   - Oxidations and Reductions
   - Rearrangements
   - Fragmentation
   - Cross-coupling
   - Metathesis

4. Reactive intermediates
   - Carbocations; Carbanions; Carbenes; Carbynes; Radicals
     - Physical properties; Detection methods; Trapping reactive intermediates; Structure; Stability; Reactions involving reactive intermediates

5. Retrosynthetic analysis
   - Planning a synthesis backwards
   - Disconnection approach
     - Retrons; Transforms; Disconnections; Synthons; Strategy algorithm
   - 'Natural reactivity' and 'umpolung'
   - Case studies

6. Concerted organic reactions & organic photochemistry
   - Molecular orbitals of conjugated π-electron systems
   - Conservation of orbital symmetry
   - Pericyclic reactions
     - Electrocyclic reactions; Cycloaddition reactions; Group transfer reactions; Sigmatropic rearrangements
   - The conceptual and mechanistic foundations of photochemistry
   - Survey of basic photochemical processes of organic chemistry
     - Photoisomerization, di-π-methane rearrangement, de Mayo Reaction, Paterno-Büchi reaction, Photoinduced Electron Transfer, Norrish Type I and II

- Photochemistry in everyday life

7. Organic chemistry of Biomolecules
    - Amino acids; Sugars; Lipids
    - Peptides; Proteins; Nucleic acids

Assigned Reading (Textbooks & References):

- 'Organic Chemistry' by Loudon & Parise
- 'Organic Chemistry' by Clayden, Greevs, Warren & Wothers
- 'A Guide Book to Mechanism in Organic Chemistry' by P. Sykes
- 'Stereochemistry of Carbon Compounds' by E. J. Eliel
- 'Frontier Orbitals and Organic Chemical Reactions' by Ian Fleming
- 'Advanced Organic Chemistry' by J. March
- 'Advanced Organic Chemistry (Part A & B)' by Carey & Sundberg
- 'Advanced Organic Chemistry: Reaction Mechanisms' By Reinhard Bruckner
- 'Modern Physical Organic Chemistry' by Eric V. Anslyn and Dennis A. Dougherty

Evaluation:

- Participation in class discussion – 5%
- Four short take-home quizzes – 25%
- On-site written mid-term examination – 30%
- On-site written final examination – 40%

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	understand various aspects of the localized and delocalized chemical bonding and molecular structure of organic molecules.
CO 2	demonstrate a thorough understanding of conformation and stereochemistry of organic molecules, including origin of optical activity, chirality and the importance of being asymmetric.
CO 3	get familiarized with various fundamental organic reactions and associated reactive intermediates.
CO 4	utilize the concept of retrosynthetic analysis for the total synthesis of complex natural products.
CO 5	implement the idea of orbital symmetry to understand concerted thermal and photochemical processes in organic chemistry.
CO 6	gain basic knowledge of organic chemistry of biomolecules involved in life processes, such as Proteins, Sugars and Nucleic acids.
CO 7	apply organic chemistry concepts and reasoning learned in the course to effectively solve problems encountered in experimental Organic Chemistry laboratory in future.

CHM-115.7: Chemistry of Main group elements and organometallic Chemistry

Syllabus:

1. Chemistry of *s*- and *p*-Block Elements (12 lectures)

[a] Periodic trends of main group elements
[b]Chemistry of compounds involving lithium and magnesium: synthesis, structure and reactivity
[c] Chemistry of boron: boranes, bonding of boranes, synthesis and reactivity, boron clusters, carboranes and metallacarboranes
[d] Aluminum and silicon chemistry: synthesis and application

[e] Chemistry of compounds involving magnesium, boron, silicon, aluminum, germanium, tin, and lead: synthesis, structure and reactivity
[f] Chemistry of nitrogen, phosphorus and sulfur (oxides and oxoacids): synthesis, structure and reactivity
[g] Chemistry of halogen, haloacids, interhalogen and polyhalogen compounds
[h] Chemistry of xenon compounds: synthesis, structure and reactivity

2. Organometallic Chemistry (12 lectures)
[a] Chemistry of main group organometallic compounds.
[b] d^n electron counting
[c] Transition metal hydrides, alkyls, aryls, carbonyls, nitrosyls: synthesis, structure and reactivity
[d] Organometallic compounds of π-bound ligands (alkene, alkyne, allyl, diene, cyclopentadienyl, and arenes): synthesis, structure and reactivity
[e] Organometallic reactions involving transition metal complexes: mechanism and their consequence on catalytic process
[f] Syntheses and application of organometallic reagents
[g] Coupling reactions: Kumada coupling, Suzuki-Miyaura coupling, Hiyama coupling, Sonogashira coupling, Negeshi coupling, Stille coupling, Buchwald-Hartwig Coupling, Heck reaction, Click Reactions
[h] Homogeneous catalysis and catalysts: Alkene isomerization, hydrogenation, hydroformylation, Monsanto acetic acid process.
[i] Alkene polymerization, cross coupling reactions, metathesis, C-H activation, and functionalization

Evaluation: Based on 6 assignments (20 % weightage) and two examination, mid-term and final (40 % each).
Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Know the various aspects of *p*-block compounds: novel bonding and reactivity.
CO 2	Know the chemistry of novel gases.
CO 3	Know the chemistry of heavier main-group compounds (synthesis, reactivity, and bonding).
CO 4	Know the organometaliic chemistry: basic fundamental to recent advances.
CO 5	Know the organometaliic chemistry involving organolithium compounds.

CHM-120.7: Biochemistry

Syllabus:

- Components of Life – proteins, nucleotides, carbohydrates, lipids and small molecules (ATP, metals, ions, etc).
- Proteins - amino acids, protein folding and protein structure
- Proteins - Analytical tools to study proteins (UV vis spectroscopy, chromatography, mass spec, sequencing)
- Proteins – protein function (enzymes, structural proteins, antibodies, ion channels, hormones)
- Proteins – Enzymes, ligand binding
- Proteins - Biological oxidation and reduction
- Proteins – Post-translational modifications
- Proteins – GPCRs and chemotaxis
- Nucleotides – Central dogma of life, DNA structure and replication
- Nucleotides – Transcription
- Nucleotides – RNA types, structure and chemistry, ribozyme
- Nucleotides – Translation
- Nucleotides – DNA repair
- Nucleotides – Role of nucleotides in synthesis/chemistry of ATP, GTP, NAD, etc.
- Carbohydrates – Photosynthesis, metabolism
- Carbohydrates – Glycolysis
- Carbohydrates – TCA cycle
- Carbohydrates – Oxidative phosphorylation
- *Buffer for delays in previous lectures*

- (If no delays, then I will teach 'Mutations and Diseases')
- Lipids – Biological membranes, transport of lipids
- Lipids – Metabolism of fatty acids, triglycerides
- Lipids – Membrane fusion and fission
- Special Topics – Virus
- Special Topics – Mitochondria
- Special Topics - *Open for suggestions*
- (my suggestion is Biological Toxins)
- Special Topics - *Open for suggestions*
  (my suggestion is Origins of Life)

Primary Text / Reference Books:

Lehninger Principles of Biochemistry by David Nelson & Michael Cox or Biochemistry by Lubert Stryer

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

Final exam - 35%, Midterm exam – 25%, Write up (summary of review papers) – 20%, Problem sets – 20%

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Get a molecular understanding of biological processes
CO 2	Download, visualize and analyze macromolecular structures using Pymol and Coot
CO 3	Understand various tools to study proteins – SDS PAGE, UV-vis spectroscopy, chromatography, centrifugation, NMR, X-ray crystallography, etc.
CO 4	Learn the atomic-level details of post-translational modification of proteins, redox biology and signal transduction pathways
CO 5	Learn from original research papers and present them succinctly and to write summaries of research papers

<u>CHM-110.7: Statistical Mechanics-I</u>

Syllabus:

Short description: An introduction to statistical mechanics with applications to systems in physics and chemistry.

1. **Brief overview of equilibrium thermodynamics:** Extensive and intensive properties, laws of thermodynamics, entropy and free energy, chemical potential, phase equilibrium (3 lectures)

2. **Ensembles in statistical mechanics:** Phase space density in classical systems and its time evolution, introduction of microcanonical, canonical and grand canonical ensembles, partition functions and connections to thermodynamic variables, fluctuations (5 lectures)

3. **Application of statistical mechanics** to the ideal gas, rotational and vibrational spectra, heat capacity of crystals, non-interacting spin systems, chemical reaction equilibrium (4 lectures)

4. **Statistical mechanics of quantum systems:** Fermi and Bose statistics, ideal Fermi gas and ideal Bose gas, discussion of the classical limit, Fermi gases at low temperature, Bose-Einstein condensation (5 lectures)

5. **Statistical Mechanics of Interacting Systems 1**: The configuration integral, virial expansion, the law of corresponding states (3 lectures)

6. **Statistical mechanics of interacting systems 2**: Correlation functions and relation to thermodynamic functions, radial distribution function in simple liquids, correlation functions in magnets (4 lectures)

7. **Computer simulation of statistical systems:** Introduction to Monte Carlo and molecular dynamics, case studies (3 lectures)

Mode of Evaluation: 4 or more assignments, 2 exams (1 mid term and 1 end term)

CHM-113.7: Spectroscopy of atoms and molecules

Syllabus:

(1) Interaction of radiation with matter:

Blackbody radiation, absorption and emission of radiation (semi – classical description)
Einstein coefficients, relaxation phenomena
Review of time – dependent perturbation theory
Transition probabilities and spectral line shapes
Coherent excitation and density matrix approach

(2) Molecular symmetry and group theory:

Symmetry operations, introduction to point groups
Review of linear algebra, matrix representation of groups
Quantum mechanics and group theory, selected applications for molecular spectroscopy

(3) Atomic spectroscopy:

One electron systems, many electron systems, selection rules
Zeeman and Stark effect

(4) Molecular spectroscopy:

Rotational spectroscopy of diatomic and linear molecules, asymmetric tops
Vibrational spectroscopy of diatomic and polyatomic molecules
Symmetry and normal modes
Light scattering and Raman spectroscopy
Electronic spectroscopy of diatomic and polyatomic molecules
Case studies: Spectroscopy of specific systems such as NO, CO_2 etc.

(5) Spectroscopic Instrumentation and introduction to nonlinear spectroscopy and optics:

Spectrograph, monochromator and interferometers, detection of light
Lasers as spectroscopic light sources
Introduction to nonlinear spectroscopy techniques
Introduction to nonlinear optical mixing techniques, phase matching, quasi – phase matching, sum/difference frequency and higher harmonic generation, optical parametric oscillators

Primary Text / Reference Books:

1)Molecular quantum mechanics, Atkins P. W. and Friedman R.
(2)Spectra of atoms and molecules, Bernath P. F.
(3)Molecular Spectra and Molecular Structure, Herzberg G.
(4)Laser Spectroscopy, Demtroder W.

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):
25% Mid term exam(s) + 25% Special reading topic + 50% Final Exam

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Understand basic models describing interaction of radiation and matter (classical and semiclassical)
CO 2	Understand the fundamentals of symmetry and group theory in the context of molecular structure and spectroscopy
CO 3	Understand molecular rotations, vibrations and electronic energy level structure and spectra
CO 4	Appreciate the experimantal tools needed for high resolution spectroscopy experiments
CO 5	Use of spectroscopic databases to extract the necessary information to estimate molecular structural properties and simulate molecular spectra

CHM-114.7: Basic Chemistry of Transition and Lanthanide Metal Ions

a) Shapes of molecules, models of bonding in chemistry, symmetry, point groups, character tables [4]

b) Ligands, Coordination compounds, Isomerism and Structure, Crystal and Ligand Field Theories. Molecular Orbital Theory of Coordination Complexes. [6]

c) Electronic spectroscopy of Coordination Complexes. Term symbols. L-S coupling. Orgel and Tanabe-Sugano diagrams. Magnetism in Coordination Complexes. Spin-cross over systems.[4]

d) New applications of Coordination Chemistry: Metal-organic frame works, Ligand-directed self-assembly of coordination complexes. Organic reactions in cages of metal complexes. [4]

e) Lanthanide complexes. f-orbital shapes and consequences. Electronic spectroscopy and photoluminescence aided by energy transfer from ligands, Organolanthanides and catalysis [5]

f) Supramolecular Chemistry: Principles and examples, Molecular Machines [4]

Course Evaluation

1. 1 Mid-sem exam: Duration 2h. Value: 100 Marks
2. 1 End-sem exam: Duration 3h. Value: 150 Marks
3. 3 Surprise quizes 30 min duration. Value: 60 Marks
4. Seminar Presentations (30 min duration) on a topic assigned by the instructor: 40 Marks
5. Assignments: 6-8. Only meant for practice not for evaluation purpose.

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Judge the point group symmetry of molecules and apply the principles of symmetry to chemical problems.
CO 2	Know about the various theories of bonding of transition metal complexes.
CO 3	Acquire knowledge of the electronic transions of transition metal complexes.
CO 4	Know about the magnetic properties of transition metal complexes.
CO 5	Know about metal-carbon bonds and basic knowledge about organometallic complexes.
CO 6	Know about catalytic reactions and the role of organometallic complexes in homogeneous catalysis.
CO 7	Acquire knowledge about lanthanide complexes and why crystal field does not perturb the lanthanide ions.

CHM-116.7: Numerical Methods and Algorithms in Chemistry Physics

Syllabus:

1) Python: Writing/running codes: Editors, Ipython; modules, matplotlib, numpy

2) Linear Equations: Gaussian elimination, LU decomposition, Direct/Iterative methods

3) Curve Fitting: Least squares fitting, polynomial interpolation, splines

4) Root finding: Graphical, bisection, Newton-Raphson

5)Numerical Differentiation: Finite difference; Error analysis

6) Numerical Integration: Newton-Cotes formulae, Romberg/Gaussian integration, Multiple integrals

7) Initial Value Problems: Euler/Runge-Ku<a methods; Stability and Stiffness

8) Boundary Value Problems: Shooting Method

9) Symmetric Matrix Eigenvalue Problems: Jacobi rotations, Power/inverse power method, Tridiagonal form

10) Minimization/Optimiztion: 1-D problems, N-D problems, Powell's method, Simplex method

11) Application to Chemical Physics: Molecular thermodynamics (Ideas, harmonic oscillator, rigid rotor partition functions), Equation of states, Schroedinger equation of Hydrogen molecule cation, Hartree Fock for He atom, Linear variational problems in Quantum mechanics (1D potentials, Tunneling prob-lems), Potential energy surface fitting, Time-dependent Schroedinger equation.

12) Optional Topic: Krylov Subspace Techniques, Lanczos iteration

Required Text 1. *Numerical Methods in Engineering with Python 3,* Jaan Kiusalaas, Cambridge university Press (2013).

Evaluation Method: Quizzes based on assignment (4x10%), closed-book mid-term exam (30%), closed-book final exam (30%).

CHM-118.7: Biophysics

Thermodynamics, kinetics and statistics in biophysics (Refresher): A refresher on the basic concepts in thermodynamics and kinetics and the tools for statistical analysis in biophysics. This will also cover basic concepts in enzyme kinetics such as Michaelis-Menten and Hill equations, analysis of co-operativity, mechanisms of inhibition, etc using case studies and simulations.

Polymer statistics and intrinsically disordered proteins, Introduction to polymer chain properties: defining radius of gyration, end-to-end distances, entropy etc. Intrinsically disordered proteins: Definition of disorder**,** Types of IDPs**,** Functions of IDPs**,** Diseases associated with IDPs

Single Molecule Biophysics: Introduction to fluorescence, FRET and smFRET, Optical tweezers, Motor proteins, Super resolution microscopy

Basic Techniques: In depth analysis of centrifugation, chromatography, calorimetry and optical spectroscopy techniques with case studies.

Metabolomics: Introduction to the use of metabolomics using NMR and Mass spectrometry to elucidate biochemical pathways and function of proteins

Biophysics of membranes: Introduction to biological membranes, lipids, lipid protein interactions, phase transitions, membrane mimetics for biophysical studies

Channels, carriers and pumps: Introduction to passive and active transport across membrane, mechanisms of transport.

Primary Text / Reference Books:

- Fluorescence—Lackowicz,
- Advances in Chemical Physics, Volume 146:
- Single Molecule Biophysics, Single-Molecule Cellular Biophysics---Leake
- Polymer physics by Colby & Rubenstein,
- Intrinsically disordered proteins by Tompa
- Channels, carriers and pumps, Stein and Litman
- Bioenergetics, Nicholls and Fergusson

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

Assignments/Quizzes	50
Midterm	20
Final	30

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Understand the principles of techniques based on fluoroscence spectroscopy and their applications to single molecule biophysics
CO 2	Understand the basics of polymer physics and its relation to biophysical problems such as protein folding and aggregation
CO 3	Develop an in-depth knowledege of aspects of enzyme function in terms of kinetic and thermodynamics parameters, and concepts such as bioenergetics, kinetic models of enzyme function, cooperativity, etc.
CO 4	Develop a working knowledge of techniques such as ITC, SPR, etc. that can be used to experimentally probe enzyme function, inhibition, activation, etc, as well as techniques in to study metabolomics.
CO 5	Develop a basic understanding of simulating complex systems using simple ODEs, as well as stochastic simulations using techniques such as a the Gillispie algorithm.
CO 6	Develp a basic understanding of membrane biophysics, with introduction to membrane transporters
CO 7	Review and critique research articles pertinant to the above topics

CHM-200.7: Principles of NMR Spectroscopy

Syllabus:

The goal of the course is to introduce one to NMR spectroscopy, so that one can understand standard solution state experiments and also follow the literature. No knowledge of NMR spectroscopy is assumed.

The following topics will be covered:

Bloch Equations, Review of Quantum Mechanics, Angular momentum, Hamiltonians in NMR, Multiple spins, Energy levels, Different basis sets, Density matrix formalism, Pulsed NMR, Fourier Transform, Line shape/width, phasing, Ernst Angle, Hahn Echoes, Studying diffusion, Finite Pulses, INEPT, 2D NMR: J resolved, COSY etc, Adiabatic pulses, Basic Solids: Pake Pattern, Magic Angle Spinning, Basics of relaxation, measuring T1, T2 etc, Solomon equations, NOESY, Chemical Exchange, Multi Quantum Spectroscopy, DQF COSY, Coherence Selection: Phase Cycling/Gradients, INADEQUATE Experiment, Product Operators. Hahn echo, Average Hamiltonian theory, Decoupling, Basic Hetero nuclear experiments HSQC, HMQC, CT-HSQC etc, Water Suppression, Protein NMR: Triple resonance, Deuteration etc. Amide/Methyl TROSY, Residual Dipolar Couplings

Primary Text / Reference Books:

1) Levitt: Spin Dynamics (2nd Edition), Wiley 2008 (ML)
2) Keeler: Understanding NMR Spectroscopy (2nd Edition), Wiley 2010 (JK)
3) Goldman: Quantum Description of High-Resolution NMR, Oxford, 1988 (MG)
4) Harris: Nuclear Magnetic Resonance Spectroscopy, Longman Scientific, 1986 (RH)
5) Cavanagh et al.: Protein NMR Spectroscopy (2nd Edition), Elsevier. 2006 (PNS)
6) Any Quantum Mechanics textbook, (For example: Shankar) (QM)
7) Slichter: Principles of Magnetic Resonance 3rd Edition Springer (CS)
8) Ernst, Bodenhausen, Wokum: Principles of Nuclear Magnetic Resonance in One and Two Dimensions, Oxford (EBW)

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

Midterm:	**30**	
Paper:	**20**	Present a summary on one recent NMR paper. (Paper should be selected in consultation with the instructor.)
Final:	**50**	

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Understand the basics of NMR spectroscopy
CO 2	Will become familiar with various techniques and tricks used in the modern NMR experiments.
CO 3	Will be able to understand how various modern solution NMR experiments work.
CO 4	Should be able to understand modern solution NMR literature.

CHM-210.7: Physics and Chemistry of materials: Bulk to Nano

Syllabus:

- Introduction to semiconductors: Metal, Semiconductor and Insulator, Formation of Energy bands, carrier concentration and transport phenomena, electrochemical potential & Fermi-Dirac statistics, metal-semiconductor contacts (ohmic & Schottky). P-N junction characteristics, Transistors-Uni polar and bi-polar, Metal-oxide-semiconductor characteristics, MOSFETs. Scaling down effects – properties at the nano-scale: change in density of states due to confinement. (12 hours)

- Introduction to magnetism: Classifications - dia, para, ferro and anti-ferromagnetism. Domain wall theory,Magnetic anisotropy, exchange interactions, Introduction to meanfield approximation, periodic table of magnetic materials, magnons, and demagnetization factor, Size effects in magnetism. (12 hours)

- Nano-materials & nano-probes : Synthesis of nanomaterials - top-down & bottom-up approaches, characterization tools - optical and electron spectroscopy & microscopy, and mechanical analysis, introduction to electrochemistry. (10 hours)

- Nanofabrication & Nano-devices: Basics of fabrication techniques: photo-lithography, Ebeam lithography, etching techniques. Nano-devices–molecular electronics, resonant tunneling devices, single electron transistors. (8 hours)

- **Extra-components:** Guest lectures, Lab tour & Student presentations (covering important characterization methods / device physics)

Primary Text / Reference Books:

1. Introduction to Solid State Physics: Charles Kittel
2. Physics of Semiconductor devices, S. M. Sze
3. Introduction to Magnetic materials, B. D. Cullity
4. Introduction to Nanotechnology, Charles P. Poole, From J. Owens
5. Electrochemical methods: Fundamental & applications: Allen J. Bard, Larry R. Faulkner.

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

- Four assignments and two examinations (closed book).
- Two students' presentations (each student/group).

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Basics of semiconductor physics, energy dispersion diagram of different classes of materials.
CO 2	Understanding of exciton physics, charge tranport and separation in heterostructured semiconductors.

CO 3	Basics of device physics and lithography techniques.
CO 4	Fundametanls of magnetism and atomistic origin of magnetism in materials and its finite size effects.
CO 5	Introduction to different materials characterisation tools: spectroscopy, microscopy, electrochemical and electronic transport assisted analyses.

CHM-214.7: Advanced Topics in Organic Chemistry and Inorganic Chemistry

First and Second Row Main Group Elements emphasizing with their low oxidation states: 6 lectures

Activation of Hydrogen by Lewis pairs, Hydrogenation and Dehydrogenation reactions (catalytic-non catalytic) involving main group reagents. Boryl Lithium, Borylene, Boron based nucleophile and Lewis Base. Classical and Non Classical Carbocation synthesis and structure, Bonding of C2 molecule, Hyper coordinated carbon and some unusual carbon based systems including carbenes.

Heavier (3rd Row Elements and Beyond) Main Group Elements: 6 lectures

Mg(I) Compound. Mg(I) as a Reducing Reagents. Chemistry of compounds involving Low Valent Low- coordinate Aluminum, Silicon, Germanium, Tin, Lead, Phosphorous, Arsenic, Antimony, and Bismuth. Bonding description of disilenes and disilynes and its comparison with alkenes and alkynes.

Recent Advances in Transition Metals: 4 lectures

Compounds involving metal metal bonding (including zinc) and its reactivity. Transition metal hydrides and fluorides. Some aspects of transition metals in bio inorganic chemistry.

New Strategy for the Installation of Organic Functional Group and Recent Trends in Organic Synthesis: 8 lectures

Application of Halonium ions (including fluoronium ion) in organic chemistry, Cascade reactions, Flow reactions, Selective oxidation-reductions involving recent developed reagents, application of boron and silicon compounds for selective functionalization, Modern approach (without protection and deprotection of functional group strategy) for natural product synthesis.

Primary Text / Reference Books:

Most of the material for this course will be accessed from primary literature viz., Journal Articles.
Some text books that will be followed are as follows:

1. F.A. Cotton, A. M, Carlos, M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Edition 2001.
2. Clayden, Greeves, Warren, and Wothers, Organic Chemistry, 1st ed, 2001
3. W. Kaim, B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons Inc., 1994.
4. E. J. Corey, X-M. Cheng, The logic of chemical synthesis, John-Wiley & Sons, New York. 1989.
5. V. Ya. Lee, A. Sekiguchi, Organometallic Compounds of Low-Coordinate Si, Ge, Sn and Pb: From Phantom Species to Stable Compounds. John Wiley and Sons, Ltd., 2010.

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):
Mid-Sem & End-Sem Examination + 6 Assignments

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Know the recent advances in fundamental developemental of synthetic organic chemistry.
CO 2	Know the recent advances in fundamental development of synthetic inorganic chemistry.
CO 3	Know the recent advances in the development (synthesis and potential applications) of new class of compounds.

CO 4	Know the novel strategy for the synthesis of uncommon compounds.
CO 5	Know the unprecedented reactivities of *p*-block compouns which are mimics with transition metal complexes.

CHM-215.7: Molecular and nonlinear dynamics

Molecular Dynamics (18 lectures):

- Broad overview of Computer simulation and application of molecular dynamics simulation. (1 lecture)
- Basic linux primer, Primer on a programming language (Fortran), Plotting data using gnuplot (4 lectures)
- **Writing your first Molecular Dynamics code**: Initialization of system, Force calculation from classical potential, Implementation of periodic boundary condition, Integration schemes of Newtonian equation of motion. Simple monoatomic liquids as the test system (6 lectures)
- **Using a software package for MD**: GROMACS to simulate simple liquid (2 lectures)
- Molecular force fields and overview of the existing bimolecular force fields, water models as case study, (**1 lecture**)
- Implementation of Thermostats and Barostat in Molecular Dynamics simulation: Introduction to Berendsen, Nose Hoover and Parrinello Rahman protocols for NVT and NPT simulation (**2 lectures**)
- Handling Electrostatics in computer simulation: Implementation of Ewald summation and Particle mesh ewald summation in computer simulation. (2 **lectures**)

Nonlinear dynamics (12 lectures) :

- **Introduction to 1D and 2D flows** (5 Lectures)
  i) Fixed points and stability,

  ii) Linear stability analysis

  iii) Bifurcations: saddle-node, transcritical, pitch-fork, imperfect bifurcations and catastropes, Hopf-bifurcation

  iv) *Phase plane*: phase portraits, existence and uniqueness, Conservative and reversible systems, fixed- point and linearization

  v) Limit cycle: Introduction, Poincare-Bendixon Theorem, Lienard systems, Relaxation oscillator, weakly nonlinear oscillators,

- **Oscillatory Reactions** (2 Lectures)

  Chemical kinetics, mechanism, Lotka-Volterra, Brusselator, B-Z reaction, (Case studies using numerical simulations)

- **Reaction-diffusion systems and pattern formation (**5 lectures)
  Turing Patterns: General theory, examples of model systems, (case studies using numerical simulations)
  Waves: traveling waves, solitons, spiral, target

Primary Text / Reference Books:

Molecular Dynamics part:
"Understanding Molecular Simulations" Frenkel and Smit.
"Statistical Mechanics: Theory and Simulation" M. Tuckerman
Nonlinear dynamics part:
"Nonlinear dynamics and chaos" by Steven Strogatz
"An Introduction to Nonlinear Chemical Dynamics: Oscillations, Waves, Patterns, and Chaos" by Irving R Epstein and John A Pojman

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

8 Assignments (computer): 50 %
2 examinations (pencil + computer): 50 %

CHM-216.7: Protein structure and synthesis

1. **Fundamentals of protein structure (4 lectures) KM**
    - Primary structure
    - Secondary structure
    - Super-secondary structure (motifs)
    - Tertiary structure
    - Quaternary structure
2. **Chemical protein synthesis (3 lectures) KM**
    - Solid phase peptide synthesis
    - Peptide ligation
    - Case studies
3. **Protein synthesis using recombinant DNA technology (5 lectures) SK**
    - Protein Engineering (DNA manipulation and vector design)
    - Protein expression
    - Protein purification and analysis
    - Protein Crystallization
4. **Protein structure determination by X-ray crystallography (5 lectures) KM**
    - Introduction to X-ray Crystallography
    - X-ray diffraction of protein crystals
    - Space group determination from diffraction intensity
    - Phase problem
    - Structure solution methods
    - Case studies
5. **Protein structure determination by NMR spectroscopy (7 lectures) VA**
    - NMR interactions
    - Polarization transfer methods
    - Assignments of protein resonances
    - Distance restraints
    - Structure calculation

Case studies: small hydrophobic domain.

Books and Reference:

- 'Proteins: Structure and Function' by David Whitford
- 'Molecular Cloning: A Laboratory Manual', Volume 1, by Joseph Sambrook, David William Russell
- 'Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology' by Bernhard Rupp
- 'Crystallography Made Crystal Clear' by Gale Rhodes
- 'Fundamentals of Protein NMR spectroscopy' by Gordon S. Rule and Kevin Hitchen
- 'Protein NMR Spectroscopy: Principles and Practice' by John Cavanagh, Wayne J. Fairbrother, Arthur G. Palmer, III, Nicholas J. Skelton, Mark Rance

Evaluation Scheme:

(Assignments (20%), Mid-term (20%), Final (60%))

- Question-answer format assignments
- Reading Assignments with short report
- Mid term written exam/presentation
- Final written exam + presentation

CHM-217.7: Solid State NMR

- ❖ Principles of solid-state NMR: Spin interactions, anisotropy of intern Frame transformations, magic-angle spinning, heteronuclear spin decoupling, cross polarization
- ❖ Sensitivity enhancement in spins-1/2: Cross polarization; theory **and pulse** schemes, transient oscillations, dipolar coupling information, adiabatic/ramped CP, Scalar coupling transfers in solids.
- ❖ Resolution enhancement in spins-1/2*:* Decoupling, various pulse schemes, experimental strategies, refocussed and non-refocussed transverse relaxation times
- ❖ Distance and Geometry information via recoupling: Separated local-field experiments, pulse schemes based on symmetry of spin interactions, applications to **correlation/distances/bond** and torsional angles/assignments
- ❖ Quadrupolar spins: Introduction of half-integer and integer spin qudrupolar nuclear spins, comment on resolution and sensitivity issues, applications
- ❖ Solid-State NMR in biomolecular applications

Books: Some elementary books in the solid-state NMR spectroscopy.

- **Introduction to Solid-State NMR Spectroscopy,** Melinda **J.** Duer, Blackwell ***Publishing,*** Oxford (2004).
- **Multidimensional Solid-state NM ~lymers** -Rohr and Hans WoIfgang Spiess, Academic, London (1 994).
- **Principles of Nuclear Magnetic Resonance in one and Two Dimensions,** R. R. Ernst,G. Bodenhausen, and A. Wokaun, Clarendon, Oxford (1990).
- **Principles of Magnetic Resonance, 3rd edition,** Charles P. Slichter, Springer, Berlin (1996).
- **High Resolution NMR Spectroscopy in Solids,** Michael Mehring, Springer-Valag, Berlin (1983).
- **The Principles of Nuclear Magnetism,** Anatole Abragam, Oxford University Press, Oxford (1983).

Course Evaluation: 6 assignments, a midterm exam and a final exam with a weight age of 20, 30 and 50% respectively.

CHM-219.7: Advanced Mathematics

Probability and Statistics:

Basic concepts: Combinatorics, Addition law of probailities, statistical inference. Dependent events: Conditional probability, Bayes' theorm, Bayesian interference with known priors, conjugate priors. Random variables: Discrete and continuous random variables, distribution functions. Probability distributions: Binomial and Poisson distribution, Normal distribution, Limit theorems: Law of large numbers, central-limit theorem. Regression: Covariance, linear regression, reduction of variables, resampling methods, bootstrapping

Functional analysis: Normed spaces: Linear space, linear maps and completeness, integrable functions. Hilbert space: Cauchy inequality, quantum states as vectors in Hilbert space, Lebesgue integral, linear operators on Hilbert space, linear functional space and dual vector space, spectral theorem, Fourier series,

Groups and group representations: General group theory: Definitions, isomorphism, homomorphism, conjugate classes, cosets, invariant subgroups. Representation theory: Complete set of commuting operators, group representations, Schur's lemma. Finite and discrete groups: Examples including reflection groups and lattices in relation with crystallography and molecular physics, permutation groups, projection operators, Young diagrams. Lie groups, Rotation groups and Unitary groups: Lie algebra, unitary groups, orthogonal groups, introduction to the representation theory of Lie algebra (Poincare and Lorentz groups, SU(2) and SU(3) groups)

Partial differential equations: First-, second-, and third-order equations, Integral transform techniques, methods of characteristics, classification of second-order PDE's, hyperbolic, parabolic, and elliptic equations, Green's function methods for PDE's, wave equation, diffusion equation, Laplace equation

Complex analysis: Review of complex analysis, analytic functions as mapping, conformal mapping, Cauchy's integral formula, general form of Cauchy's theorem, calculus of residues, harmonic functions

Special functions: Gamma functions, Beta functions, Stirling's series, Reimann Zeta function, Bessel functionsof the first and second kind, Hankel functions, Legendre functions of the first and second kind, physical interpretation of the generating function, spherical harmonics and irreducible tensor operators, Wigner-Eckart theorm

CHM-220.7: Electronic structure theory of matters

1. Bonds and Bands (4 lectures) Qualitative molecular orbital theory, orbital interaction theory, perturbative molecular orbital theory, Jahn-Teller distortion, from molecules to solids, Peierls distortion, Brillouin zone, Fermi surface, Hückel and tight-binding methods, zero differential overlap, electronic structure theory – literature survey. **2. Many Electron Wavefunctions and Operators (4 lectures)** Born-Oppenheimer approximation, diabatic and adiabatic states, conical intersections, Slater determinant, configuration state functions, Slater-Condon rules for matrix elements, spin-adapted wavefunctions, second-quantization, Feynman-Kac formula, Slater-Jastrow wavefunction.

3. Hartree-Fock Approximation (2 lectures) Fock operator, self-consistent-field procedure, Koopman's theorem, orbital relaxation, Roothan equations, basis-set Ansatz.

4. Configuration Interaction (6 lectures) Many-electron correlation, Brillouin's theorem, natural orbitals, many-body perturbation, coupledcluster method, size-consistency, size-extensivity, Goldstone's graphical method for many-body

perturbation, Wick's theorem, linked graphs, Brueckner theory, quasi-particles, Green's function and self-energy, random-phase approximation, Bethe-Salpeter equation.
5. Stochastic Methods (1 lecture) Quantum Monte-Carlo (quantum dots, jellium clusters), diffusion Monte-Carlo, Jastrow's method.
6. Density Functional Theory (6 lectures) Reduced density, pair density, Thomas-Fermi model, Fermi and Coulomb hole, self-interaction, Hohenberg-Kohn theorems, Kohn-Sham equations, performance of various recipes, exchangecorrelation functionals.
7. Time-dependent Theories (2 lectures) Excited states, time-dependent Hartree-Fock, Frenkel-Dirac variational theorem, Runge-Gross theorem.
8. Application-Related Topics (5 lectures) Structure relaxation, transition-state search (popular methods), potential energy surfaces, partial atomic charges, density of states, solvent effects, energy derivatives as molecular response properties.

CHM-222.7: Molecular Dynamics Simulation and application in chemical physics

- Broad overview of Computer simulation and application of molecular dynamics simulation. (2 lecture)
- Basic linux primer, Primer on a programming language (Fortran) (6 lectures)
- **Writing your first Molecular Dynamics code**: Initialization of system, Force calculation from classical potential, Implementation of periodic boundary condition, Integration schemes of Newtonian equation of motion. Simple monoatomic liquids as the test system (6 lectures)
- Implementation of Thermostats and Barostat in Molecular Dynamics simulation: Introduction to Berendsen, Velocity-rescale, Nose Hoover and Parrinello Rahman protocols for NVT and NPT simulation. Implementation using Fortran and Gromacs (**4 lectures**)
- Handling Electrostatics in computer simulation: Implementation of Ewald summation and Particle mesh ewald summation in computer simulation. Illustration using Fortran and Gromacs (2 **lectures**)
- Introduction to molecular force fields and overview of the existing molecular force fields, water models as case study (**1 lecture**)
- Free energy calculations, Introduction to Enhanced sampling approaches, Illustration using Umbrella sampling and Metadynamics simulation using GROMACS (4 lectures)
- QM/MM: Basics; Additive vs Subtractive schemes, Different types of embedding, Adaptive QM/MM models (3 lectures)
- Ab Initio MD (1 lecture)
- Beyond Born-Oppenheimer approximation (1 lecture)

Grading policy:

8 Assignments (computing based): 50 %, 2 examinations (Both Pencil and Computer based): 50 %

Reference: "Understanding Molecular Simulations" Frenkel and Smit., "Statistical Mechanics: Theory and Simulation" M. Tuckerman

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Get theoretical knowledge of Molecular dynamics simulation
CO 2	Get hands-on numerical programming skills of simulating simple system
CO 3	Would get introduced to quantum mechanical approach
CO 4	Would learn how to simulate macromolecule's movements

CHM-224.7: Chemistry of Materials Based on p-Block Elements

Syllabus:
Preamble: This course will mostly deal with material chemistry of *p*-block elements. This course has been designed considering as an elective course for IPhD and PhD students.
1. **Boron:** Borole, Borafluorene, Borophene, BODIPY (boron-dipyrromethene), Borazylene, Amine-Borane, Boron Nitride, Cycloborazane, Diboraanthracene, 9,10-Azaboraphenanthrene, Azaborine, Ethynyleneborane (6)
2. **Aluminium:** Aluminoxane, Methylaluminoxane, Aluminium Alloy, Aluminium Based Composite Material (3)

3. **Gallium:** Gallium Nitride, Gallaferrocenophane (1)
4. **Silicon:** Polysiloxane, Polysilanes, Polycarbosilanes, Silicon Based Nanomaterials (2)
5. **Nitrogen:** Nitrogen-Doped Carbon Material, Nitrogen-Rich Polymers, Nitrogen Based Energetic Materials (3)
6. **Phosphorus:** Phosphole, Phosphole Oxide, Phosphaalkenes, Phosphazene, Cyclophosphazene, Carbaphsphazene, Phosphorus-Based Alloy Materials, Phosphorus-Based Mesoporous Materials (5)
7. **Sulfur:** Sulfides, Polysulfur, Poly(arylenesulfide), Thiophene, Benzothiophene, Dibenzothiophene, Thienothiophene (3)
8. **Selenium:** Selenides, Selenophene (1)

Evaluation: Based on assignments / term papers (20 % weightage) and two examination, mid-term and final (40 % each).

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Know the various materials aspects of *p*-block compounds (except carbon): synthesis and isolation
CO 2	Know the chemistry of energetic molecules.
CO 3	Know the chemistry of polymers.
CO 4	Know the chemistry of molecules which are exhibit striking photo-physical properties.
CO 5	Know the chemistry of molecules which are exhibit application in varios fields: materials, catalysis, and medicinal chemistry.

CHM-225.7: Organic and Perovskite materials

- Carbon Based Macromolecules and Polymers – Polyethene, Polystyrene, Polyacetylene, Electroactive Conjugated Polymers, Donor and Acceptor Blended Polymers – 2 L
- Diamond, Graphite – Graphene, Nanocarbons – Fullerene and Nanotubes, Cyclo[18]Carbon-*sp*-Hybridized Molecular Carbon Allotrope, Diatomic Carbon – 2 L
- Molecular Switches – Acidochromic, Photochromic, Host–guest, Mechanically-Interlocked – 3 L
- Molecular Motors – Rotor, Axle, Stator – 2 L
- Molecular Propeller, Molecular Shuttle, Molecular Tweezers, Molecular Sensor, Molecular Logic Gate, Molecular Assembler, Molecular Hinge – 4 L
- Radicals, Diradicals, and Diradicaloids, Polyradicals, Distonic Radical Cations, Distonic Radical Anions – 3 L
- Molecules of Interests for Photophysical Properties – Absorbance at NIR Range, Fluorescence, Aggregation-Induced Emission, Vibration-Induced Emission, Singlet Fission, Two-Photon Absorption – 2 L
- General and Targeted Perovskite Materials, Structures of Perovskite Materials, Physical Properties of Perovskite Materials, Applications of Perovskite Materials – 6 L

Evaluation: Based on assignments / term papers (20 % weightage) and two examination, mid-term and final (40 % each).

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Know the various materials aspects of carbon compounds: synthesis and isolation
CO 2	Know the chemistry of open-shell compounds.
CO 3	Know the chemistry of carbon compounds which are known for application in varios fields: materials and catalysis.
CO 4	Know the basis of development of semincondctor materials based on organic and halide perovskite materials
CO 5	Working principles of devices like solar cells, light emitting devices, transistors based on perovskite and organic materials.

CHM-253.7: NMR Instrumentation

(A) Basics of NMR Spectroscopy [3 classes, 2 assignments]
1. Phenomenological modelling of time and frequency domain NMR signals, relaxation, the concepts of phase, quadrature detection, linewidths and signal-to-noise analysis, basics of processing NMR data, (window functions, zero filling, etc) [1.5 classes]
2. Basics of multidimensional NMR: Data collection and processing [1.5 class]
(B) NMR of small molecules
1. Analysis and Interpretation of small molecules structure using proton NMR chemical shifts, scalar couplings, area under the signal, paramagnetic shifts. [1 hour]
2. The basics of 13C-detected or 13C-edited NMR experiments routinely used for analyzing small molecules structure. [1 hour]
3. The role correlation experiments (proton-proton, proton-X Nuclei) for structure analysis. basic correlation experiments like COSY, TOCSY, HSQC, HMQC, HMBC, and NOESY, etc. will be covered. [2 hours]
4. X- nuclei NMR, analysis and Interpretation. (X = 19F, 31P, 11B, 29Si, 15N, 207Pb, 117Sn, 2H) [1 hour]
5. Exercise on on two small molecule structure interpretation. [2 hours]
6. Practical training on NMR instrument [3 hours]
7. NMR spectrometer hardware and general trouble shooting. [2 hours].
(C) Understanding NMR using simulations
1. Propagators, hamiltonians and simulating a simple 1D signal [1 class]
2. Strong and weak coupling patterns in J-coupled spectra, dipolar coupled spectra, and chemical shifts [1 class]
3. Basic experiments: INEPT/Cross-polarization/Composite Pulses [2 classes]
4. Chemical Exchange [1 class]
In preparation for the first class:
1. The class requires extensive use of the Python programming, although no background in programming is required. All concepts necessary for the class will be covered. The following libraries must be installed in preparation for the class: Python, Numpy, Scipy, Matploltib, Jupyter. If you are unsure of how to install all of these, we recommend the Anaconda distribution of the scientific stack which can be downloaded for any OS from here: https://www.anaconda.com/distribution/. Although any other programming language can be used for the material taught in this course, we will be supporting only Python for assignments and exams for consistency.

2. The Topspin software from Bruker used to acquire and process data can be downloaded from here. This is available for free for academic users and will require you to make an account.

Grading
• Part (A): 2 assignments (10% each)
• Part (B): 2 assignments (10% each)
• Part (C): 2 assignments (10% each)
• Final Exam (40%)
Reference material for the course
1. Nuclear Magnetic Resonance Spectroscopy: A Physicochemical View *by Robin K. Harris*
2. Understanding NMR Spectroscopy *by James Keeler*
3. High-resolution NMR Techniques in Organic Chemistry *by T. D. W. Claridge*
4. Modern NMR spectroscopy- A workbook of chemical problems *by J. K. M. Sanders, et al.*

CHM-255.7: Introduction to Data Science

Syllabus: 1) Data Science: Big Data, Facets of data (structured/unstructured data)
2) Toolboxes: Python libraries, SCIKIT-Learn, PANDAS
3) Statistics: Distributions, Outlier, Skewness, Pearson's/Spearman's/Kendall's coefficient, Kernel densi-ty
4) Statistical Inference: Hypothesis testing, Confidence Intervals
5) Supervised Machine Learning: What is machine learning? Learning curves, Support Vector Ma-chines, Random Forest
6) Regression: Linear Regression, Logistic Regression
7) Unsupervised Machine Learning: Clustering, Case studies
8) Big Data concepts: Handling large data, Hadoop, Spark, NoSQL, Graph databases, Natural lan-guage processing, MapReduce

Required Text 1. *Introduction to Data Science. A Python Approach to Concepts, Techniques and Applications,* Laura Igual, Santi Segu, Springer (2017). 2. *Introducing Data Science,* Davy Cielen, Arno D. B. Meysman, Mohamed Ali, Manning (2016).

Evaluation Method: Assignment (50%), Presentations (50%)

Course Outcome:

Sr. No.	On completing the course, the student will be able to:
CO 1	Appreciate the various terminology used in data science applications.
CO 2	Get an idea of the algorithm used in popular data analysis techniques.
CO 3	Develop a simple Python code to perform elementary data analysis.
CO 4	Use publicly available data science platforms in their research.

CHM-211.7 / PHY-206.7: Advanced Quantum Mechanics / Quantum Mechanics-II:

1. Theory of angular momentum (3L) ˆ
Rotations and spherical tensor operators ˆ
Matrix elements of spherical tensor operators: Wigner-Eckart theorem ˆ
(HW-1)
2. Time Independent Perturbation Theory (2L) ˆ
Projection operator technique ˆ
Examples ˆ
(HW-2)
3. Adiabatic principle and Berry phase (4L) ˆ
Adiabatic principle ˆ
Berry phase ˆ
Modern theory of polarization
4. Time dependent QM (4L) ˆ
Different representations, TDSE in interaction picture: Exact solution for 2-state system V = constant, periodic perturbation
Extension to 1 → continuum, Green operator ˆ
TDPT: with coeff (historical): 1st order, application V = constant, Fermi's golden rule ˆ
examples ˆ
(HW-3)
5. Quantum scattering theory (4L) ˆ
Elastic scattering ˆ
Born Approximation and Born series ˆ
Optical theorem 1 ˆ
Plane wave analysis: method of partial waves ˆ
Some examples: Hard sphere Scattering, Coloumb Scattering
6. Review (1L)
7. Midterm
8. Introduction to QED (12L) ˆ
Quantization of EM field (8L)

- Introduction, Total free field energy density → collection of uncoupled harmonic oscillators
- Second quantization
  * Bosonic and fermionic ladder operators
  * 1- and 2- particle operators in second quantization
  – Lagrangian, conjugate variables, canonical quantization
  – Examples: Spontaneous emission, photoelectric effect
  – (HW-4)
  – Lamb shift (Bethe's derivation)
  – Four vector and Lorentz gauge, other ways of quantization ˆ

Relativistic QM (4L)
– Review of Special relativity
– Relativistic Hamiltonian
– Dirac Equation and Klein Gorden equation
– Free particle solution and Central force problem
– Hole theory
– CPT invariance
– (HW-5)
9. Review (1 extra lecture)
10. Final

Referece Texts (i) Modern Quantum Mechanics, Sakuari (Addison and Wesley) (ii) Advanced Quantum Mechanicw, Sakuari (Addison and Wesley) (iii) Relativistic Quatum Mechanics , Bjorken and Drell (McGraw Hill)

CHM-212.7 / BIO-101.7: Basic Cell Biology

- Basic processes of transcriptional, translational and post-translational regulation:
  Endocytosis, exocytosis and protein export
    - RNA production, splicing and export
    - Regulatory roles of non-coding RNA
    - Biochemical processes in specific cellular organelles like the endoplasmic reticulum, golgi, mitochondria, nucleus and nucleolus and the plasma membrane
    - Protein sorting in the cell - discovery of the Sec and SNARE proteins and their roles in regulating subcellular trafficking.
- Physical and chemical processes regulating cellular function:
    - The cell cycle and its regulation
    - Maintenance of pluripotency in stem cells; mechanobiology, effects of substrate stiffness and mechanical forces on cell fate and development
    - Chemical modifications of DNA and histone proteins regulating gene expression (Epigenetics)
    - Phosphorylation cascades that regulate chromatin function and DNA repair
    - Nuclear architecture and its regulatory role in controlling gene expression
    - Roles of membrane heterogeneity in regulating endocytosis and signaling
    - Mitochondria, energy production and apoptosis
    - Sources and use for noise in gene expression
- Roles of the cytoskeleton and associated motor proteins:
    - Structure of actin, microtubules, cytoskeletal intermediate filaments, nuclear intermediate filaments (lamins)
    - Discovery and function of molecular motor proteins like myosin, kinesin and dynein.

Course Evaluation: There will be papers assigned every week after a lecture. The students will be expected to provide written reports of what they understand from the papers and also discuss them in class. They are expected to convey not just the philosophical content of what is claimed, but the actual methods that led to the conclusions. In addition to these and other written components, the final examination will constitute of seminar presentations on specific topics chosen by the students. A student will be expected to perform extensive literature survey on the topic of their choice, write a comprehensive report and make a cogent presentation critically evaluating the current state of knowledge on the topic. A major aim that this course hopes to achieve is to inculcate students with the ability to critically evaluate studies in Cellular Biology and Biochemistry, in addition to conveying knowledge of the current state of the fields.

Weightage of marks - 70% from written assignments, 30% from presentations

CHM-213.7 / BIO-202.7: Fluorescence Methods in Cellular Biophysics

1. Basics of fluorescence - Jablonski diagrams, Stokes shifts, structures of fluorophores, quantum yields, fluorescence instrumentation - fluorescence microscopy and spectroscopy, light sources, filters, and detectors.

2. *Forster Resonance Energy Transfer* (*FRET*), Time-Correlated Single Photon Counting (TCSPC), fluorescence lifetime, quenching - theoretical ideas, technical details behind measurements and applications. Fluorescence polarization measurements - steady-state and time-resolved fluorescence anisotropy - theory, instrumentation and technical details.

3. Widefield microscopy, effects of objective numerical aperture on resolution, diffraction limit of resolution of light microscopy.

4. Confocal microscopy - point-scanning and spinning disk confocal microscopy; light sheet microscopy; Total Internal Reflection Fluorescence (TIRF) microscopy; considerations for temporal resolution; multiphoton microscopy.

5. GFP technology and dynamics measurements in live cells - Single Particle Tracking (SPT), Fluorescence Correlation spectroscopy (FCS), Fluorescence Recovery After Photobleaching (FRAP), live cell dynamics measurements.

6. Super-resolution microscopy methods - stimulated emission depletion (STED), structured illumination microscopy (SIM), stochastic optical reconstruction microscopy (STORM), photo activated localization microscopy (PALM), point accumulation for imaging in nanoscale topography (PAINT) and others.

Course Evaluation:

There will be papers assigned every week after a lecture. The students will be expected to provide written reports and present what they understand from the papers. They are expected to convey not just the philosophical content, but the actual methods that led to the conclusions. In addition to these written assignments. The final examination will have a written element and seminar presentations on specific topics chosen by the students. A student will be expected to perform extensive literature survey on the topic of their choice, write and make a cogent presentation critically evaluating the current state of knowledge on the topic. A three-member committee convened by the course instructor will grade the presentations. A major aim that this course hopes to achieve is to inculcate students with the ability to critically evaluate topics, in addition to conveying of the basics and the current state knowledge in fields pertaining to the applications of fluorescence in Cellular Biophysics.

Weightage of marks - 70% from written assignments/examinations, 30% from presentations.

CHM-223.7 / PHY-325.7: Polymer Physics and Soft Matter

Syllabus:

- Polymer Science, Soft Matter, Some problems (1 lecture)
- Ideal Chains: Conformations of ideal chain, Ideal chain models, Radius of gyration, free energy, pair correlations, measurements (basic concepts) (3 lectures)
- Real Chains: Excluded volume, Flory theory, Temperature and strain (polymer under shear flow) effects, scaling theory (3 lectures)
- Computer simulation approach using polymer based model (2 lectures)
- Thermodynamics of phase separation, spinodal and binodal. Brief overview of phase separation in biology (2 lectures)
- Polymer solutions, quality of solvent, Alexander-de Gennes brush (2 lectures)
- Percolation, gelation, Flory-Stockmayer theory, phase separation, glass transition (basic overview of the problem and some theoretical models) (8 lectures)
- Dynamics: Rouse model, Zimm model, branched polymers, entanglements, elastic regime (4 lectures)

Evaluation Method:
4 assignments: 25%, Presentation on term-paper based on application of polymer physics in biology: 25%, 2 class-room examinations: 50%

CHM-119.7 / BIO-205.7: Biological Thermodynamics

Syllabus:
Thermodynamics is the study of heat, energy, and work. Originally introduced to maximize the work-efficiency of heat engines, thermodynamics soon became one of the most fundamental branches of physics. Its laws are so general that they are applicable to all systems from inanimate machines to living cells. In this course, we will visit the core concepts of thermodynamics and statistical mechanics and explore their applicability to numerous biochemical and biophysical phenomena.

- *Brief review of thermodynamics*: Introduction to the laws of thermodynamics. Thermodynamics and statistical mechanics. Phase transition and equilibria. Enthalpy and free energy of reaction. Gibbs free energy.
- *Significance of free energy and statistical mechanics in biology*: Energetics of biochemical reactions. Protein stability. DNA melting and polymerase chain reaction (PCR). Analysis of thermodynamic data and multistate equilibriums in biology. Heat capacity of proteins. Cooperative transitions. Free energy of protein-protein interactions. Applications in Molecular pharmacology.
- *Applications of the first and second laws in biology*: Specific examples from biochemistry. Energy, information, and life. Non-equilibrium thermodynamics and living systems. Cells as active gels. Special emphasis on the distinction between equilibrium states and steady states of the nonequilibrium variety with relevance to cellular processes.
- *Metabolism as energy flow*: Investigation of hypotheses related to primordial metabolism. Energy conversion at Hydrothermal vents. Acquisition of mitochondria – endosymbiotic event that broke the energy constraint for creating complex structures. Glycolysis and oxidative phosphorylation. ATP synthesis. Donnan equilibrium. Membrane transport.
- *Thermodynamics and chemical kinetics of enzymes:* Binding equilibria and reaction kinetics. Single-site model. Scatchard and Hill plots. Rate constant and order of reaction. Multiple independent sites. First and second order reactions. Transition state theory. Enzyme kinetics, inhibition, and allosteric effect.
- *Thermodynamics of molecular machines inside cell:* Polymerization of various and thermodynamics of acto-myosin contractile system. Thermodynamics of molecular motors.

Primary Text / Reference Books:
Biological Thermodynamics by D. T. Haynie, Cambridge University Press. *Understanding Thermodynamics* by H. C. Van Ness, Dover Publication. *Statistical Physics* by F. Mandl, Wiley.

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):
Evaluation method: Assignments and Presentations: 40, one mid-term: 30, and one final exam: 30.

CHM-218.7 / BIO-203.7: Mechanobiology

Syllabus: The field of mechanobiology explores how mechanical forces influence many cellular and multicellular processes. The main objective of mechanobiology is to eventually explain these processes with a few relatively simple mechanical laws. This course intends to cover the history of mechanobiology, provide the conceptual foundations to fluid and solid mechanics for making a mechanical approach to the biological problems, explore fundamental structural elements that generate and transmit forces within cells and tissue, and finally, discuss the experimental methods towards measuring and perturbing forces in biology. The course also intends to provide several case-studies of mechanobiology-regulated physiological processes, including morphogenesis, wound healing, and cancer.

- Introductory part: Concept of length and time-scales in biology. Diversity of biological forces. Classic works in mechanobiology. Rudimentary solid and fluid mechanics, with examples from biology. Introduction to viscoelasticity and surface tension and how do they operate at cellular and tissue level.
- Biology, chemistry, and physics of cellular force-bearing structures: How do the cells generate force? Actin filaments and actomyosin network. Actomyosin contractility and contraction of muscle and non-muscle cells. Microtubules and their force-sensitive participation in cell division. Diversity of cytoplasmic and nuclear intermediate filaments. Polymer mechanics of cytoskeletal elements. Nuclear mechanics and force transduction. Force sensitive molecular complexes, including focal adhesions and adherens junctions. Extracellular matrix (ECM) mechanics. The physiological range of ECM stiffness and its effect on cellular differentiation. Force transmitting proteins or mechanotransducers including cadherins and integrins. Molecular motors. Mechanoresponsive ion channels.
- Techniques of mechanobiology: How can we measure forces at molecular and cellular level? Traction force microscopy, micropillar assays, monolayer stress microscopy, atomic force microscopy, optical traps, magnetic tweezers, molecular tension sensors, DNA-based force sensing, fluorescence speckle microscopy, oil inclusions, micropipette aspiration, and indirect computational methods. Experimental perturbative approaches to cellular mechanical structures. Measuring forces on cellular organelles. Discussion on the limitations of the current techniques and on futuristic mechanobiological methods and paper presentations.
- Forces in tissue and organism development: Forces that shape a developing embryo. Forces in the epithelium. How the cells build the tissue stiffness: molecular assembly and collective effect. Epithelial constriction, invagination, bending, folding, and hydraulic fracture. Density-dependent and independent jamming and unjamming of the epithelium in asthma and cancer. Force measuring techniques at tissue level: current approaches and limitations. Mechanobiology of cancer.

Primary Text / Reference Books:
Physical Biology of the Cell by Rob Phillips *et al.*, Garland Science
Biological Physics: Energy, Information, Life by Philip Nelson, W.H.Freeman & Co Ltd
Biological Physics of the Developing Embryo by Gabor Forgacs and Stuart A. Newman, Cambridge University Press
Introduction to the Physics of Fluids and Solids by James S. Trefil, Dover Books on Physics.

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):
Assignments and Presentations: 60, Mid-term exam: 20, and End-term exam: 20.

CHM-121.7 / BIO-208.7: Chemical Biology-I

1. Introduction to chemical biology **(1 lecture, ATV)**
• Central dogma of molecular biology
• Historical perspective
• Bringing chemical solutions to biological problems
2. Chemistry of Nucleic acids (DNA and RNA) **(3 lectures, ATV)**
• Historical perspective, modern methods for chemical synthesis of DNA and RNA, backbone-modified nucleic acids (PNA, LNA, therapeutic nucleic acids (ASO) and morpholinos), aptamers and systematic evolution of ligands by exponential enrichment (SELEX), chemical modifications of DNA and RNA, expanding genetic code and new alphabets of DNA, DNA-sequencing chemistry, DNAencoded libraries for drug discovery, DNA-nanotechnology, DNA for digital data storage and computing
3. Protein chemistry **(6 lectures, KM)**
• Protein design
– Designing α-helices (rational design, peptide stapling, amphiphilic helix); Coiled coils; 4 helix bundles
• Protein synthesis
– Ribosomal and non-ribosomal peptide and protein synthesis; Missing-link between ribosomal and non-ribosomal protein synthesis; Chemical protein synthesis; Synthesis of proteins with unusual topology
• Inteins
– Protein splicing, Expressed protein ligation
• Expanding the genetic code
– Incorporating non-canonical amino acids into proteins

• Covalent protein modification
• Protein engineering
– Directed evolution; Phage-display; Bacterial display; Yeast display; mRNA display; Ribosomal display
4. Bio-orthogonal labeling - tools and techniques **(2 lectures, KM)**
• Bio-conjugation chemistry (NHS chemistry, maleimide chemistry, click-chemistry and photo-cross linking reagents)
• Antibody-drug conjugates
5. Chemical Glycobiology **(2 lectures, ATV)**
• Chemical constituents of glycans, synthetic modifications of glycans, automated glycan synthesis, tools for molecular imaging of glycans in cells, glycoengineering and its therapeutic applications
6. Chemigenetic technologies and their applications in biology **(2 lectures, ATV)**
• HaloTag chemistry, SNAP-tag chemistry, biotin-ligase chemistry, small-molecule-based protein dimerization techniques, applications of chemigenetic tools in biology
7. Fluorescent probes for cellular and *in vivo* imaging **(2 lectures, ATV)**
• Fundamentals of fluorescent probe design, genetically encoded fluorescent sensors, chemigenetic indicators, small-molecule-based fluorescent probes for biology
8. Interfacing chemistry with immunology (chemical immunology) and neuroscience (chemical neurobiology) **(2 lectures, ATV)**
• Basic components of immune system, chemical modulators of immune cell signaling pathways, drug targets of the immune system.
• Chemical biology on the brain, neuromodulation using smallmolecules, caged neurotransmitters, photo-pharmacology in neurons, therapeutic targets in the brain and chemical probes for brain imaging.
9. Chemical biology & drug discovery **(4 lectures, KM)**
• Chemical genetics
– Small Molecules as a Means to Perturb Biological Systems
– Forward and Reverse Chemical Genetics
• High throughput and imaging-based high-content screening technologies
• Mirror-image phage display
• Targeted protein degradation and stabilization in live cells
– Ubiquitin-proteasome system; Autophagy; Chemistry, design principles and case studies of proteolysis-targeting chimera (PROTAC), lysosome-targeting chimera (LYTAC), autophagytargeting chimera (AUTAC), molecular glues, Deubiquitinase Targeting Chimera (DUBTAC)

Assigned Reading (Textbooks & References):
• Introduction to Bioorganic Chemistry and Chemical Biology; David Van Vranken & Gregory A Weiss
• 'New Frontiers in Chemical Biology: Enabling Drug Discovery'; Edited by Mark E. Bunnage
• 'Chemical and Biological Synthesis: Enabling Approaches for Understanding Biology'; Edited by Nick J. Westwood & Adam Nelson
• 'Chemical Biology: Learning through Case Studies'; Edited by Herbert Waldmann & Petra Janning
• 'Bioconjugate Techniques. Greg. T. Hermanson, Pierce Biotechnology, 3rd Edition.

Evaluation:
• Participation in class discussion – 5%
• Four short take-home quizzes – 25%
• On-site written mid-term examination / Presentations – 30%
• On-site written final examination – 40%

CHM-221.7 / PHY-417.7: Magnetism

Syllabus:

Moments and Susceptibility
Local moments; Curie Law; Pauli paramagnetism; General formula for susceptibility

Magnetic Moment of a Single Atom or Ion
Spin and Orbital effects; (A) Hund's Rules; (B) Spin-orbit coupling; (C) Crystal fields
Transition Metals (C>B); Rare Earths (B>C)

Exchange Interactions in Insulators
Direct (potential) exchange; Kinetic exchange; Superexchange; Dzyaloshinski-Moriya interactions

Local Moments in Metals and their Interactions
Anderson impurity Hamiltonian; Kondo limit and the Kondo effect; RKKY interactions; Kondo Lattices

The Hubbard Model
The atomic limit; Half-filling → the spin 1/2 Heisenberg model; Single hole: the Nagaoka result

Magnetic States
Ferromagnets; Antiferromagnets: Neel and Resonating valence bond (RVB) states; Ferrimagnets; Helimagnets; Spin glasses

Magnetism in Metals
Itinerant magnetism

Primary Text / Reference Books:
"Lecture Notes on Electron Correlation and Magnetism" by P. Fazekas (World Scientific)

Evaluation

Homework: 30, Mid Term: 30, Final: 40

CHM-300.7 / PHY-418.7: Quantum Thermodynamics

Syllabus:

I. Classical Thermodynamics: temperature, heat, work; first law; entropy and second law; specific heats; heat engines, refrigerators and their efficiencies; entropy of mixing; chemical reactions and entropy constants; Nernst and Nernst-Planck formulations of the third law; cooling rates; dilution refrigerators.
II. Classical Statistical Mechanics: microcanonical, canonical and grandcanonical ensembles; ideal gases.
III. Brief introduction to non-equilibrium stat mech, thermalisation.
IV. Quantum Statistical Mechanics: quantum ideal bose gas; specific heats and entropy.
V. Quantum Thermodynamics of first kind: quantum modifications of classical thermodynamics; third law in the light of QSM;; entropy constants for monatomic and di-atomic ideal gases; He3-He4 mixtures and revision of entropy of mixing; chemical reactions revisited.
VI. Open Quantum Systems.
VII. Classical and Quantum Information
VIII. Quantum Thermodynamics of the other kind: emergence of thermodynamic behavior in quantum systems; quantum-work, quantum-heat and quantum-entropy; quantum first law; many entropies and many second laws; quantum third law; quantum heat engines, refrigerators and their efficiencies.

Primary Text / Reference Books:

- Principles of Thermodynamics by N.D. Hari Dass, CRC Press.
- Statistical Mechanics by R.P. Feynman
- The Principles of Statistical Mechanics by R.C. Tolman
- Elements of Non-equilibrium Statistical Mechanics by V. Balakrishnan
- Advanced Quantum Mechanics by J.J. Sakurai
- Quantum Thermodynamics by Jochen Gemmer and M. Michel

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):
60 percent final exam; 40 percent assignment

PHY-215.7: Error Analysis and Statistical Inference in Experiments

1. Errors in experimental science: Errors as uncertainties. Inevitability of uncertainty. Importance of knowing the uncertainties. Estimating uncertainties in repeatable measurements.
2. How to report and use uncertainties: Best estimate ± Uncertainty. Significant figures. Discrepancy. Comparison of measured and accepted values. Comparison of two measured numbers. Fractional uncertainties. Significant figures and fractional uncertainties. Multiplying two measured numbers.
3. Propagation of uncertainties: Uncertainties in direct measurements. Sums and differences, products and quotients. Independent uncertainties in a sum. Arbitrary function of one variable. General formula for error propagation.
4. Statistical analysis of random uncertainties: Random and systematic errors. The mean and standard deviation. The standard deviation as the uncertainty in a single measurement. The standard deviation of the mean.
5. The normal distribution: Histogram and distributions. Limiting distributions. The normal distribution. The standard deviation as 68% confidence limit. Justification of the mean as the best estimate. Justification of addition in quadrature. Standard deviation of the mean. Confidence.
6. Averaging data: Weighted averages
7. Rejection of data: The problem of rejecting data. Chauvenet's criterion.
8. Least-square fitting: Maximum likelihood and Fitting data to a straight line.

9. The binomial distribution and the Poisson distribution: Probabilities in dice throwing. Definition of the binomial distribution. Properties of binomial distribution. Definition of the Poisson distribution. Properties of Poisson distribution

10. The χ 2 test for a distribution: Introduction to χ 2 . General definition of χ 2 . Degrees of freedom and reduced χ 2 . Probabilities of χ 2 .

11. Some special topics: Use of covariance. Confidence limits on estimated parameters.

CHM-254.7 / PHY-201.7: Computer Programming using Python language

1. Simple programs with input and output
2. Variables, operations, expressions, statements
3. Numbers, characters, strings
4. Tuples, lists, dictionaries, sets
5. Functions
6. Scoping
7. Conditionals
8. Iteration
9. Manipulating text
10. Files
11. Packages
12. Computing with random numbers Along the way, we will learn some simple algorithms.

CHM-112.7: Inorganic Chemistry

1. Chemistry of *s*- and *p*-Block Elements (6 lectures)

[a] Chemistry of compounds involving lithium and magnesium: synthesis, structure and reactivity
[b] Chemistry of boron: boranes, bonding of boranes, synthesis and reactivity, boron clusters, carboranes and metallacarboranes
[c] Aluminum and silicon chemistry: synthesis and application
[d] Chemistry of compounds involving magnesium, boron, silicon, aluminum, germanium, tin, and lead: synthesis, structure and reactivity

2. Transition Metal and Lanthanide Chemistry (10 lectures)

[a] Synthesis and structure of mononuclear and multinuclear transition metal complexes
[b] Theories of bonding: crystal-field and molecular orbital theory, effects of ligand-field
[c] Concepts of orbital symmetries for d-orbital splitting diagrams in different stereochemistry
[d] Spectroscopy of transition-metal complexes
[e] Magnetism of transition-metal complexes
[f] Supramolecular structures involving transition metal complexes
[g] Coordination complexes in applied chemistry
[h] Introduction of lanthanide chemistry
[i] Synthesis of organo-lanthanide complexes
[j] Applications of lanthanide complexes - magnetism and catalysis

3. Organometallic Chemistry (8 lectures)

[a] dn electron counting
[b] Elimination and addition Reactions involving transition metal complexes and their consequence on catalytic process
[c] Syntheses and application of organometallic reagents
[d] Coupling reactions: Kumada coupling, Suzuki-Miyaura coupling, Hiyama coupling, Sonogashira coupling, Negeshi coupling, Stille coupling, Buchwald-Hartwig Coupling, Heck reaction, Click Reactions
[e] Homogeneous catalysis and catalysts: Alkene isomerization, hydrogenation, hydroformylation, Monsanto acetic acid process.
[f] Alkene polymerization, cross coupling reactions, metathesis, C-H activation, and functionalization

Books:

[1] N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, Pergamon Press, 2nd Edn., 2002.
[2] R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 5th Edn., John Wiley and Sons, 2009.
[3] J. E. Huheey, K. E. Keiter, R. L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4th Edn, Pearson Education, 2008.
[4] D. F. Shriver, P. W. Atkins. C. G. Langford, Inorganic Chemistry. 3rd Edn., Oxford University, Oxford, 1999.
[5] F. A. Cotton,; C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley Interscience, 2001.
[6] B. D. Gupta, A. J. Elias, Basic Organometallic Chemistry, University Press, 2013.

Evaluation: Based on 6 assignments (20 % weightage) and two examination, mid-term and final (40 % each).

<u>CHM-100.7: Research Methodology – SRS, AM & GR:</u>

Scientific research involves a mature understanding of past literature, providing contextual motivation for current work; a judicious analysis of generated data; good presentational skills; and an appreciation of the foundational role of scientific ethics and scientific method. The course will cover diverse areas such as research ethics, literature survey, quantitative methods of data and statistical analysis with practical applications to real- world data, and field visits. Because of the universal need for these research methods, values and skillings, this course is mandatory for graduate students of all the three subject-boards relevant to TIFR Hyderabad (Physics, Chemistry and Biology). The course includes topics below. (Square brackets show [No. of classes]. Smaller font is (informal teacher's notes on the topics to be covered)).

1.SKILLING STUDENTS TO:

* Sketch a Function [2] (Function *and* slope. Symmetries, Special pts, asymptotes, draw segments. Join up!)

* Write a CV [1] (First impression. Show professionalism! CV content. Fonts, topics, and sequencing.)

* Write a Letter [1] (Apply for postdoc. Ask to visit. Request to be cited.)

* Talk about research work [1] (10 minute talk, 1 minute talk, coffee conversation, the elevator pitch,140-character tweet.)

* Give a Research Talk [2] (Judge audience! 1 slide ~ 2 mins. Intro/Motivation/Methods/Results/Takeaways. Questions.)

* Write a Research Paper [2] (Abstract, Text, Fig Caps, Refs, Acknowledgements. Proof-reading. Good/Bad writing examples.)

* Read a Research Paper [1] (Quick-read. Skim text, main refs. Go to Origins, trace Evolutions. Detailed reading.)

* Make Quantitative Estimates [2] (Memorize basic constants, sizes. Internal conversation. Compare others, on Log scale.)

2. METHOD OF SCIENCE [2] (Theoretical model, predict⍰Quantitative experimental test⍰Keep/ Modify model, predict⍰...Ideas of Bacon, Occam, Popper, Kuhn.)

3. RESEARCH ETHICS AND AVOIDING PLAGIARISM [2] (Dangers of copy-paste. Plagiarism. Proper citing. Indian Academy of Sciences Report)

4. VISUAL REPRESENTATION OF RESEARCH DATA [2] (Optimal design of plots, charts, schematics, posters etc for graphic display of empirical relationships in complex data.)

5. ERROR ANALYSIS OF RESEARCH DATA [3] (Random and systematic errors. Statistical errors and probability distributions. Error propagation or addition of errors.)

6. STUDENT PRESENTATIONS

(Research Literature. *25+5 min talks,3 per class. Graded. Two cycles, if class-size permits*.)

7. LAB VISITS

(Students split up for Bio/ Chem/ Phys tours, guided by Senior PhD students)

Primary Text / Reference Books:

- Scientific Writing and Communication, Angelika Hofmann, (Oxford 2014).
- Back-of-the-Envelope Physics, Clifford Swartz, (Johns Hopkins 2003).

- The Visual Display of Quantitative Information, Edward Tufte (Graphics Press 1982); Bang Hong, Nature Methods articles.
- Measurements and their Uncertainties, IG Hughes and TPA Hase, (Oxford 2014)
- Advice to a Young Scientist, Peter B Medawar, (Basic Books 2008)
- A PhD Is Not Enough, Peter Feibelman (Basic Books 2011)

Evaluation Method (Weightage for Internal Assessment, Mid Term / Term End exams, Presentations etc.):

Based on student written hand-ins (50%) and student oral presentations (50%)

Course Outcome:

Sr. No.	On completing the course, the student will be able to have a deep perspective on the following topics from emerging literature:
CO 1	Students are taught what senior people already know from experience, namely how to survive a PhD programme, and how to function as an academic professional.
CO 2	There are lectures on Scientific Method and Scientific Ethics. But the core of the course is a series of How To lectures telling them things that, for earlier students at least, were not written down anywhere.
CO 3	How to sketch a function. How to do a CV. How to give a talk. How to write a paper. How to read a paper. How to converse with others about your work. How to write an application letter. How to give an interview, including an online one. How to think,and to feed and keep healthy, your two minds (M1 eats logic. M2 eats analogies.)
CO 4	The course ends with 10 min talks by students on topics that are Not in their area of specialization, that count for 50% of the grade.
CO 5	The RM course is unusual, but seems to work, with students giving quite positive comments