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BASANTSING INSTITUTE OF SCIENCE
&
J. T. LALVANI COLLEGE OF COMMERCE
(AUTONOMOUS)

"A" Road, Churchgate, Mumbai - 400 020, India.

Affiliated to
University of Mumbai

Program: M.Sc. Chemistry

(Physical)

Course: Thermodynamics, Surface and Biophysical

Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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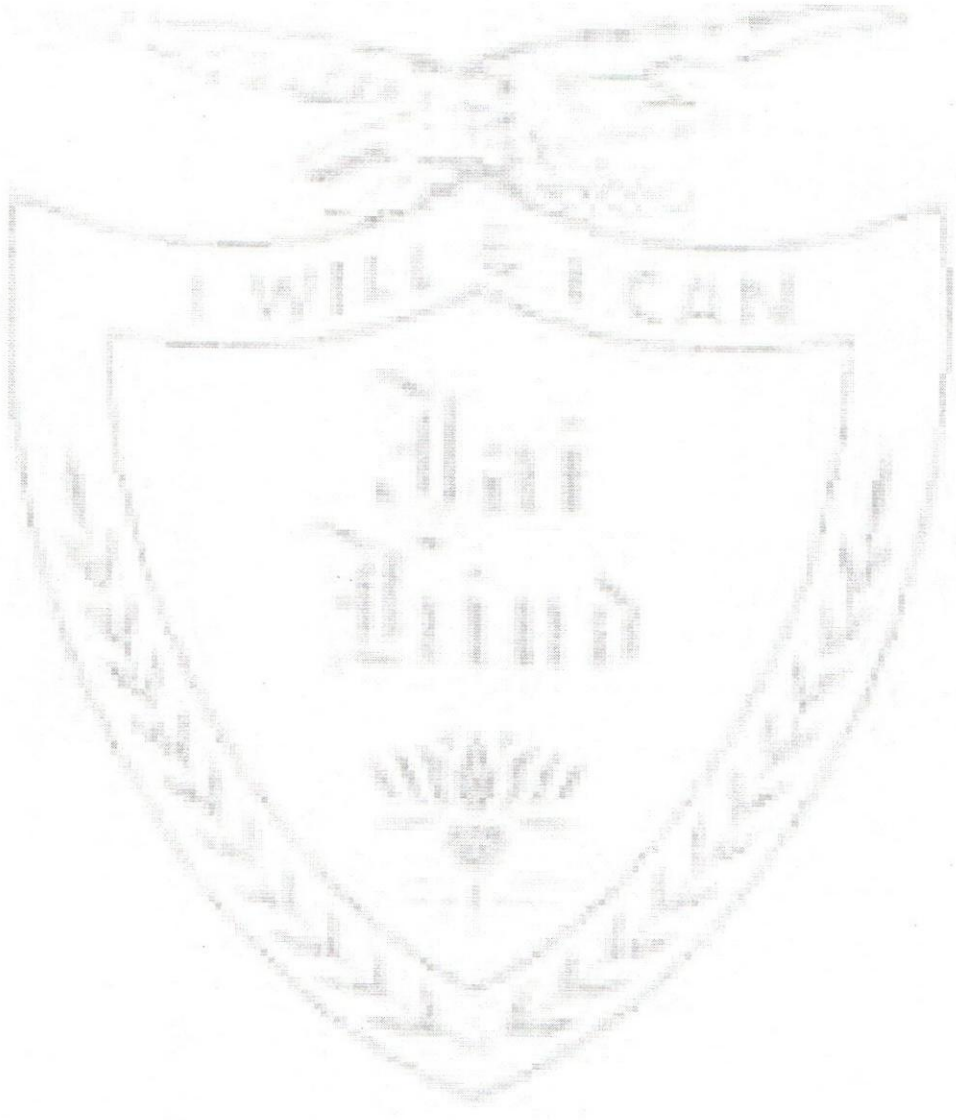
M.Sc. Thermodynamics, Surface and Biophysical Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE1401	**Thermodynamics, Surface and Biophysical**	**04**	**04**



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Semester IV – Theory

Course: PSCHE1 401	**Thermodynamics, Surface and Biophysical (Credits: 04 Lectures/Week: 04)**	
	Non-equilibrium thermodynamics, Voltametric methods, surface and interfacial chemistry & physical chemistry of biomolecules	
	Objectives: **1. To introduce the concept and phenomena of irreversible thermodynamics.** **2. To understand the application of different voltametric methods.** **3. To explain the advanced concept of surface and interfacial chemistry.** **4. To understand the physical chemistry of biomolecules.** **Outcomes:** **1. To describe the Onsager's reciprocal relation and verify the Onsager relation.** **2. To illustrate the application of Cyclic voltammetry in organic synthesis.** **3. To summarise the concept of surface and interfacial chemistry.** **4. To describe the principles of protein structure and stability.**	
Unit I	**Irreversible Thermodynamics** 1.1 Phenomenological laws and Onsager's reciprocal relation, conservation of mass and energy in closed and open systems**[3L]** 1.2 Entropy production due to heat flow & in chemical reactions. Entropy production and entropy flow in open systems. Transformation properties of fluxes and forces**[4L]** 1.3 Principle of microscopic reversibility and the Onsager reciprocal relations, verification of the Onsager relations**[3L]** 1.4 Electrokinetic effects, Thermomolecular pressure difference and Thermomechanical effect **[2L]** 1.5 Stationary non-equilibrium thermodynamics. Applications of irreversible thermodynamics to biological systems**[2L]** 1.6 Nonlinear thermodynamics of irreversible processes**[1L]**	**15L**
Unit II	**Voltametric Methods** 2.1 Recapitulation: DC polarography, DME, Introduction to three electrode system; modern polarography and voltammetry necessity and development of new voltametric techniques and their comparison with classical DC polarography**[2L]** 2.2 Voltametric methods:Sampled DC polarography (TAST), Linear sweep voltammetry (LSV), Cyclic voltammetry (CV), diagnostic	**15L**

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	criteria of cyclic voltammetry**[3L]** 2.3 Normal pulse polarography (NPP), Differential pulse polarography (DPP), Double differential pulse polarography (DDPP)**[4L]** 2.4 Sinusoidal AC polarography, square wave polarography**[4L]** 2.5 Applications of electrochemical methods in Organic synthesis**[2L]**	
Unit III	**Surface and Interfacial Chemistry** 3.1 **Surface active agents:** Introduction and their classification, hydrophile lipophile balance**[2L]** 3.2 **Micellization:** shape and structure of micelles, hydrophobic interaction, critical Micelles concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, micelle catalysis, reverse micelles**[4L]** 3.3 **Emulsions:** Solubilization, micro emulsions, characterization of microemulsions**[2L]** 3.4 **Solid surfaces:** Surface energy and imperfections, adsorption at solid surfaces **[1L]** 3.5 **Solid-liquid interfaces:** Work of adhesion and cohesion, wetting and contact angles, adsorption from solution at solid/ liquid interfaces, critical surface tension**[3L]** 3.6 **Electrical properties of double layers:**Models of EDL, colloidal stability, DVLO theory, electrokinetic phenomena, zeta potential-measurement and applications**[3L]**	**15L**
Unit IV	**Biophysical Chemistry** 4.1 **Principles of protein structure and stability:** Forces in protein folding, Primary structure; Secondary structure alpha and beta confirmation, collagen structure, stability of alpha helix, Ramchandran plot, Tertiary structure, structure of myoglobin and haemoglobin, Quaternary structure, symmetry consideration, Analysis of subunits and chain arrangement of subunits, stability of globular quaternary structure. Protein folding rules, pathways and kinetics. Protein Denaturation**[8L]** 4.2 **Structure of Nucleic acids:** compositions of nucleic acid, Chargaff's rule in DNA, RNA base compositions, Primary & Secondary structure of DNA & RNA**[3L]**	**15L**

	4.3 **Electrophoresis:** Principle, Types and factors affecting Electrophoresis. Zone Electrophoresis (Paper, Gel, Capillary, Cellulose acetate electrophoresis), applications **[4L]**	

Standard References:

Unit I

1. I.Prigogine, Introduction to Thermodynamics of Irreversible
2. Processes,3rded., Interscience,NewYork, 1967.
3. Principles of Physical Chemistry B.R. Puri, L.R. Sharma, M.S. Pathania, Vishal Publishing Company, 2008.

Unit II

4. Bard A.J., Faulkner L.R., Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley 2000
5. D.A.Skoog,F.J.Holler, J.A.Nieman,Principles of Instrumental analysis, 6thEd.
6. Bagotsky, V.S., Fundamentals of Electrochemistry, 2nd Edition, Wiley-Interscience, 2006

Unit III

7. M. J. Rosen. Surfactants and Interfacial Phenomena (3rd edn.), John Wiley (2004).
8. An introduction to the principles of surface chemistry- Aveyard
9. Micelles- Theoretical and applied aspects- Y.Morai
10. Fundamentals of colloid science- Robert J Hunter- Vol I and II

Unit IV

11. Nelson, D. L., & Cox, M. M. (2017). Lehninger principles of biochemistry (7th ed.). W.H. Freeman
12. Klostermeier, D., & Rudolph, M. (2018). Biophysical Chemistry (1st ed.). CRC Press.
13. Biophysical Chemistry: Principles & Techniques Handbook by Avinash Upadhyay, Kakoli Upadhyay and Nirmalendu Nath, Himalaya Publishing House.
14. Allen, James P. "Biophysical Chemistry." Wiley.com, 8 Aug. 2008.

Additional References:

15. Seddon J.M., Gale J.D., Thermodynamics and Statistical Mechanics, Tutorial Chemistry Texts series, Vol. 10, Royal Society of Chemistry, 2001
16. Silbey R.J., Alberty R.A., Physical Chemistry, 3rd Edition, John Wiley and Sons, Inc. 2002
17. Laidler K.J., Meiser J.H., Physical Chemistry, 2nd Edition, CBS publishers and distributors 1999
18. Agarwal B.K., Eisner M., Statistical Mechanics 1988, Wiley Eastern, New Delhi
19. Lingane J.J., Electroanalytical Chemistry, 2nd Edition, Interscience publishers, Inc., New York (1958)
20. Bard A.J., Electro-analytical Chemistry, Marcel Dekkre Inc., New York
21. Noel M., Vasu K.J., Cyclic Voltammetry and Frontiers of Electrochemistry, IBH, New Delhi, 1990

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Evaluation Scheme

- **Continuous Assessment (CA) – 40 Marks**
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- **Semester End Examination (SEE)- 60 Marks**

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Program: M.Sc. Chemistry

(Physical)

Course: Practical Coursework III

Semester IV

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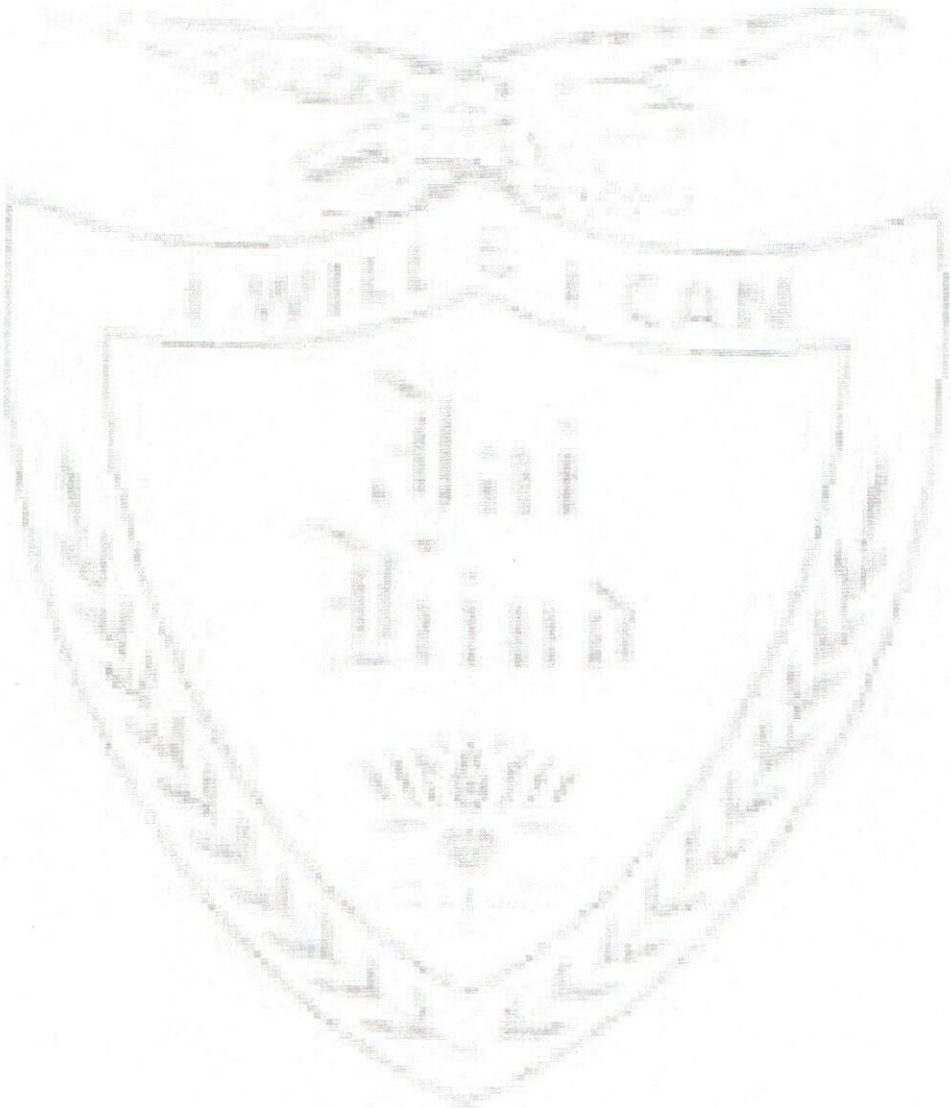
M.Sc. Practical Coursework III Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP1401	**Practical Coursework III**	**02**	**02**



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Semester IV – Practical

Course: PSCHEP1401	**Practical Coursework III (Credits: 02, Practical /Week: 02)**
	Objectives: **To solve problems in chemistry through experiments.** **Outcomes:** **Learner will be able to design experiments and will gain experimental skills to solve problems in chemistry**
	PSCHEP1401: Practical Coursework III 1. Determination of the transport number of Silver(I) ions by Hittorf's method. 2. To study the order of the reaction between bromate and bromide. 3. To determine the Van't Hoff's factor by cryoscopic method. 4. To determine K_1 and K_2 of a dibasic acid by titration with a base by pHmetry. 5. To determine the composition of a mixture of HCl, KCl and NH_4Cl by titration with NaOH and $AgNO_3$. 6. To determine the liquid junction potential with a concentration cell with and without transference. REFERENCES: 1. Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 1989 2. Woolins J.D., Inorganic Experiments, VCH, Weinheim, 1994 3. Palmer W.G., Experimental Inorganic Chemistry, CUP Archive 1954 4. Raj G., Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd, 2013 5. Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo 6. Athawale V.D., Mathur P., Experimental Physical Chemistry, New Age International Publishers, 2017. 7. Vishwanathan B., Raghavan P.S., Practical Physical Chemistry, Viva Books Private Limited, 2005 8. James A.M., Prichard F.E., Practical Physical Chemistry, 3rd Edition, Longman, 1974 9. Lewitt B.P., Findlay's Practical Physical Chemistry, 9th Edition, 1973 10. Brennan C.D., Tipper C.F.H., A Laboratory Manual of Experiments in Physical Chemistry, McGraw Hill 1967 11. Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo

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Evaluation Scheme

- **Semester End Examination (SEE)- 50 Marks**

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Program: M.Sc. Chemistry

(Physical)

Course: Solid State Chemistry

Semester IV

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M.Sc. Solid State Chemistry Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE1402	**Solid State Chemistry**	**04**	**04**

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Semester IV – Theory

Course: PSCHE1402	**Solid State Chemistry (Credits: 04 Lectures/Week: 04)**	
	Solid state- structure, properties and synthesis; defects and non-stoichiometry, electrical, magnetic, thermal and optical properties of solids	
	Objectives: **1. To understand the Structure, properties and Synthesis of solids.** **2. To understand the crystal defects and non-stoichiometry.** **3. To introduce the Electrical and Magnetic Properties of solids.** **4. To summarise the thermal and optical properties of solids.** **Outcomes:** **1. To distinguish between different structure of solids and various method to synthesize it.** **2. To identify different type of defects and its applications.** **3. To describe the electrical, magnetic, thermal and optical properties of solid.**	
Unit I	**Structure, properties and Synthesis of solids** 1.1 **Simple structures:** (i) **AB** type compounds (PbO & CuO) (ii) **AB_2**type (β cristobalite, CaC_2 and Cs_2O) (iii) **AB_3**type (ReO_3, Li_3N) (iv) **ABO_3**type, relation between ReO_3 and perovskite $BaTiO_3$, its polymorphic forms, oxide bronzes, ilmenite structure (v) **AB_2O_4**type, normal, inverse, and random spinel structures 1.2 **Linked Polyhedra** (i) Corner sharing: tetrahedral structure (silicates) and octahedral structure (ReO_3) and rotation of ReO_3 resulting in VF_3, RhF_3 and calcite type structures (ii) Edge sharing: tetrahedral structures (SiS_2) and octahedral structures (BiI_3 and $AlCl_3$), pyrochlores, octahedral tunnel structures and lamellar structures 1.3 **Methods of synthesis:** Chemical method, high pressure method, arc technique and Skull method (with examples). 1.4 **Single crystal growth:** Crystal growth from melt- Bridgman (i) Crystal growth from melt: Bridgman and Stockbargar, Czochralski and Vernuil methods (ii) Crystal growth from liquid solutions: Flux growth and temperature gradient methods (iii) Crystal growth from vapour phase: epitaxial growth methods	**15L**

Unit II	**Crystal defects and non-stoichiometry** 2.1 **Point defects:** Point defects in metals and ionic Crystals – Frenkel defect and Schottky defect;thermodynamic formation of these defects (mathematical derivation to find defect concentration); defects in non-stoichiometric compounds, color centers 2.2 **Line defects:** Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids 2.3 **Surface defects:** Grain Boundary and Stacking Fault. Dislocation and Grain Boundaries, Vacancies and Interstitial Space in Non-Stoichiometric Crystals, Defect Clusters, Interchangeable Atoms and Extended Atom Defects	**15L**
Unit III	**Electrical and Magnetic Properties of Solids** 3.1 **Electrical properties of solids:** Conductivity of solid electrolytes, fast ion conductors, mechanism of conductivity, hopping conduction, Thomson and Seeback Effects; Thermocouples and their applications, Hall effect, Dielectric, ferroelectric, piezoelectric and pyroelectric materials and their inter-relationships and applications 3.2 **Magnetic properties:** Behaviour of substance in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering, Hysteresis, Hard and soft magnets; Structures and magnetic Properties of Metals and Alloys; Transition metal Oxides; Spinels; garnets, Ilmenites;Perovskite and Magneto plumbites, Application in transformer cores, information storage, magnetic bubble memory devices and as permanent magnets	**15L**
Unit IV	**Thermal and Optical Properties of Solids** 4.1 **Thermal properties:**Introduction, heat capacity and its temperature dependence; thermal expansion of metals; ceramics and polymers and thermal stresses **4.2 Optical properties:** Color Centres and Birefringence; Luminescent and Phosphor Materials; Coordinate Model; Phosphor Model; Anti Stokes Phosphor	**15L**

Standard References:

1. L. E. Smart and E. A. Moore, Solid State Chemistry-An introduction, 3rd edition, Taylor and Francis, 2005.
2. A.R.West, Solid State Chemistry and Its Applications, John Wiley & sons, 1987.
3. C.N.R. Rao and J.Gopalkrishnan New Directions in Solid State Chemistry, 2nd

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Ed., Combridge University Press. 1997
4. D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Ed. Wiley and sons, New York, 1966.
5. J.M. Hollas, Symmetry in Molecules, Chapman adn Hall Ltd.,1972.
6. Robert L carter, Molecular Symmetry and Group Hohn Wiley and Sons, New York, 1988.
7. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, John Wiley and Sons, Chichester, 1993.
8. R.N.Kutty and J.A.K.Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.
9. H.V.Keer, Principles of the Solid state, Wiley Eastern Ltd., 1993. Gary L.Miessler and Donald A.Tarr, Inorganic Chemistry, 3rd edition , Pearson Education, Inc., 2004.
10. D.K.Chakraborty, Solid State Chemistry, New Age International Publishers, 1996.
11. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press,N.Y. (1966)

Evaluation Scheme

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Course: Practical Coursework IV

Semester IV

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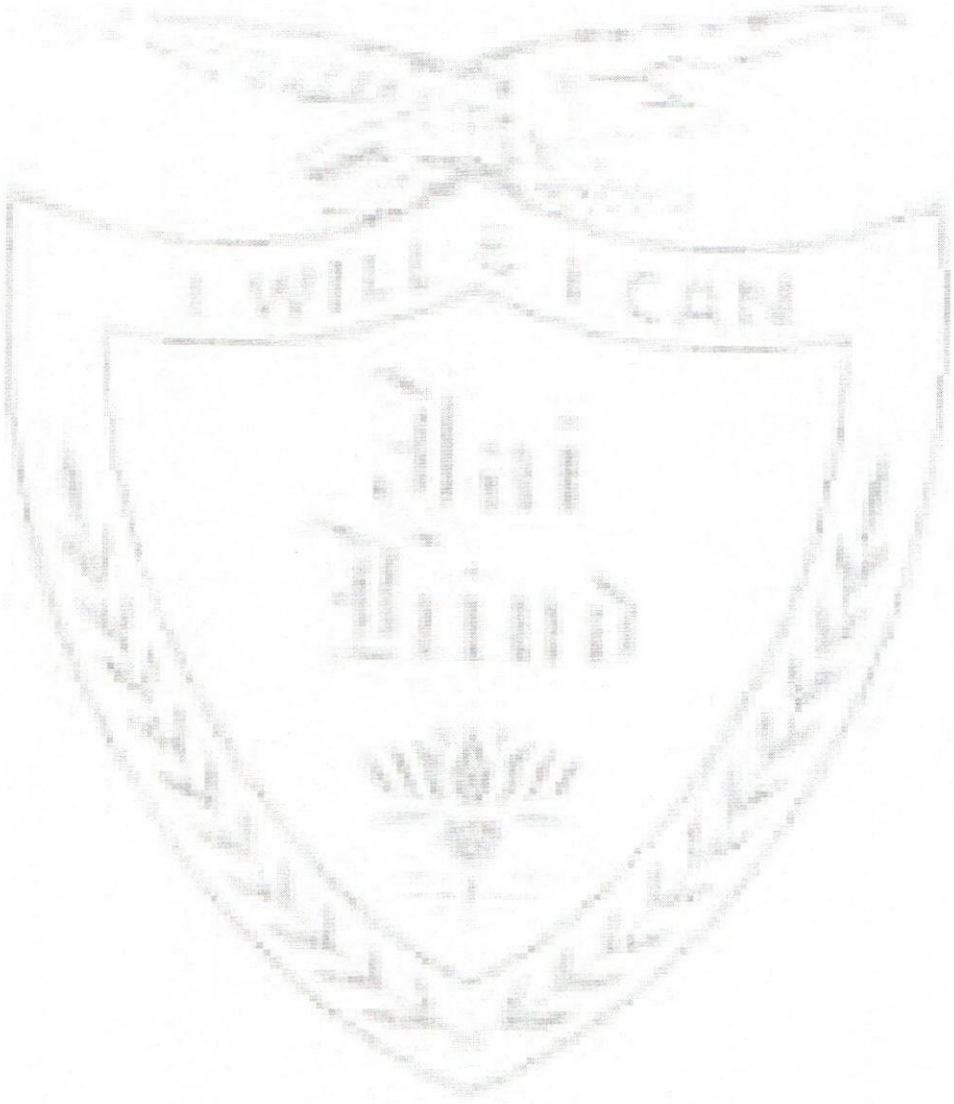
M.Sc. Practical Coursework IV Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP1402	**Practical Coursework IV**	**02**	**02**



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Semester IV – Practical

Course: PSCHEP1402	Practical Coursework IV (Credits: 02, Practical /Week: 02)
	Objectives: **To evaluate commercial samples, ores and alloys for their percentage assay** **Outcomes:** **Learner will be introduced to quality control procedures, errors in measurement and comparison against standards.**
	PSCHEP1402: Practical Coursework IV a. Analysis of commercial sample of electral powder for Na+ content by flame photometer b. Analysis of commercial sample of sea water for percentage salinity by Volhard's method. c. Analysis of commercial sample of Fasting salt for chloride content by conductometrically d. Determination of Stability constant of $[Ag(en)^+$ by potentiometry e. Analysis of of Galena ore for Pb content by gravimetry & Fe by colorimetry f. Analysis of Brass alloy for Cu content by iodometrically and Zn complexometricaly REFERENCES: 1. Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 1989 2. Woolins J.D., Inorganic Experiments, VCH, Weinheim, 1994 3. Palmer W.G., Experimental Inorganic Chemistry, CUP Archive 1954 4. Raj G., Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd, 2013 5. Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo 6. Athawale V.D., Mathur P., Experimental Physical Chemistry, New Age International Publishers, 2017. 7. Vishwanathan B., Raghavan P.S., Practical Physical Chemistry, Viva Books Private Limited, 2005 8. James A.M., Prichard F.E., Practical Physical Chemistry, 3rd Edition, Longman, 1974 9. Lewitt B.P., Findlay's Practical Physical Chemistry, 9th Edition, 1973 10. Brennan C.D., Tipper C.F.H., A Laboratory Manual of Experiments in Physical Chemistry, McGraw Hill 1967 11. Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo.

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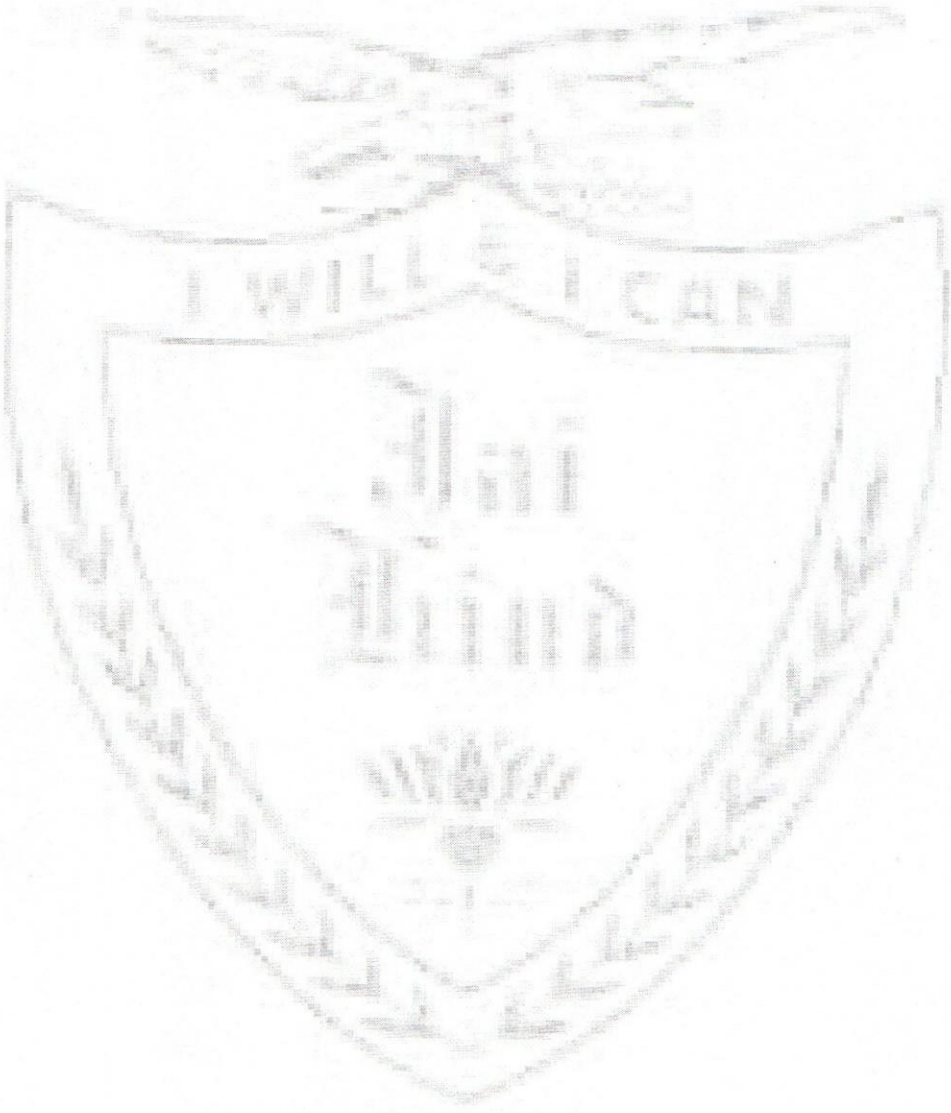
Evaluation Scheme

Semester End Examination (SEE)- 50 Marks



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Program: M.Sc. Chemistry

(Physical)

Course: Photochemistry and Advanced Spectroscopy

Semester IV

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M.Sc. Photochemistry and Advanced Spectroscopy Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHE1403	Photochemistry and Advanced Spectroscopy	04	04

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Semester IV – Theory

Course: PSCHE1403	**Photochemistry and Advanced Spectroscopy (Credits:04 Lectures/Week:04)**	
	Photochemistry and photocatalysis, fluorescence phenomenon and its applications, advanced techniques in NMR spectroscopy & mass spectrometry	
	Objectives: **1. To introduce the concept of Photochemistry & Photocatalysis.** **2. To understand the principal and application of fluorescence phenomena.** **3. To describe the principal, instrumentation and applications of advanced Spectroscopic Techniques-I& II.** **Outcomes:** **1. To apply the principles of Photochemistry & Photocatalysis in water splitting, CO_2 reductions etc.** **2. To describe the phenomena and mechanism of fluorescence quenching.** **3. To elucidate the structure of molecules applying advanced Spectroscopic Techniques-I & II.**	
Unit I	**Photochemistry & Photocatalysis** **1.1 Photochemistry [8L]** 1.1 **General Introduction:** Laws of photochemistry, selection rules for transitions, shapes of absorption bands and Frank Condon Principle. 1.2 **Properties of excited state:** Environmental effect on absorption and emission spectra, solvatochromic shifts, properties of excited state- dipole moment, acidity constant, redox potential. 1.3 **Photophysical pathways:** types of photophysical pathways, types of radiationless transitions, fluorescence emission, triplet state and phosphorescence, delayed fluorescence: e-type and p-type. **1.2 Photocatalysis [7L]** 1.4 **Photocatalytic activity:** Photocatalytic reactions, mechanism, influence of different parameters on catalytic activity. 1.5 **Types of photocatalysts:** SMOs (TiO_2, ZnO), metal chalcogenides (MoS_2, WS_2), quantum dots (C, S), mesoporous materials for photocatalysis and their synthesis (one each)	**15L**

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	1.6 **Application of photocatalysis:** photodegradation of organic pollutants, CO_2 photoreduction, water splitting.	
Unit II	**Applications of Fluorescence Phenomena** a. **Introduction & Fluorescence Characteristics:** Fluorescence phenomenon, Characteristics of fluorescence- mirror image rule, exceptions, Kasha's Rule; Stokes shift, fluorescence lifetimes and quantum yields, steady state fluorescence and fluorescence anisotropy **[2L]** b. **Structural effects on Fluorescence emission:** π-electron system, substituted aromatic hydrocarbons- internal heavy atom effect, EDG, EWG, Sulfonates, heterocyclic compounds- Nitrogen heterocycles, coumarins, BODIPY; Luminescence of nanostructures- carbon nanostructures, quantum dots. **[2L]** c. **Fluorescence quenching**: mechanism of quenching- static and dynamic; derivation of Stern-Volmer equations for static and collisional quenching, quenching by added substances- charge transfer mechanism (CT) and energy transfer mechanism (RET) **[3L]** d. **Instrumentation and sensing:** instrumentation of a steady state spectrofluorophotometer, modes of measurement- fixed excitation wavelength, fixed emission wavelength, fixed excitation and emission wavelength, variable excitation and emission wavelengths- 3D spectrum, synchronous spectrum; analytical terms associated with sensing- sensitivity, selectivity & ICH guidelines- LOD, LOL, dynamic range **[4L]** e. **Applications of Fluorescence:** Sensing modes and mechanisms, Photoinduced Electron Transfer (PET), Photoinduced Charge Transfer (PCT); design of sensor; miscellaneous applications of fluorescence **[4L]**	**15L**
Unit III	**Advanced Spectroscopic Techniques-I** 3.1 **Basic Concepts in NMR:** Nuclear spin states, magnetic moments, absorption of energy, mechanism of absorption, population densities of nuclear spin states, chemical shift and shielding, NMR spectrometer- CW v/s FT NMR **[4L]** 3.2 **Spin-spin coupling:** spin-spin splitting (n+1) rule, origin of spin-spin splitting and Pascal's triangle, coupling constant J, mechanism of coupling, Karplus relationship, long range coupling, magnetic equivalence, first order splitting and complex multiplets- more than one value of J, second order spectra and Pople spin notations; second order effects and	**15L**

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	field strength of NMR. **[5L]** 3.3 **^{13}C & Heteronuclear NMR:** ^{13}C nucleus, chemical shifts, proton coupled and decoupled ^{13}C NMR, NOE & cross polarization, molecular relaxation processes & integration of spectra, Off-resonance decoupling, solvents used in NMR; ^{19}F, ^{31}P, ^{11}B NMR; heteronuclear coupling of ^{13}C with fluorine and phosphorus. **[4L]** 3.4 **Other topics in 1D NMR:** proton exchange, dynamic NMR, quadrupole broadening of NH protons **[2L]**	
Unit IV	**Advanced Spectroscopic Techniques II:** 4.1 **Pulsed techniques in NMR:** FT-NMR, Attached Proton Test (APT), INEPT & DEPT **[4L]** 4.2 **2D NMR techniques:** Homonuclear 2D NMR- COSY, NOESY; Heteronuclear 2D NMR- HETCOR, HSQC, HMQC, HMBC **[4L]** 4.3 **Mass spectrometer:** Overview, block diagram & sample introduction **[1L]** 4.4 **Ionization methods:** Electron ionization (EI); Chemical ionization (CI); Desorption ionization methods (SIMS, FAB, MALDI); Electron spray ionization (ESI) **[3L]** 4.5 **Mass analyzers:** Magnetic sector, double focusing, Quadrupole, TOF; detection and quantitation; determination of molecular weight & molecular formulae **[3L]** **Spectral problems:** Application of NMR & Mass Spectrometry in structure elucidation.	**15L**

Standard References:

Unit I

1. Rohatgi-Mukherjee, K. K. (1992). Fundamentals of photochemistry. New Delhi: Wiley Eastern Ltd.
2. Photocatalysis- Principles and Applications, Rakshit Ameta, Suresh C.Ameta, CRC Press, Taylor &Francis group, Boca Raton, London, New York, 2017.
3. Zhang, J., Tian, B., Wang, L., Xing, M., Lei, J. - Photocatalysis_ Fundamentals, Materials and Applications-SPRINGER VERLAG, SINGAPORE (2018)

Unit II

4. Lakowicz, J. R. (2006). Principles of fluorescence spectroscopy. New York: Springer.
5. Valeur, B. (2002). Molecular fluorescence: Principles and applications. Weinheim: Wiley-VCH.

Unit III & IV

6. Pavia, D. L., Lampman, G. M., & Kriz, G. S. (1979). Introduction to spectroscopy: A guide for students of organic chemistry. Philadelphia: W.B. Saunders Co
7. Field, L. D., Li, H. L., & Magill, A. M. (2015). Organic structures from 2D NMR spectra.

Additional References:

8. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
9. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
10. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
11. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
12. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
13. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.

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University of Mumbai

Program: M.Sc. Chemistry

(Physical)

Course: Spectral Interpretation

Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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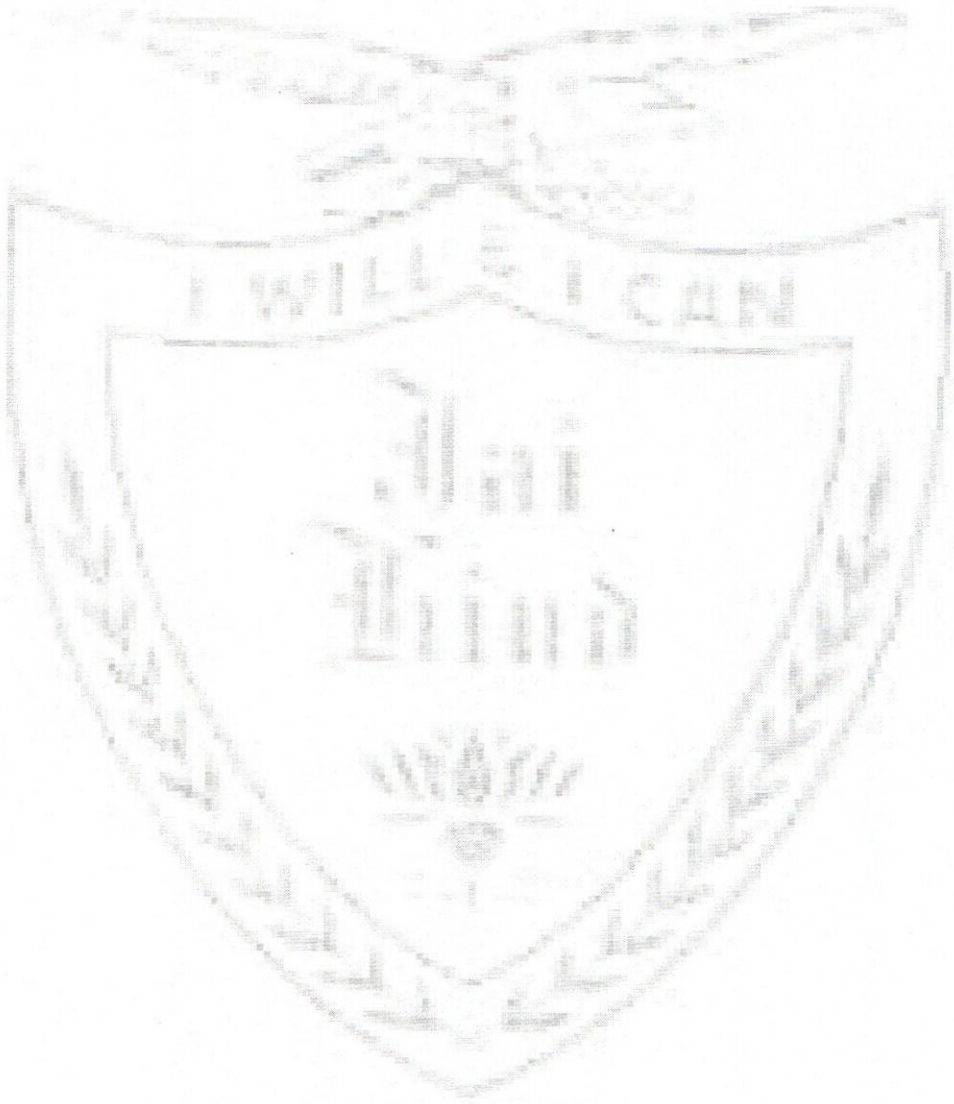
M.Sc. Spectral Interpretation Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP1403	**Spectral Interpretation**	**02**	**02**



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Semester IV – Practical

Course: PSCHEP1403	Spectral Interpretation (Credits: 02, Practicals/Week: 02)
	Objectives: **To elucidate structural information about molecules from their spectral data.** **Outcomes:** **Learner will be able to interpret of UV/IR/NMR/Mass/XRD spectra and its analysis.**
	PSCHEP1403: Spectral Interpretation Interpretation of Uv/IR/NMR/Mass/XRD spectra and its analysis. REFERENCES: 1. Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 1989

Evaluation Scheme

- **Semester End Examination (SEE)- 50 Marks**

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(AUTONOMOUS)
"A" Road, Churchgate, Mumbai - 400 020, India.

Affiliated to
University of Mumbai

Program:M.Sc. Chemistry

(Physical)

Course: Materials, Devices and Computational Chemistry

Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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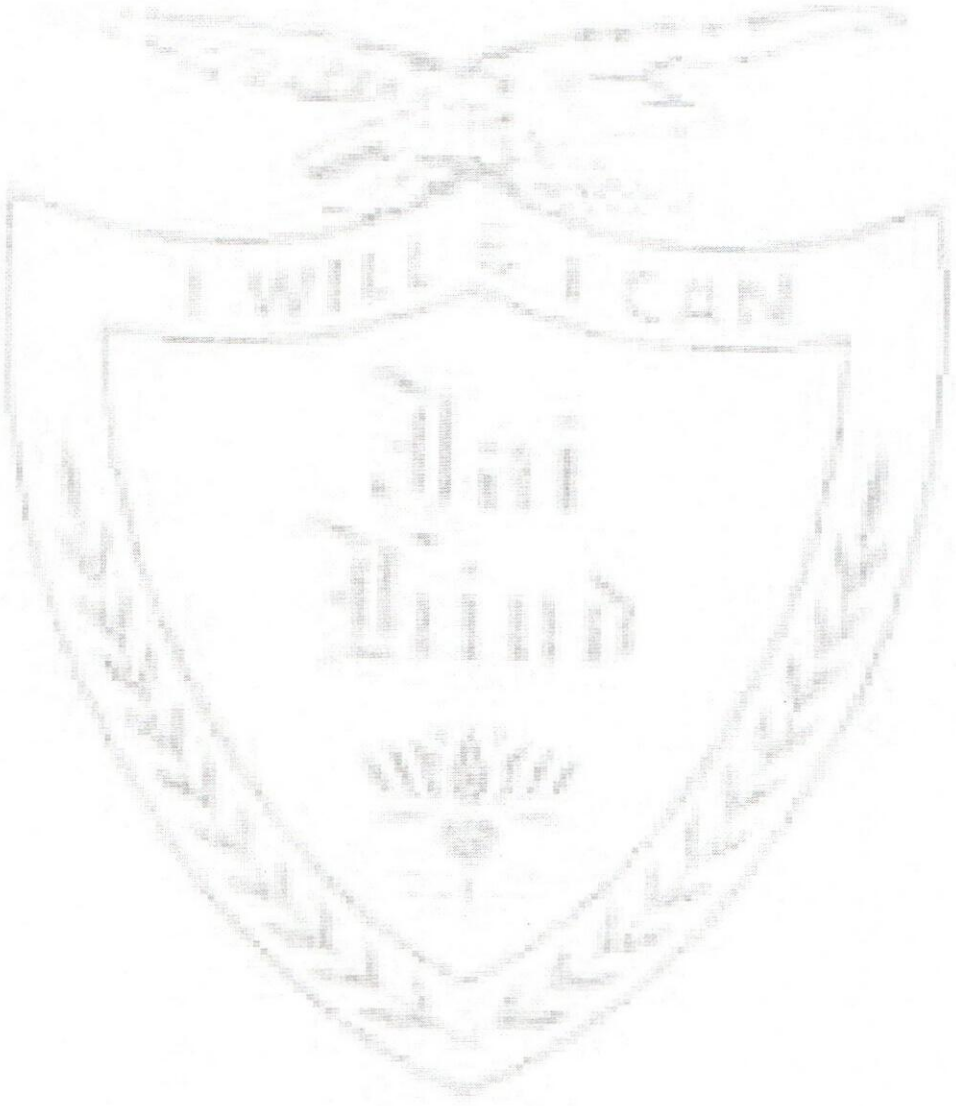
M.Sc. Materials, Devices and Computational Chemistry Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHE1404	Materials, Devices and Computational Chemistry	04	04



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Semester IV – Theory

Course: PSCHE1404	**Materials, Devices and Computational Chemistry (Credits:04 Lectures/Week:04)**	
	Solar photovoltaics, batteries and supercapacitors, organic electronic and photonic materials, Intellectual Property Rights & Cheminformatics	
	Objectives: **1. To describe different photovoltaic cells and its applications in batteries and supercapacitors.** **2. To introduce the concept of organic semiconductors, optoelectronic devices.** **3. To introduce the of Intellectual Property Rights & Cheminformatics.** **Outcomes:** **1. To identify different type photovoltaic cells and its applications in batteries and supercapacitors.** **2. To explain the working of organic semiconductors, optoelectronic devices.** **3. To describe Intellectual Property Rights & Cheminformatics.**	
Unit I	**Energy Conversion and Storage Devices** 1.1 **Solar Photovoltaics:** P-n junction, light generating current, I-V equation, solar characteristics, effects of various parameters on efficiency, losses in solar cells, Solar cell design, Antireflective coating (ARC), solar simulator, Quantum efficiency. **[5L]** 1.2 **Sensitized and polymer photovoltaics:** DSSC, Quantum dot sensitised solar cells, Perovskite sensitised solar cells, Planar and bulk heterojunction polymer solar cells, Exciton generation and dissociation, Advantages, disadvantages, and types of materials. **[4L]** 1.3 **Batteries and Supercapacitors:** Recapitulation of batteries: primary batteries, rechargeable batteries, electrochemical energy storage: laws, parameters, heat effects. Types of batteries (Lead-acid, Ni/Cd, Ni/metal hybrid), charging methods and techniques, characteristic curves, comparison of supercapacitor and batteries, Energetics, Double layer electrostatic capacitor, Pseudocapacitance, Impedance, materials for supercapacitors. **[6L]**	**15L**
Unit II	**Organic Electronic & Photonic Materials [15L]** 3.1 **Introduction:** Brief history of organic electronics, organic	**15L**

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	semiconductor materials, electronic states, and transitions **[2L]** 3.2 **Organic semiconductors:** Charge formation- By injection, By absorption, By doping; determining energy levels of charged molecules- cyclic voltammetry, photoemission spectroscopy; difference between electrical and optical gap; **[5L]** 3.3 **Semiconductor materials:** Transport in organic materials- electrode contacts, transport regimes & magnetic field effects on transport; preparation of semiconductor materials- synthetic approaches, preparation of thin films & patterning for devices **[3L]** 3.4 **Optoelectronic devices:** Basic processes- photon absorption, spontaneous photon emission, stimulated photon emission; Devices- OFET, OPV, OLED; molecular materials for OLEDs- hole transporting, electron transporting, emitting materials: fluorescent, phosphorescent & TADF. **[5L]**	
Unit III	**Intellectual Property Rights [15L]** 3.1 **Introduction to Intellectual Property:** Definitions and types of IP, importance of protecting IP, economic value of IP- intangible assets and their valuation, licensing, and technology transfer laws. **[2L]** 3.2 **Patents:** Definition, Historical perspective, Basic and associated right, WIPO, PCT system, databases in patent search- google patents, reading and writing patents **[5L]** 3.3 **Industrial Designs:** Definition, how to obtain, features, international design registration **[2L]** 3.4 **Copyrights:** Introduction, how to obtain, differences from Patents **[2L]** 3.5 **Trademarks:** Introduction, how to obtain, different types of marks- collective marks, certification marks, service marks, trade names etc. **[2L]** 3.6 **Geographical indications:** Definition, rules for registration, prevention of illegal exploitation, importance to India. **[2L]**	**15L**
Unit IV	**Cheminformatics [15L]** 4.1 **Introduction to Cheminformatics:** History & evolution of cheminformatics, fundamental questions & learning, major tasks **[2L]**	**15L**

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	4.2 **Representation of molecules:** Nomenclature, different types of notations, Line notations- SMILES coding, InChi notation; Graph theory & matrix representations, input and output of chemical structures, standard structure exchange formats, structures of molfiles and sdfiles, Tools- academic programs: Marvin Sketch, ACD labs; commercial tools: ChemDraw, Shrodinger, Accelrys **[5L]** 4.3 **Representation of chemical reactions:** Reaction types, reaction center, chemical reactivity, Hendrickson's scheme **[2L]** 4.4 **Searching Chemical Structures:** Full structure search, sub-structure search, basic ideas, similarity search, basics of computation of physical and chemical data and structure descriptors, data visualisation **[2L]** 4.5 **Applications:** QSPR, Spectra correlations, Computer aided synthesis design, docking & computer aided drug designing **[4L]**	

Standard References:

Unit I

1. https://www.pveducation.org/pvcdrom/solar-cell-operation
2. Solar photovoltaics, Fundamentals, Technologies and Applications by Chetan Singh Solanki, PHI Learning Private Limited, Delhi-110092.
3. Dye Sensitized Solar Cells by K. Kalyansundaram, EPFL Press, A Swiss academic publisher distributed by CRC press.
4. Battery Technology Handbook by H. A. Kiehne , Marcel Dekker, Inc. , New York, Basel.
5. Electrochemical Supercapacitors, Scientific fundamentals and Technological Applications by B. E. Conway, Kluwer Academic/ Plenum Publishers, New York,Boston, Dordrencht, London, Moscow.

Unit II

6. Kohler, A., & Bassler, H. (2015). *Electronic processes in organic semiconductors: An introduction.*
7. Muller, T. J. J., & Bunz, U. H. F. (2007). *Functional organic materials: Syntheses, strategies and applications*. Weinheim: Wiley-VCH.
8. Ostroverkhova, O. (2019). *Handbook of organic materials for electronic and photonic devices.*
9. Sun, S.-S., & In Dalton, L. R. (2019). *Introduction to organic electronic and optoelectronic materials and devices.*

Unit III

10. Duran, N., Fonseca, L. C., & Seabra, A. B. (2019). *Intellectual property in chemistry: A guide to applying for and obtaining a patent for graduate students and postdoctoral scholars.*

Unit IV

11. Gasteiger, J., & Engel, T. (2008). *Chemoinformatics: A textbook*. Weinheim: Wiley-

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VCH.
12. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
13. Karthikeyan, M., & Vyas, R. (2014). *Practical chemoinformatics.*
14. In Engel, T., & In Gasteiger, J. (2018). *Applied chemoinformatics: Achievements and future opportunities.*

Evaluation Scheme

- **Continuous Assessment (CA) – 40 Marks**
  - Knowledge and Application based: Objective test of 20 Marks
  - Skill based (20 marks): Learner will be assessed on relevant skills pertaining to the course content of a particular paper which could involve but not limited to
    Oral Presentations on relevant topics
    Review writing/Worksheets etc.
- **Semester End Examination (SEE)- 60 Marks**

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"A" Road, Churchgate, Mumbai - 400 020, India.

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University of Mumbai

Program: M.Sc. Chemistry

(Physical)

Course: Research Project

Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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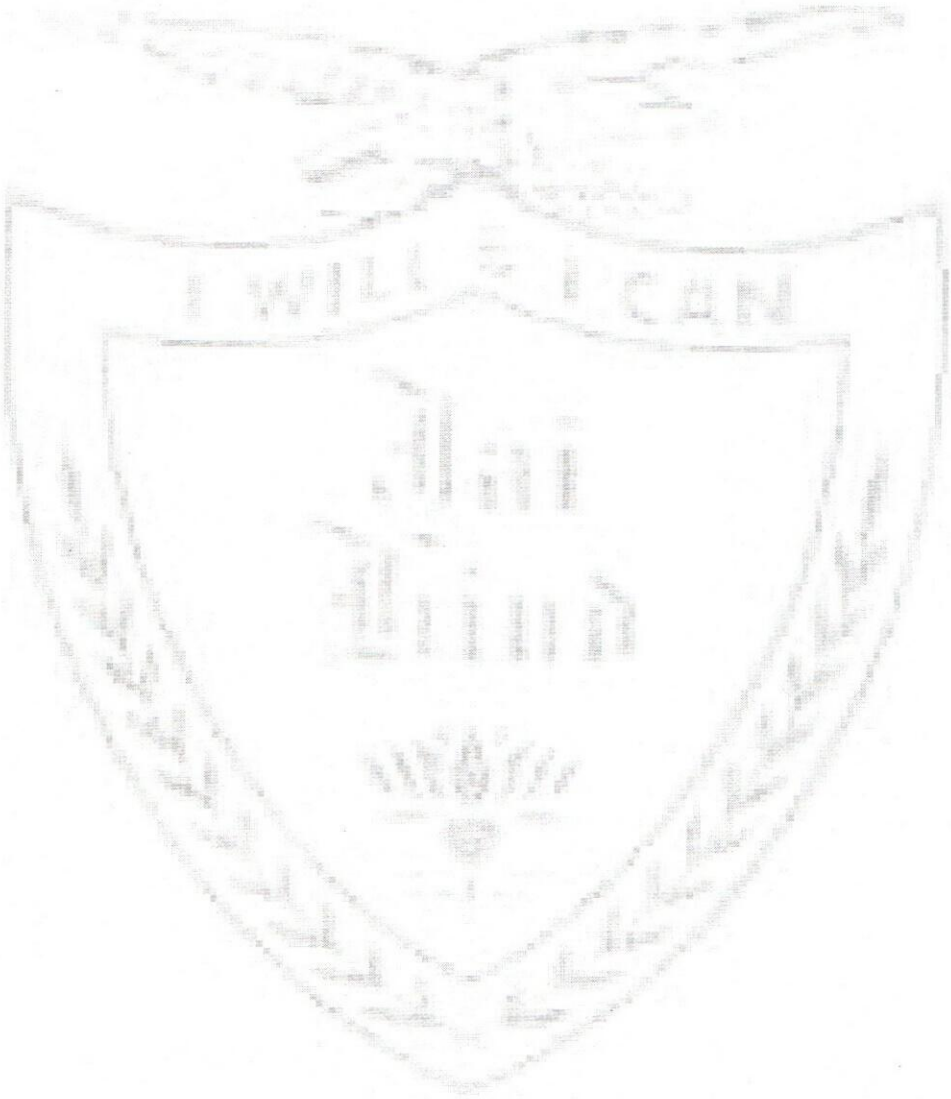
M.Sc. Research Project Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP1404	**Research Project**	**02**	**02**



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Semester IV – Practical

Course: PSCHEP1404	Research Project (Credits: 02, Practical/Week: 02)
	Objectives: **To design a research problem and investigate it experimentally through project.** **Outcomes:** **Learners will be able to understand research workflow- literature review, identification of research problem and investigation.**
	PSCHEP1404: Research Project Short term research project culminating in a dissertation and presentation of the work done.

Evaluation Scheme

- **Semester End Examination (SEE)- 50 Marks**

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