



UNIVERSITY OF CALICUT

Abstract

General and Academic IV -Faculty of Science -Scheme and Syllabus of M.Sc Chemistry (Nano Science) Programme w.e.f 2022 Admission in tune with Regulations under Choice-based Credit Semester System for Post Graduate Programmes (CCSS PG-2022) - Implemented - Subject to ratification by Academic Council -Orders Issued.

G & A - IV - J

U.O.No. 11070/2022/Admn

Dated, Calicut University.P.O, 03.06.2022

*Read:-*1.U.O.No. 8481/2022/Admn dated, 11.04.2022

2. U.O.No. 9278/2022/Admn dated, 28.04.2022

3. Item No.1 of the Minutes of the meeting of the Board of Studies in Nanoscience and Technology held on 07.05.2022.

4. Remarks of the Dean Faculty of Science, dated 27.05.2022.

5. Orders of the Vice chancellor in the file of even no, Dated 28.05.2022.

ORDER

1. The Regulations under Choice-based Credit Semester System for Post Graduate Programmes (CCSS PG-2022) of all Teaching Departments / Schools of the University of Calicut, has been implemented with effect from 2022 Admission, vide paper read (1) above.
2. The existing M Tech Nanoscience and Technology programme under the Department of Nanoscience and Technology has been restructured in to two separate programmes, M.Sc Physics (Nano Science) and M.Sc Chemistry (Nano Science), w.e.f 2022 admission, vide paper read (2) above.
3. The meeting of the Board of Studies in Nanoscience and Technology (Single Board), held on 07.05.2022, vide paper read (3) above, has resolved to approve the scheme & syllabus of M.Sc Chemistry (Nano Science) in tune with Regulations under Choice-based Credit Semester System for Post Graduate Programmes (CCSS PG-2022) of all Teaching Departments / Schools of the University of Calicut, w.e.f. 2022 admission.
4. The Dean, Faculty of Science, vide paper read (4) above, has approved the above resolution of the Board of Studies in Nanoscience and Technology (Single Board) held on 07.05.2022.
5. Considering the urgency, sanction has been accorded by the Vice Chancellor, to implement the scheme & syllabus of M.Sc Chemistry (Nano Science) in tune with Regulations under Choice-based Credit Semester System for Post Graduate Programmes (CCSS PG-2022) of all Teaching Departments / Schools of the University of Calicut, w.e.f. 2022 admission, vide paper read (5) above, subject to ratification by the Academic Council.

6. The scheme & syllabus of M.Sc Chemistry(Nano Science), in tune with Regulations under Choice-based Credit Semester System for Post Graduate Programmes (CCSS PG-2022) of all Teaching Departments / Schools of the University of Calicut, is therefore implemented with effect from 2022 Admission , subject to ratification by the Academic Council.
7. Orders are issued accordingly. (Syllabus appended).

Abdussamad M

Assistant Registrar

To

The Head, Department of Nanoscience & Technology

Copy to: PS to VC/PA to PVC/ PA to R/PA to CE/JCEI/JCEV/JCEVII/CHMK
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Forwarded / By Order

Section Officer

DEPARTMENT OF NANOSCIENCE AND TECHNOLOGY

Programme:

1. **M.Sc. CHEMISTRY (NANOSCIENCE)**
Program Code: **FSCNSCHMSC**

SCHEME, CURRICULUM & SYLLABUS



UNIVERSITY OF CALICUT

(A State University Accredited with “A” Grade by NAAC)

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APRIL 2022

UNIVERSITY OF CALICUT

Department of Nanoscience and Technology, School of Physical Sciences,

University of Calicut

Scheme and Syllabus for

M.Sc. Chemistry (Nanoscience) (Code: FSCNSCHMSC)

Under (CCSS-PG-2022), (w.e.f. 2022 admission onwards)

ELIGIBILITY FOR ADMISSION

B.Sc. Degree of this University with Chemistry/ Industrial Chemistry/ Polymer Chemistry (Main/core) or an equivalent degree with Mathematics & Physics as compulsory complementary, having 50% marks or equivalent grade in Part III (Core and complementary put together) are eligible to apply for this programme. OBC/OEC Candidates are eligible for relaxation up to 5 %. SC/ST Candidates need only to get a pass.

ADMISSION PROCEDURE

Admission to this MSc program shall be based on entrance examination conducted among eligible candidates and successful candidates shall be ranked according to the entrance test marks. Program structure, evaluation and grading will be as per the Choice-based Credit Semester System PG - CCSS Regulations for Post Graduate Programmes of Teaching Departments/Schools of the University of Calicut. Intake is 10.

SCHEME AND CURRICULUM OF THE PROGRAM

- M.Sc. Chemistry (Nanoscience) is a PG program of 2 years duration with 4 semesters. The program includes Core, Elective and Audit courses. The total credit of the program (excluding audit courses) is **80**.
- The total credits of the Audit courses shall be 4 and this credit point will not be considered while calculating the SGPA/CGPA.
- Total credits for the core courses (Theory, Practical, Project) shall be **64**.
- The Project work is compulsory for all students and the credit points assigned is **8**.
- Total credits for the elective courses shall be **16**
- Accumulated minimum credits required for successful completion of the program is **80 (+ 4 credits of the Audit course)**
- Minimum credits required from core courses (Theory, Practical, Project) is **64**
- Minimum credits required from elective courses is **16**
- Minimum attendance required is **75 %**
- Evaluation and grading will be done as per CCSS PG Regulations 2022 - Regulations for Post Graduate Programmes of Teaching Departments/Schools of the University of Calicut

Program Educational Objectives (PEOs)

The PG programme, **M.Sc. Chemistry (Nanoscience)**, offers a well-balanced curriculum that ensures the career prospects of the students with due consideration is given to capacitate the students to face the challenges posed by the specialized areas of knowledge in the global arena. Since Nanoscience being an applied science and has application in various fields, in other words, being a vastly interdisciplinary area with great fluidity, the competence of the students can be improved with specialization and focus on chosen areas.

| | |
|--------------|--|
| PEO-1 | To bring students from different branches of Science under one roof to get benefits of each other's to develop a purely multidisciplinary group to work in the area of applied research focusing the science and technology close to nano regime |
| PEO-2 | Solid foundation in their respective core subjects such as physics and chemistry in addition to nanoscience and technology |
| PEO-3 | Good theoretical and practical knowledge so as to comprehend, analyse, design, and create products and solutions for the real-life problems |
| PEO-4 | Facilitate the students to develop research attitude to do innovative research in diverse area of Nanoscience and Technology |
| PEO-5 | Facilitate research ambiance and practical experiences with advanced technologies for the understanding of exceptional properties shown by matter at nanoscale |
| PEO-6 | Professional and ethical attitude, effective communication skills, teamwork skills, multidisciplinary approach, and an ability to relate nanotechnology to address energy, environmental and biomedical applications |
| PEO-7 | Train the student to design a research problem and the selection of methodologies for meeting the fixed objectives to solve the problem. |
| PEO-8 | Facilitate the student to interact with the peers in other disciplines in industry and society and contribute to the economic growth of the country. |

| Program Specific Outcomes (PSOs) | |
|---|---|
| PSO-1 | Recognise and relate the theories and principles of physics and chemistry for understanding the scientific phenomenon in nano domain |
| PSO-2 | Understand and apply the mathematical techniques for describing and deeper understanding of nano systems. |
| PSO-3 | Understand the quantum mechanical concepts and apply the same in various physical systems and processes at nano regime |
| PSO-4 | Understand and apply the inter-disciplinary concepts and computational simulationsto describe natural phenomenon. |
| PSO-5 | Understand the core of organic, inorganic and physical chemistry and apply the knowledge to explain different phenomenon observed at nano regime. |
| PSO-6 | Provide exposure in various specializationsin the field of Nanoscience with frequent updates |
| PSO-7 | Provide exposure to advanced experimental/theoretical methods for measurement, observation, and fundamental understanding of phenomenon at nanoscale and nanosystems. |
| PSO-8 | Provide practical experience in both physical and chemical sciences with judiciously designed experiments for imparting the research attitude. |
| PSO-9 | Contribute adaptive thinking and adaptability to protect the environment for sustainable development |
| PSO-10 | Well-tempered professional ethics essential to maintain a transparent career |
| PSO-11 | The basic understanding of how interdisciplinary science works to coordinate Nanoscience and Technology. |
| PSO-12 | The vital awareness of computational/mathematical programs to solve the bottleneck issues in different aspects of science and technology. |
| PSO-13 | New ideas to develop advanced nanomaterials for sustainable/eco-friendly energy, clean water, pollution-free air, and modern biology. |

| Program Outcomes (POs) | |
|-------------------------------|---|
| PO-1 | Illustrate the fundamental concepts of classical mechanics and relate it to the progression towards quantum mechanics. |
| PO-2 | Provide extensive knowledge to solve quantum mechanical and solid state physics or chemistry problems and relate them to nanoscience. |
| PO-3 | Provide comprehensive understanding on physics and chemistry of solids, to explain the working of semiconductor based electronic and photonic devices and relate them to nanoscale electronics. |
| PO-4 | Provide a comprehensive understanding of statistical mechanics and chemical kinetics and relate them to the growth of nanoparticles. |
| PO-5 | To familiarize fundamental concepts of nuclear and particle physics and relate them to the characterization of nanomaterials. |
| PO-6 | Illustrate fundamental concepts of size and shape dependent changes in the properties of nanostructured materials for various applications. |
| PO-7 | Provide comprehensive understanding on organic, physical and inorganic chemistry and demonstrate the ability to synthesize and characterize nanostructured materials. |
| PO-8 | Demonstrate ability to design new nanostructured materials, characterize, interpret and analyse the data using the theories related physics and chemistry for catering the needs of the industry. |
| PO-9 | Demonstrate new ideas for addressing the problems of the 21 st century viz., energy crisis and environmental remediation using the knowledge provided through specific electives. |
| PO-10 | Develop confidence in self-educating new knowledge and gain the ability for life-long learning. |
| PO-11 | Develop the knowledge to use computational methods to address the activities of different bio-active compounds. |

University of Calicut, Kerala- 673635

M.Sc. Chemistry (Nanoscience)

Course and Credit Distribution Summary (2022 admission onwards)

| Semester | Code | Subject | Type | Total Marks | Credits |
|------------------------|-------------|---|-------------|--------------------|----------------|
| First Semester | NSC1C 01 | Conceptual Organic Chemistry | Core | 100 | 3 |
| | NSC1C 02 | Chemistry of Transition Metals | Core | 100 | 3 |
| | NSC1C 03 | Kinetics, Photochemistry and Catalysis | Core | 100 | 4 |
| | NSC1C 04 | Quantum Mechanics -I | Core | 100 | 4 |
| | NSC1C 05 | Physics and Chemistry of Solids | Core | 100 | 4 |
| | NSC1P 01 | Practical-I | Core | 100 | 2 |
| | NSC1A 01 | Ability Enhancement Course (AEC) | Audit | | 2* |
| | | TOTAL | | 600 | 20 |
| Second Semester | NSC2C 06 | Organic Reactions and Re-arrangements | Core | 100 | 3 |
| | NSC2C 07 | Thermodynamics and Electrochemistry | Core | 100 | 3 |
| | NSC2C 08 | Quantum Mechanics -II | Core | 100 | 4 |
| | NSC2C 09 | Introduction to Nanomaterials | Core | 100 | 4 |
| | NSC2C 10 | Advanced Analytical Techniques | Core | 100 | 4 |
| | NSC2P 02 | Practical – II | Core | 100 | 2 |
| | NSC2A 02 | Professional Competency Course (PCC) | Audit | | 2* |
| | | TOTAL | - | | 600 |
| Third Semester | NSC3C11 | Organometallic and Bio-inorganic Chemistry | Core | 100 | 3 |
| | NSC3C 12 | Spectroscopy | Core | 100 | 3 |
| | NSC3C 13 | Design, Synthesis and Properties of Nanomaterials | Core | 100 | 4 |
| | NSC3C 14 | Computational Nanotechnology | Core | 100 | 4 |
| | NSC3E 01 | Elective – I (Open Elective) | Elective | 100 | 4 |
| | NSC3P 03 | Practical-III | Core | 100 | 2 |
| | | TOTAL | - | | 600 |
| | NSC4E -- | Elective -II | Elective | 100 | 4 |

| | | | | | |
|------------------------|--------------|----------------|----------|------------|-----------|
| Fourth Semester | | | | | |
| | NSC4E -- | Elective – III | Elective | 100 | 4 |
| | NSC4E -- | Elective – IV | Elective | 100 | 4 |
| | NSC4PR 01 | Project | Core | 100 | 8 |
| | TOTAL | - | | 400 | 20 |
| Total Credits | | 80 | | | |

*The credits for the audit courses (NSC1A 01 and NSC2A 02) will not be counted for computing the SGPA/CGPA of the student. Students have to obtain only pass minimum requirements in the audit courses.

| Code | Subject | Type | Total Marks | Credits |
|----------|--|----------|-------------|---------|
| NSC4E 01 | Nanstructured Solar Cells | Elective | 100 | 4 |
| NSC4E 02 | Nanomaterials for Photocatalysis and Solar Fuel Generation | Elective | 100 | 4 |
| NSC4E 03 | Micro/Nano Electro-mechanical Systems (MEMS/NEMS) | Elective | 100 | 4 |
| NSC4E 04 | Sustainable Nanomaterials | Elective | 100 | 4 |
| NSC4E 05 | Nanomaterials for Supercapacitor Applications | Elective | 100 | 4 |
| NSC4E 06 | Computational Studies on Bio-active Compounds | Elective | 100 | 4 |
| NSC4E 07 | Precision Nanoclusters: Origin and Applications | Elective | 100 | 4 |
| NSC4E 08 | Materials in Medicine | Elective | 100 | 4 |

More Elective courses will be added in near future.

Audit courses:

Two audit courses **Ability Enhancement Course (AEC) & Professional Competency Course (PCC)**, each with 2credits are to be done within the first two semesters of the PG program. The credits will not be counted for computing the overall SGPA/CGPA of the student. The concerned department shall conduct examination for these courses and shall intimate /upload the results of the same to the University on the stipulated date during the III Semester. The student has to obtain only minimum pass requirements in these two courses. Detailed syllabus is framed for both audit courses.

EVALUATION AND GRADING: As per the Calicut University Regulations under Choice Based Credit Semester System for Postgraduate Programmes (CCSS-PG) of the University Campus Departments.

PATTERN OF QUESTION PAPER FOR CORE AND ELECTIVE COURSES

M.Sc. Chemistry (Nanoscience)

Time: 3 hours

Total Marks = 50

Section A

Ten Compulsory short answer type questions of one mark each
(Total Marks = $10 \times 1=10$ Marks)

Section B

Eight paragraph answer type questions, the students shall answer 4 question each of four marks (Total Marks = $4 \times 4 = 16$ marks)

Section C

Eight essay/problem type questions, the students shall answer four questions, each of six marks
(Total Marks = $4 \times 6=24$ marks)

SYLLABUS

For

**M.Sc. Chemistry (Nanoscience)
(Code: FSCNSCHMSC)**

CORE PAPERS

| | | | | | | |
|---|--|-------------------------------------|-------------------------|----------|-------------|----------|
| Course Code | NSC1C 01 | CONCEPTUAL ORGANIC CHEMISTRY | L | T | P | C |
| Core | | | 3 | 0 | 0 | 3 |
| Pre-requisite | Basic knowledge in general Organic Chemistry. | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ul style="list-style-type: none"> • Understand the fundamental concepts and principles in organic chemistry. • Learn different reagents and reactions. • Understand the concepts of stereochemistry and conformations. • Learn different kinds of supramolecules. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of organic chemistry – K1 2. Understand the applications of hetrocyclic compounds and supramolecules – K2 3. Understand the concepts of stereochemistry and conformations solving problems based on it – K2, K3, K5 4. Understand the importance of green chemistry – K1 | | | | | | |
| K1- Remember K2 – Understand K3 – Apply K4 – Analyse K5 – Evaluate | | | | | | |
| UNIT-I | Stereochemistry & Conformations | | 20 Hours | | | |
| <p>Configuration and conformation, Internal factors affecting the stability of molecules -dipole interaction, bond opposition strain, bond angle strain. Perspective and Newman projections. Conformation of acyclic compounds - Ethane, n-butane, alkane dihalides, glycols, tartaric acid, erythro and threo isomers, aldehydes and ketones (acetaldehyde, acetone). Introduction to isomerism, racemisation, resolution, asymmetric synthesis, atrop-isomersim, restricted rotation and asymmetry, reactivity in acyclic compounds, non-carbon chiral centers, Introduction to stereochemistry of cyclohexane, fused rings and bridged compounds, Stereochemistry of organic compounds other than carbon center, Carbohydrate-Stereochemistry and configuration of glucose, mannose, and xylose.</p> | | | | | | |
| UNIT-II | Reactive Intermediates & Synthetic Reagents | | 16 Hours | | | |
| <p>Free radicals: Generation, characterization, Stability, detection, Structural and stereochemical properties. Reactions: Rearrangement and fragmentation reactions. Applications of free radicals: Gomberg-Bachmann reaction and Wohl-Ziegler reaction, Hunsdiecker reaction and Reed Reaction. Carbenes and nitrenes: generation, stability, addition, cyclisation, insertion and ring enlargement reactions, Skattebol re-arrangement, Wolff rearrangement, synthetic applications of the following reagents: N-Bromo-succinimide(NBS), Diazomethane, Dicyclohexyl carbodiimide (DCC), Selenium dioxide, Dichloro-dicyano-benzoquinone(DDQ), Di-isobutyl aluminium hydride(DIBAL), Lithium di-isopropylamide (LDA)</p> | | | | | | |
| UNIT-III | Heterocyclic Compounds | | 15 Hours | | | |
| <p>Aromatic heterocycles and nonaromatic heterocyclic compounds. Five membered ring compounds with one heteroatom. Synthesis, reactions and applications of Pyrrole, Furan, Thiophene, Benzofuran, Benzo-thiophene. Synthesis and reactions of six membered ring</p> | | | | | | |

compounds. Iso-quinoline, Pyrylium salts, 2H-pyran-2 ones, 4H-pyran-4 ones. Five and six membered ring with two or more heteroatoms-pyrimidines and purines, quinazoline, oxazine, Thiazine, Imidazole.

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| UNIT-IV | Supramolecular and Green Chemistry | 16 Hours |
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The concept of recognition, host-guest receptor concept, Forces involved in molecular recognition- hydrogen bonding, Pi stacking, van der Waals and hydrophobic interactions and their significances. Supramolecular chemistry-molecular receptors like calixarenes, crown ethers, Cryptands, Cyclophanes, Cyclodextrins in detail. Self-assembly of supramolecular structures. Introductory study of Combinatorial chemistry. Principles of Green Chemistry. E factor. Atom economic (Diels-Alder reaction, Claisen rearrangement and Michael addition), and atom uneconomic reactions (Wittig reaction, Mitsunobu reaction, and Amide formations). Alternative energy sources: Microwave assisted synthesis, sonochemical synthesis. Emergence of solid acids and zeolites as green catalysts. Discussions on Solvent free Synthesis and Organic reactions in water. Use of super critical carbon dioxide and super critical water as a green media for organic reactions. Fluorous solvents in green organic chemistry. Immobilized Enzyme Catalysis in Green chemistry. Major methods for immobilization of enzymes. Ionic Liquids and Supported Catalysts/reagents. Green Chemistry in Core Organic Synthesis: Multicomponent, Domino and Tandem reactions)

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| UNIT-V | Contemporary Issues | 5 Hrs. |
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Expert lectures, General Seminars, online seminars – webinars

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| | Total Lecture Hours | 72 Hours |
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Text Books/References

1. N.S. Issac, Reactive Intermediates in Organic Chemistry, John Wiley & Sons (1974).
2. Nasipuri - Stereo Chemistry of Organic Compounds, 1993, Edn.
3. Kalsi-Stereochemistry of Organic Compounds Wiley Eastern.
4. F.A. Carey, R.J. Sunberg - Advanced Organic Chemistry, Plenum Press
5. P.Y. Bruice, Organic Chemistry, Prentice Hall.
6. Gilchrist, Heterocyclic Chemistry.
7. P.Y. Bruice, Organic chemistry, Prentice Hall.
8. I.L. Finar, Organic chemistry, Prentice Hall.
9. Carruthers, Modern Synthetic Methods, Cambridge.
10. Fieser & Fieser, Synthetic Reagents, Vol. 1-4.
11. P.T. Anastas and J.C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, Oxford, 1998.
12. H. Vogtle, Supramolecular Chemistry, John Wiley and Sons

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|--|--|---------------------------------------|-----------------|----------|----------|----------|
| Course Code | NSC1C 02 | CHEMISTRY OF TRANSITION METALS | L | T | P | C |
| Core | | | 3 | 0 | 0 | 3 |
| Pre-requisite | Basic knowledge in general inorganic Chemistry. | Syllabus Version | 2022 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ul style="list-style-type: none"> • Understand the importance of coordination chemistry. • Learn different kinds of spectral properties of coordination compounds. • Understand the importance of coordination compounds. • Learn reaction mechanism and photochemistry of inorganic compounds. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of coordination compounds – K1 2. Understand the concepts of MOT in coordination chemistry– K2 3. Understand different kinds of spectral properties of coordination compounds – K2 4. Understand reaction mechanism and photochemistry of inorganic compounds– K1 | | | | | | |
| 1. Problem solving, evaluation and analysis capacity – K3, K4, K5 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 - Analyse K5 – Evaluate | | | | | | |
| UNIT-I | Introduction to Coordination Chemistry | | 15 Hours | | | |
| <p>Coordination compounds. Formation constants, Step-wise and overall stability constants-factors affecting stability- methods of determination of stability constants. Chelate, macrocyclic and macrobicyclic effects. Geometrical and optical isomerism. ORD and circular dichroism. Linkage isomerism. symbiosis-hard and soft ligands. Valance bond theory. Crystal Field and Ligand filed theories (Orbital splitting in octahedral, tetrahedral, cubic, square planar, square pyramidal and trigonal bipyramidal fields). Significance of $10Dq$, factors affecting crystal field splitting, spectrochemical and nephelauxetic series, Jahn-Teller effect, Causes and consequences.</p> | | | | | | |
| UNIT-II | Molecular Orbital Theory and Electronic Spectra of Coordination Compounds | | 16 hours | | | |
| <p>Correlation diagrams (d_1 and d_2 systems). Molecular Orbital Theory of Coordination Compounds. Symmetry adapted linear combination of atomic orbitals in tetrahedral, octahedral, Square planar complexes, formation of symmetry adapted group of ligand, Charge transfer spectra. Charge Transfer spectra ($KMnO_4$). Electronic spectra of complexes – Terms of dn configurations, selection rules for $d-d$ transitions. Orgal diagrams, calculation of Dq, B and β. Correlation diagram. Tanabe and Sugano diagrams. Charge transfer spectra.</p> | | | | | | |
| UNIT-III | Reaction Mechanism of Coordination Compounds | | 16 Hours | | | |
| <p>Reaction mechanisms of metal complexes, rate laws, Metal and ligand substitution reactions in octahedral complexes – A, D and I mechanisms and associated energetic, aquation and base hydrolysis, stereo chemical changes, isomerisation and recemisation.</p> | | | | | | |

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| <p>Fuoss-Eigen equation and factors determining A and D mechanisms. Lability and inertness of the complexes, trans-effect, cis-effect. Reactions of coordinated ligands: hydrolysis, acid dissociation, aldol condensation, transamination, template effect and macrocyclisation. Redox reaction mechanisms – classification, outer-sphere electron transfer, chemical activation, Marcus theory and thermodynamics. Inner-sphere electron transfer – kinetics, effect of the nature of metal and ligand, bridging group effects. Metal-ligand redox reactions. Two electrons, inner-sphere electron transfer processes.</p> | | |
| UNIT-IV | Photochemistry and spectroscopy of Coordination Compounds | 20 Hours |
| <p>Prompt and delayed reactions. Charge transfer excited states and redox processes, communication between excited states, radical pair models. Properties of ligand field excited states, rules for photo substitution, photo-aquation and ligand exchange reactions. Substitution and redox reactions of Cr(III) and Rh(III) complexes. Photo-isomerisation and photo-racemisation. Metal complex sensitizers, chemical actinometry and photo-chromism. Water photolysis and dinitrogen splitting. IR and NMR of simple inorganic compounds and metal complexes. Changes in ligand vibrations on coordination with metal ion. Vibrational spectra of metal carbonyls. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin-spin coupling. ESR spectra of metal complexes-Hyperfine splitting and A parameter, g values, zero field-splitting and Kramer's degeneracy, application to simple copper complexes. Mossbauer spectroscopy-the Mossbauer-effect, hyperfine interactions (qualitative treatment). Application to simple iron and tin complexes.</p> | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. D. J. Shriver and P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford University press, 2010. 2. J.E. Huheey, Inorganic Chemistry – Principles of Structure and Reactivity, IV ed., Pearson, 1993. 3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry. 5th ed. John Wiley, 1999. 4. G. Wulfsberg, Inorganic Chemistry, Viva Books, 2002. 5. B.E. Douglas, D.H. Mc Daniel and J. J. Alexander, Concepts and models of Inorganic chemistry, 3rd edition, John Wiley, 1994. 6. F. A. Cotton, Basic Inorganic Chemistry, 3rd edition, John Wiley, 2004. | | |

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|---|---|---|-------------------------|----------|-------------|----------|
| Course Code | NSC1C 03 | KINETICS, PHOTOCHEMISTRY AND CATALYSIS | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in general physical chemistry | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| The main objectives of the course are to: <ul style="list-style-type: none"> • Understand the fundamental concepts of physical chemistry. • Learn the method of solving problems mathematically. • Understand the concepts of kinetics, photochemistry and catalysis. • Learn the method of evaluation of kinetics of chemical and photochemical reactions. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of kinetics – K1 2. Understand some mathematical concepts – K2 3. Understand different kinetic pathways and problems based on it – K2, K3 4. Understand photochemistry of different systems – K1 5. Problem solving, evaluation and analysis capacity – K3, K4, K5 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate | | | | | | |
| UNIT-I | Chemical Kinetics I | | 16 Hours | | | |
| Reaction rate. The Arrhenius equation. The energy of activation. Collision theory. Transition state theory. Thermodynamic treatment of reaction rates. The London equation. Potential energy surfaces (brief). Various theories of Unimolecular reactions. Lindemann-Hinshelwood and RRKM theories (no derivation). The kinetics of complex reactions. Chain reactions. The rate laws of chain reactions. Explosions (brief only). Polymerization kinetics. Stepwise polymerization. Chain polymerization. | | | | | | |
| UNIT-II | Chemical Kinetics II | | 16 hours | | | |
| Kinetic of reaction in solution. Comparison of solution and gas kinetics. Diffusion controlled reactions. Influence of solvent on rate. Cage effect. Effect of dielectric constant on rate. Primary and secondary kinetic salt effects. Structural effects on rate. Hammett and Taft Equations. Study of fast reactions. Flash photolysis. Flow techniques. Relaxation methods. | | | | | | |
| UNIT-III | Photochemical Reactions | | 20 Hours | | | |
| Reactions of electronically excited species. Laws of Photochemistry, quantum yield and its determination. Radiation-chemical reactions – primary processes, pulse radiolysis, hydrated electrons. Chemi-luminescence. Radiative and non-radiative transitions. Jablonski diagram. Fluorescence: quantum efficiency of fluorescence, Stern-Volmer equation; delayed fluorescence. E-type and P-type phosphorescence. Laser photochemistry, Multiphoton excitation. Effect of temperature, wavelength and intensity of radiation on photochemical reaction. Different types of photochemical reactions. Kinetics of H ₂ -Br ₂ and H ₂ -Cl ₂ reaction, photo stationary states. Excimers and Exciplexes. Photosensitization by | | | | | | |

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| Hg. Photo-physical phenomena. Luminescence, chemiluminescences and thermo luminescence. Chemistry of photography. | | |
| UNIT-IV | Catalysis | 15 Hours |
| Classification. Theories of homogeneous catalysis. Acid base catalysis, Bronsted catalysis law. Enzyme catalysis: features, Michaelis Menten Mechanism. Auto catalysis. Oscillating reactions. BZ reaction. Heterogeneous catalysis: Adsorption and catalysis. Kinetics and mechanism of surface catalyzed reactions. Unimolecular surface reaction: Eley – Rideal Mechanism. Bimolecular reactions: Langmuir – Hinshelwood Mechanism- Discussion on carbon monoxide oxidation reaction on catalyst surface. Industrial Applications (brief mention). | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. K K Rohatgi and Mukherjee, Fundamental of Photochemistry, New Age International. 2. Dupoy and Chapmann, Molecular Reactions and Photochemistry, Prentice-Hall. 3. Fundamental Chemical Kinetics, Margaret Robson Wright. Horwood publishing Limited. 4. E. K Rideal, Concepts in catalysis, academic press. 5. Physical Chemistry, Peter Atkins, Julio de Paula, Oxford University Press. 6. A. Clark, theory of adsorption and catalysis, Academic press. | | |

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| Course Code | NSC1C 04 | QUANTUM MECHANICS- I | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in general physics, Chemistry and mathematics. | Syllabus Version | 2022 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ul style="list-style-type: none"> • Understand the fundamental concepts and principles in quantum mechanics for different systems. • Learn the method of solving problems quantum mechanically. • Understand the concepts of statistical mechanics. • Learn the method of evaluation of kinetics and thermodynamics of chemical reactions. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of classical mechanics – K1 2. Understand some mathematical concepts – K2 3. Understand different postulates of QM and solving problems based on it – K2, K3 4. Understand QM of different systems – K1 5. Problem solving, evaluation and analysis capacity – K3, K4, K5 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate | | | | | | |
| UNIT-I | Origin of Quantum Mechanics & its Postulates | | | | 16 Hours | |
| Plank's quantum hypothesis, Einstein's photoelectric effect, wave particle duality, de Broglie matter waves, Electron diffraction, Heisenberg's Matrix Mechanics (brief mention), Schrodinger wave mechanics, Deduction of Schrodinger equation from classical wave equation. Polar and spherical coordinates. Schrodinger Equation and Wave Packets, Poisson Brackets and Commutators, State function postulate, Operator postulate, Eigen value postulate, Expectation value postulate, Postulate of time dependent Schrodinger Equation of motion, Conservative system and time-independent Schrodinger equation, Stationary states, Formulation of quantum mechanical problem. | | | | | | |
| UNIT-II | Quantum Mechanics of Different Systems & Angular Momentum | | | | 20 hours | |
| Quantum mechanics of translational motion- particle in 1D and 3D box. Tunneling. Vibrational motion- One-dimensional harmonic oscillator. Rotational motion- Rigid rotator. Spherical harmonics. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((Lx, Ly, Lz), commutation relations between these operators. Clebsh-Gordon coefficients. Spin Angular Momentum- Spin 1/2 and the Pauli Matrices. Coupling of Orbital and Spin Angular Momenta. | | | | | | |
| UNIT - III | Quantum Mechanics of Hydrogen Like Atoms | | | | 16 Hours | |
| Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates, Separation of variables. The R, Theta and Phi equations and their solutions. Laguerre and Associate d Laguerre polynomials. Wave functions and energies of hydrogen-like atoms, Orbitals. Radial functions and Radial distribution of functions and their plots Angular functions and their plots, Orbital diagrams. Explanation of Hydrogen spectrum, Fine structure, The postulate of spin by Unlebeck and Goldsmith, Dirac's Relativistic Schrodinger | | | | | | |

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| equation for hydrogen atom and discovery of spin, Hydrogen wave functions including spin or spin orbitals, construction of Spin orbitals from Orbitals and Spin functions. | | |
| UNIT - IV | Conservation and Scattering | 15Hours |
| Space-time symmetries- Space translation and conservation of linear momentum, Time translation and conservation of energy, Space rotation and conservation of angular momentum, Space inversion and time reversal. Identical particles- Identical Particles in Classical and Quantum Mechanics, Exchange Degeneracy, Scattering cross section and scattering amplitude, Low energy scattering by a central potential, The method of partial waves, Phase shifts, Optical theorem, Convergence of partial wave series, Scattering by a rigid sphere, Scattering by a square well potential, High energy scattering, Scattering integral equation and Born approximation. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. A Text Book of Quantum Mechanics, P.M. Mathews & K. Venkatesan, Tata McGraw Hill, (2010). 2. Quantum Chemistry, Donald, A. McQuarrie, University Science Books, 1983 (first Indian edition, Viva books, 2003). 3. Modern Quantum Mechanics, J. J. Sakurai and Jim Napolitano, Cambridge University Press, third edition, 2020. 4. Problems and solutions in quantum mechanics, K. Tamvakis, Cambridge University Press, 2005. 5. Quantum Physics, Florian Scheck, Springer Science & Business Media, 2007. 6. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press. 7. Quantum Chemistry, I.N. Levine, 6th Edition, Pearson Education Inc., 8. Molecular Quantum Mechanics, P.W. Atkins and R.S. Friedman, 4th Edition, Oxford University Press, 2005. 9. Quantum Mechanics in Chemistry, M.W. Hanna, 2nd Edition, W.A. Benjamin Inc., 1969. 10. Physical Chemistry – Quantum Mechanics, HoriaMetiu, Taylor & Francis, 2006. 11. Introduction to Quantum Mechanics, L. Pauling and E.B. Wilson, McGraw-Hill, 1935 (A good source book for many derivations). 12. Quantum Chemistry, R.K. Prasad, 3rd Edition, New Age International, 2006. 13. Lectures on Chemical Bonding and Quantum Chemistry, C.N. Datta, Prism Books Pvt. Ltd., 1998. | | |

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| Course Code | NSC1C 05 | PHYSICS AND CHEMISTRY OF SOLIDS | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in crystals and solids | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ul style="list-style-type: none"> • Understand the fundamental concepts and principles of material science. • Learn the method of solving problems mathematically. • Understand the concepts of crystalline and solid state. • Learn different properties of solid materials. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of solid state – K1 2. Understand different postulates of theories in solid state – K2 3. Understand different properties of solid materials – K2 4. Evaluating different types of defects and packing of solids – K2, K4, K5 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate | | | | | | |
| UNIT-I | Crystalline State | | | | 15 Hours | |
| Crystal morphology: symmetry elements, crystal systems; Point group symmetry: derivation of point groups, space groups and Bravais lattices; Crystal planes and directions: Miller indices, interplanar separations. Crystal symmetry, Symmetry elements and symmetry operations. Structure analysis by X-rays: Atomic scattering factor; Laue conditions for diffraction and Bragg's law; Geometrical structure factor, systematic absences; Powder X-ray diffraction. | | | | | | |
| UNIT-II | Crystal Packing, Defects and Theories | | | | 16 hours | |
| Packing in a crystal: BCC, FCC, HCP structures with examples, Description of X-Ray diffraction using reciprocal lattice, Brillouin zones, Van der Waals interaction, Madelung interaction, Cohesive energy of ionic crystals, Covalent bonding, Metallic bonding, Hydrogen-bonded crystals. Point defects, line defects, plane defects. Free electron theory of metals, Band theory of solids, Effective mass; Direct and Indirect bandgaps: Determination of bandgap; Donors and acceptors, carrier concentration at thermal equilibrium; Calculation of Fermi level; Degenerate and Non-degenerate semiconductors. MO band and zone theories. | | | | | | |
| UNIT-III | Electronic and Dielectric Properties | | | | 16 Hours | |
| Free electron gas in three dimensions, heat capacity of electron gas, electrical conductivity and Ohm's law, Experimental electrical resistivity of metals, Motion in magnetic fields, Hall effect, Thermal conductivity of metals (Wiedemann-Franz law), Nearly free electron model-origin of energy bands, Magnitude of energy gap, Bloch functions, Kronig Penny model, Semiconductor crystals: band gap, direct/indirect bad gap SCs, Equation of motion, Holes, Effective masses in semiconductors, Intrinsic carrier concentration, Impurity conductivity, Thermoelectric effects. Theory of Dielectrics: Polarisation, Dielectric constant, Local Electric field, Dielectric polarisability, Clausius- Mossotti relation, Polarisation from dipole orientation, Dielectric losses, Ferroelectric crystals, Order-disorder type ferroelectrics, Polarisation catastrophe, Displacive type ferroelectrics, Landau theory of ferroelectric phase | | | | | | |

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| transitions, Ferroelectric domain, Antiferroelectricity, Piezoelectricity, Applications of Piezoelectric Crystals | | |
| UNIT-IV | Magnetic & Super Conductivity Properties | 20 Hours |
| <p>Diamagnetism and Paramagnetism: Langevin's diamagnetism equation, Quantum theory of diamagnetism of mononuclear systems, Quantum theory of paramagnetism, Hund's rule, Paramagnetic susceptibility of conduction electrons, Ferro, Anti and Ferri magnetism: Curie point and the exchange integral, Magnons, Ferrimagnetic order, Curie temperature and susceptibility of ferrimagnets, Antiferromagnetic order. Weiss theory of ferromagnetism, Ferromagnetic domains, Bloch walls, Origin of domains, Novel magnetic materials: GMR-CMR materials.</p> <p>Meissner effect, Type I and Type II superconductors, Heat capacity, Microwave absorption, Energy gap, Isotope effect, Free energy of superconductor in magnetic field and the stabilization energy, London equation and penetration of magnetic field, Cooper pairs and the BCS theory, DC and AC Josephson effects.</p> | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| Total Lecture Hours | | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. D.A McQuarrie and J.D. Simon, Physical Chemistry, a molecular approach, University Science Books. 2. Tareen and Kutty, Solid state chemistry. 3. Lesley Smart & Elaine Moore, SolidState Chemistry, nelson Thornes. 4. A.K. Galway, Chemistry of Solids, Science Paperbacks and Chapman and Hall Ltd., London 91967). 5. A.R. West, basic Solid State Chemsitry, John Wiley & Sons Ltd. (1991). 6. B.S.Skoog and D.M. West, Principles of Instrumental Analysis, Sanndes College, Philadelphia (1980). 7. Atomic structure and chemical Bond, Manas Chanta Publisher: McGraw-Hill Inc.,US (1 December 1974) ISBN-10: 0070965110 8. Concise Inorganic chemistry, J.D.Lee Publisher: Wiley; 5th edition edition (18 December 1998) ISBN-10: 0632052937 9. Inorganic Chemistry, G. Wwfsberg Unit IV Publisher: Pearson; 4 edition (31 May 2012) ISBN-10: 0273742752 10. Introduction to solids – L.V. Azaroff □ Publisher: McGraw Hill Education; New edition edition (14 June 2001) ISBN-10: 0070992193 11. Introduction to solid state Physics – C. Kittel □ Publisher: John Wiley & Sons Inc (23 July 1996) □ ISBN-10: 0471142867 12. Elements of solids state physics, J.P. Srivastava □ Publisher: Prentice Hall India Learning Private Limited; 4th Revised edition edition (17 December 2014) ISBN-10: 8120350669 13. Superconductivity and Superconducting Materials – A V Narlikar and S N Ekbote (South Asian Pub., 1983). 14. Physics of high T_c superconductors – J C Phillips (Academic Press, 1989) 15. Introduction to superconductivity – A C Rose-Innes and E H Rhoderick (Pergamon Press, 1978) | | |

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| Course Code | NSC1P 01 | PRACTICAL -I | L | T | P | C |
| Core | | | 0 | 0 | 2 | 2 |
| Pre-requisite | Basic knowledge in general Physics and Chemistry | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ul style="list-style-type: none"> • To experimentally realize the concepts in Physics, Chemistry and nanoscience • To expose students to common topics in Physics and Chemistry to understand nanoscience | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Gain practical knowledge by applying the experimental methods to correlate with the theory – K4 2. Apply and understand the various procedures and techniques for the experiments in physics and chemistry experiments – K2, K3 3. Apply the analytical techniques and graphical analysis to interpret the experimental data – K3, K5 4. Develop intellectual communication skills and discuss the basic principles of scientific concepts in a group – K3 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate | | | | | | |
| List of Experiments: | | | | | | |
| <ol style="list-style-type: none"> 1. Method of separation and purification of organic compounds: fractions, steam and low-pressure distillation, fractional crystallization, and sublimation 2. Quantitative separation and identification of a binary mixture of organic compounds by semimicro analytical techniques. 3. Multi-step preparation of well-known organic compounds. 4. Estimation of metal ions via titrimetric method 5. Determination of Heat of solution from solubility data. 6. Determination of molecular weight from depression in freezing point. 7. Determination of molecular weight from depression in transition point. | | | | | | |

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| Course Code | NSC2C 06 | ORGANIC REACTIONS AND REARRANGEMENTS | L | T | P | C |
| Core | | | 3 | 0 | 0 | 3 |
| Pre-requisite | Basic knowledge in general organic Chemistry | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| The main objectives of the course are to: <ul style="list-style-type: none"> • Understand the fundamental concepts and principles in organic chemistry. • Learn different rearrangements. • Understand the mechanisms of different types of reactions. • Learn the concepts of green chemistry and supramolecular chemistry. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of molecular rearrangements – K1 2. Understand some named organic reactions and their mechanisms – K2 3. Understand different photochemical and pericyclic reactions – K1 4. Problem solving, evaluation and analysis capacity with chemical reactions – K3, K4, K5 | | | | | | |
| K1 – Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate | | | | | | |
| UNIT-I | Molecular Re-arrangements | 15 Hours | | | | |
| Concepts, Types of Rearrangements, Rearrangement to electron deficient carbon: (carbon migration) Wagner-Meerwin rearrangement, Pinacol-Pinacolone rearrangement. Rearrangement to electron rich carbon: Stevens rearrangement, Sommelet-Hauser rearrangement, Wittig rearrangement. Rearrangement to electron deficient nitrogen: Hofmann rearrangement, Curtius rearrangement, Schmidt rearrangement, Beckmann rearrangement. Rearrangement to electron deficient oxygen: Baeyer Villiger reaction, Hydroperoxide rearrangement, Dakin reaction. Intra-molecular migration from nitrogen to carbon: Jacobsen rearrangement. Intermolecular migration from nitrogen to carbon: Aromatic arrangements: Orton rearrangement, Fischer-Hepp rearrangement, Hofmann-Martius rearrangement, Bamberger Rearrangement, Migratory aptitude in rearrangements, cross-over experiments and its significance. | | | | | | |
| UNIT-II | Named Organic Reactions | 16 hours | | | | |
| Castro-Stephens coupling, Baylis Hillman reaction, Eschenmoser methenylation, Evans Aldolreaction, Staudinger reaction, Horner-Wadsworth-Emmons reaction, McMurry coupling, Nazarov cyclization, Nef reaction, Ritter reaction and Pauson-Khand reaction. Eschenmoser-Tanabe Fragmentation, Hofmann-Löffler-Freytag reaction, Julia-Lythogoe olefination, Koenig-Knorr glycosidation, Mitsunobu reaction, Mukaiyama aldol reaction, Peterson olefination, Hayashi reaction, Shapiro reaction, Sharpless asymmetric epoxidation, Sommelet reaction, Von Braun reaction, Hofmann-Löffler Freytag reaction, Ramburg-Backland reaction. Hell- Volhard- Zelinski reaction. Haloform reaction. Claisen | | | | | | |

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| ester condensation, Darzen reaction, Dieckmann, Perkin and Prins reactions. Mannich reaction. Michael reaction, Robinson anulation. Wittig reaction. | | |
| UNIT-III | Photochemistry & Pericyclic Reactions | 20 Hours |
| General principles, Photosensitization and PET reactions, Photochemistry of carbonyl compounds. Photochemistry of alkenes, Photochemistry of aromatic compounds, Norrish Type I and II, Patterno Buchi reaction, Barton reactions, chemi and bioluminescence reactions, Photochemical rearrangements- aromatic rearrangements, Dienone rearrangements, Di-pimethane rearrangements, Photo-Fries rearrangements. Definition and types of reactions classified as pericyclic actions - (a) Cycloaddition and cyclo-conversion (b) Electrocyclic ring closing and ring opening (c) Sigmatropicre-arrangements (d) Cheletropic reactions (e) Group transfers, Stereochemistry of pericyclicreactions and theory of molecular orbital symmetry. Application of theory of M.O.Symmetry by the method of correlation diagram by both thermal and photochemical paths. Stereochemistry of Pericyclic reactions-thermal and photochemical by "Method of transition state atomaticity". Basic principles of perturbation molecular orbital (PMO)theory, significance of Frontier Molecular orbitals, Stereochemistry of pericyclic reactions by the "Frontier molecular orbital (FMO) method". | | |
| UNIT-IV | Oxidation-Reduction Reactions & Multistep Organic Synthesis | 16 Hours |
| Elements of a synthesis (Reaction methods, reagents, catalysts, solvents, protecting groups (Hydroxyl, Amino Carbonyl and Carboxylic acid protecting groups), activating groups, leaving groups, synthones and synthetic equivalents. Types of selectivities (Chemo, Regio and Stereo selectivity). Synthetic Planning illustrated by simple molecules, disconnections and functional group inter conversions. Umpolung reactions and use in synthesis. Retro synthetic analysis of a complex molecule-a case study. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| Total Lecture Hours | | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. J. March, Advanced Organic Chemistry. 4th Edition, Wiley Interscience New York. 2. R.O.C. Norman and E.M. Coxon, Principles in Organic Synthesis, 2005, CRC Press, New York. 3. Jie Jack Li – Name Reactions: A Collection of Detailed Reaction Mechanisms. Laszlo Kurti and Barbara Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005. 4. J. Singh, Photochemistry and Pericyclic Reactions, New Age International, 2005. 5. John McMurry, Organic Chemistry, 5 Ed., 2000 or newer. 6. Stuart Warren, Designing organic synthesis: programmed introduction to the synthon approach, 1994. 7. Carruthers, Modern Synthetic Methods, Cambridge. | | |

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| Course Code | NSC2C 07 | THERMODYNAMICS AND ELECTROCHEMISTRY | L | T | P | C |
| Core | | | 3 | 0 | 0 | 3 |
| Pre-requisite | Basic knowledge in general physical Chemistry. | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ul style="list-style-type: none"> • Understand the fundamental concepts of thermodynamics. • Learn the method of solving problems mathematically. • Understand the concepts of statistical mechanics, thermodynamics and electrochemistry. • Learn some important analytical methods | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of analytical methods – K1 2. Understand some electrochemical systems – K2 3. Understand different statistical systems – K1 4. Problem solving, evaluation and analysis capacity – K3, K4, K5 | | | | | | |
| K1 – Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate | | | | | | |
| UNIT-I | Thermodynamics | 16 Hours | | | | |
| <p>Basic concepts – laws. Maxwells relations. Partial molar quantities. Chemical potential. Gibbs –Duhem equation. Ideal and non-ideal solutions. Fugacity of gases and its determination. Raoul'ts laws and its deviation. Gibbs-Duhem-Margules equation. Thermodynamics of mixing. Excess thermodynamic functions. Thermodynamics of irreversible process. Principle of local equilibrium. Forces and fluxes. The phenomenological relations. Onsagar relations: Linear relations. Reciprocal relation (no derivation). Entropy of production in simple irreversible system (closed systems). Application of reciprocal relation to diffusions. Thermal diffusion, thermo-osmosis and thermo-molecular pressure difference. Electro kinetic phenomena entropy production, electro osmosis, streaming potential, streaming current, electro-osmotic pressure.</p> | | | | | | |
| UNIT-II | Statistical Thermodynamics | 16 hours | | | | |
| <p>Probability distribution. Ensembles. Micro states and macro states. Statistical weight. Thermodynamic probability and entropy. Maxwell-Boltzmann distribution law. The partition function and its relation to the thermodynamics functions. Factorization of the partition function in to the translational, rotational, vibrational and electronic parts. The perfect gas-ideal monatomic and diatomic gases. Sackur-Tetrode equation. Heat capacity of gases. Classical and quantum theories. The anomalous heat capacity of hydrogen. The atomic crystal – Einstein theory of atomic crystals, Debyes modification of Einsteins model. Imperfect gases, the virial expressions and the virial coefficients, relation between the virial coefficients and the cluster integrals. Need for Quantum statistics-The ideal Fermi Gas. Fermi-Dirac distribution law. Gas Degeneracy. Application to electrons in metals. The ideal Bose gas. Bose-Einstein distribution law. Gas Degeneracy. Bose-Einstein condensation. Application to liquid helium. Comparison of the three statistics.</p> | | | | | | |

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| UNIT-III | Electrochemistry | 20 Hours |
| <p>Electrolytes and non-electrolytes. Activities and activity coefficients. Ionic strength, Debye – Huckel Theory, Debye- Falkenheigen effect, Debye-Huckel limiting law (Qualitative and quantitative tests). Debye-Huckel-Onsagar equation of conductivity (Validity and Deviations) Conductance ratio. EMF and concentration, Formaland standard electrode potentials, Concentration cells. Electrical double layer and its different models, Liquid junction potential and its determination. Fuel cells. Electrochemical cells and reactions. Current – potential curves. Irreversible electrode processes. Faradaic and non-Faradaic processes, polarizable and non-polarizable electrodes and their I-V characteristics, Factors affecting electrode reaction rate and current, Effect of electrode potential on Gibbs free energy of activation, Butler – Volmer equation, Exchange current density and activation over potential, Tafel equation and Tafel plots, Concentration polarization, Dissolution and decomposition potentials. Hydrogen over voltage, Ionic diffusion as the slow process, Ionic discharge as the slow process.</p> | | |
| UNIT-IV | Electro-analytical Methods | 15 Hours |
| <p>General principles of Potentiometry, different types of electrodes, Amperometry, Coulometry, Principle of chrono-potentiometry. Fundamental law of spectrophotometry, nephelometry and turbidometry and Fluorimetry. Spectrophotometric titrations. Principles of polarography, Voltammetry, Linear sweep, differential pulse and cyclic voltammetry (Brief mention only).</p> | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| <p>Expert lectures, General Seminars, online seminars – webinars</p> | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. I Prigogine, An introduction to the Thermodynamics of Irreversible processes. Inrterscience. 2. Allen J. Bard and Larry Faulkner, Electrochemical methods : Fundamentals and applications, Wiley 3. Gurdeepraj, Advanced Physical Chemistry, Goel Publishing 4. L K Nash, Elements of Statistical Thermodynamics, Addison Wesley Publishing Co. 5. G K Vemulapalli, Physical Chemistry, Prentice-Hall of India. 6. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of AnalyticalChemistry, 8th Edn., Saunders College Pub., 2007. 7. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, BlackwellScience, 2000. | | |

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| Course Code | NSC2C 08 | QUANTUM MECHANICS II | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in general physics, Chemistry and mathematics. | Syllabus Version | 2022 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ul style="list-style-type: none"> • Understand the fundamental concepts and principles in quantum mechanics for different systems. • Learn the method of solving problems quantum mechanically. • Understand the concepts of statistical mechanics. • Learn the method of evaluation of kinetics and thermodynamics of chemical reactions. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Evaluation of multi-electron systems by QM – K5 2. Understanding and evaluation of different approximation methods – K2, K5 3. Understand the concepts of relativistic QM – K2 4. Understand the fundamentals of group theory – K2 5. Application of GOT to derive character tables – K2, K3 6. Understanding applications of group theory in spectroscopy and chemical bonding – K2, K3, K4 | | | | | | |
| K1– Remember, K2 – Understand, K3 – Apply, K4 – Analysis, K5 – Evaluate, K6- Create | | | | | | |
| UNIT - I | Approximation Methods | 16 hours | | | | |
| <p>Perturbation theorem: The WKB approximation, Connection formulae, Barrier tunneling, Application to decay- bound states, Penetration of a potential barrier, Time- independent perturbation theory. Illustration by application to particle in 1D-box with slanted bottom, Perturbation treatment of the ground state of the helium atom. Transition probability, Harmonic perturbation, Interaction of an atom with the electromagnetic field, Induced emission and absorption.</p> <p>Variation theorem: The variational equation with proof, ground state and excited states, the variation method for bound states, Application to ground state of the hydrogen and helium atoms.</p> <p>HFSCF method: Hartree-Fock Self-Consistent Field (HF-SCF) method.</p> | | | | | | |
| UNIT-II | Relativistic Quantum Mechanics | 16 Hours | | | | |
| <p>The Dirac equation, Dirac matrices, Solution of the free-particle Dirac equation. Spin-orbit coupling, Covariance of the Dirac equation, Bilinear covariants, Hole theory, The Weyl equation equation for the neutrino, Nonconservation of parity, The Klein Gordon equation, Charge and current densities, The Klein- Gordon equation, Charge and current densities, The Klein –Gordon equation equation with potentials, Wave equation for the photon, Charge conjugation for the Dirac, Weyl and Klein Gordon equation.</p> | | | | | | |
| UNIT-III | Theories of Molecular Symmetry | 15 Hours | | | | |

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| Introduction to symmetry and point groups. Group multiplication tables. Similarity transformation. Reducible and irreducible representations. Construction of irreducible representations by reduction (similarity transformation). Great orthogonality theorem (GOT) and properties of irreducible representations using GOT, Construction of character Table (C _{2v} , C _{3v} , C _{2h} , C _{4v}). Nomenclature of irreducible representations - Mulliken symbols, Symmetry species. Reduction formula using GOT. | | |
| UNIT- IV | Applications of Group Theory | 20 Hours |
| <p>a. Molecular vibrations, symmetry species of normal modes of vibration, Construction of Γ_{cart}. Normal coordinates and drawings of normal modes, Selection of rules for IR and Raman activities, complementary character of IR and Raman spectra, Determination of IR active and Raman active modes of molecules.</p> <p>b. Vanishing and non vanishing integrals. Transition moment integral and selection rules. Overlap integrals and conditions for overlap.</p> <p>c. MO theory for more complex molecules - HMO theory of linear conjugated hydrocarbons (Ethylene, Butadiene, Allylic anion Frost-Huckel circle mnemonic device for cyclic polyenes).</p> <p>d. Molecular orbital treatment of molecules using Group theory. Treatment of H₂O. Electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.</p> <p>e. Group theoretical treatment of hybridization, Construction of hybrid orbital in BF₃ and Inverse transformation.</p> | | |
| UNIT-V | Contemporary Issues | 5 Hours |
| Expert lectures, General Seminars, online seminars – webinars | | |
| Total Lecture Hours | | 72 Hours |
| Text Books/References | | |
| <p>7. A Text Book of Quantum Mechanics, P.M. Mathews & K. Venkatesan, Tata McGraw Hill, (2010).</p> <p>8. Quantum Chemistry, Donald, A. McQuarrie, University Science Books, 1983 (first Indian edition, Viva books, 2003).</p> <p>9. Modern Quantum Mechanics, J. J. Sakurai and Jim Napolitano, Cambridge University Press, third edition, 2020.</p> <p>10. Problems and solutions in quantum mechanics, K. Tamvakis, Cambridge University Press, 2005.</p> <p>11. Quantum Physics, Florian Scheck, Springer Science & Business Media, 2007.</p> <p>12. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press.</p> <p>13. Quantum Chemistry, I.N. Levine, 6th Edition, Pearson Education Inc.,</p> <p>14. Molecular Quantum Mechanics, P.W. Atkins and R.S. Friedman, 4th Edition, Oxford University Press, 2005.</p> <p>15. Quantum Mechanics in Chemistry, M.W. Hanna, 2nd Edition, W.A. Benjamin Inc., 1969.</p> <p>16. Physical Chemistry – Quantum Mechanics, HoriaMetiu, Taylor & Francis, 2006.</p> | | |

17. Introduction to Quantum Mechanics, L. Pauling and E.B. Wilson, McGraw-Hill, 1935 (A good source book for many derivations).
18. Quantum Chemistry, R.K. Prasad, 3rd Edition, New Age International, 2006.
19. Lectures on Chemical Bonding and Quantum Chemistry, C.N. Datta, Prism Books Pvt. Ltd., 1998.

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| Course Code | NSC2C 09 | INTRODUCTION TO NANOMATERIALS | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Fundamentals of Physics and Chemistry at Undergraduate level | Syllabus Version | 2022 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Recognize the interdisciplinary area of Nanoscience and Technology 2. Realize different nano systems and recognize the advanced tools used for their analysis 3. Understand the reasons behind size dependent physical or chemical properties of nanomaterials 4. Analyze the phase transformation process and understand how to control that process for nanostructure creation 5. Introduce different methods available for the fabrication of nanostructures | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Recognize different nanosystems and the tools for their analysis (K2) 2. Understand the size dependent physical phenomena observed in nanomaterials (K2) 3. Realize the origin of surface energy, energy minimization and stabilization processes in nanosystems (K2) 4. Understand and apply the kinetics of phase transformation in nanosystems (K2,K3) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Introduction to Nano-systems | 11 Hours | | | | |
| Feynmann's vision on nanoscience & technology, bulk vs nanomaterials, natural and synthetic nanomaterials. Quantum confinement in nanostructures- size dependent physical phenomena in semiconductor and metal nanoparticles. Classification of nanostructures, 0D, 1D and 2D nanostructures. Visualization of nanostructures and techniques related. | | | | | | |
| UNIT-II | Surface Energy | 20 Hours | | | | |
| Surface energy and surface stress-origin and estimation of surface energy. Surface Energy minimization:- Sintering Ostwald ripening and agglomeration. Energy minimization by Isotropic and anisotropic surfaces. Surface energy and surface curvature, Surface energy stabilization- electrostatic stabilization, steric stabilization, electro-steric stabilization.. | | | | | | |
| UNIT-III | Growth Kinetics of Nanomaterials | 20 Hours | | | | |
| Kinetics of phase transformations, Homogeneous & Heterogeneous nucleation. Controlling nucleation, growth and aggregation in nanoparticle growth. Growth Mechanisms: Spontaneous growth, Evaporation condensation growth, growth controlled by diffusion and surface process, VLS growth, fundamentals of thin film growth. | | | | | | |

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| UNIT-IV | Special Nanostructures | 16 Hours |
| Diamond – Graphite- Fullerenes, CNTs and Graphene. Synthesis: CVD, Laser and Electrochemical and other methods. Functionalization and reactivity of CNTs. | | |
| Micro & Mesoporous Materials, Ordered mesoporous structures, Random mesoporous structures, and crystalline microporous materials: zeolites. Core – Shell Structures - Metal-oxide structures, Metal-polymer structures, Oxide-polymer structures. Organic-Inorganic Hybrids- Class I hybrids, Class II hybrids, Intercalation Compounds. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| Text Books: | | |
| <ol style="list-style-type: none"> 1. Nanostructures and Nanomaterials- Synthesis, Properties & applications by Guozhong Cao, Imperial College Press, (2006). (for UNIT I & II, 2nd Chapter, Unit III – Chapter 4 (3.2), Unit IV- Chapter 7 2. Nanomaterials and Nanochemistry by C. Brechignac.P. Houdy M. Lahmani Springer-Verlag (2007). (For Unit III-Part I Chapter I) 3. Materials Science and Engineering-An Introduction 7e, William D. Callister, (Wiley, 2007). (Chapter 10. section 1-.2 and 10.3) Unit II. | | |
| Reference: | | |
| <ol style="list-style-type: none"> 1. Introduction to Nanoscience & Nanotechnology by Gabor L. Hornyak, Harry F. Tibbals, Joydeep Dutta, John J. Moore, CRC Press, Tylor & Francis Group New York, 2009. Publisher: CRC Press (15 December 2008) ISBN-13: 978-1420047790 2. Introduction to Nanoscale Science & Technology, Di Ventra, Evoy, Heflin, Springer Science, NY, 2004. Publisher: Springer; 1 edition (30 June 2004) Sold by: Amazon Asia-Pacific Holdings Private Limited. | | |

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| Course Code | NSC2C 10 | ADVANCED ANALYTICAL TECHNIQUES | L | T | P | C |
| Core Course | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in, Physical, Chemical or Biological sciences | Syllabus Version | 2022 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. To familiarize and understand the fundamental principles and concepts of characterization of nanostructured materials. 2. To categorize and understand the different techniques used for studying the structural, optical, morphological, thermal, magnetic and electrochemical properties of nanomaterials. 3. To understand the working principle and instrumentation of the characterization instruments. 4. Evaluation and analysis of experimental data obtained from different instrumentation techniques | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Recognize various characterization techniques available for the studying different properties of nanostructured materials. (K1) 2. To apply the knowledge gained to correctly choose the most suitable characterization technique for studying the properties of nanomaterials.(K3) 3. To effectively use the knowledge gained in analyzing the obtained characterization data. (K4,K5) 4. To evaluate the characterization data and nurture the ability to explain the underlying mechanism.(K5) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Microscopic Techniques: | 20 Hours | | | | |
| Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM). Scanning Probe Microscopy: Atomic Force Microscopy, Scanning Tunnelling Microscopy (STM), Near field scanning optical microscopy (NSOM). Principles of Fluorescence microscopy. Confocal Laser Scanning Microscopy. | | | | | | |
| UNIT-II | Techniques for Thermal & Mechanical Analysis | 15 Hours | | | | |
| Thermal Analysis: TGA, DTG, DTA, DSC - combustion calorimetry- Thermal diffusivity by the laser flash technique- simultaneous techniques including analysis for gaseous products. Mechanical testing- Introduction, tension testing, High strain rate testing of materials, Fracture Toughness testing methods, Hardness testing. | | | | | | |
| UNIT-III | Magnetic & Electrochemical Techniques | 15 Hours | | | | |
| Magnetic Vibrating Sample Magnetometer, Mossbauer spectroscopy, ESR, NMR. Magneto-optic Kerr effect. Electrochemical Techniques:Cyclic voltammetry, | | | | | | |

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| Electrochemical Impedance, Scanning electrochemical Microscopy, The quartz crystal micro balance. | | |
| UNIT-IV | Structure and Surface Analysis Techniques | 17 Hours |
| X-ray powder diffraction: principles and practices. Small angle X-ray diffraction, GIXRD, and Single crystalline X-ray diffraction. Hydrophobic and hydrophilic surfaces, Super hydrophobicity and hydrophilicity, Contact angle, BET surface area and porosity analysis. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Introduction to Nanoscience and Nanotechnology, by K K Chattopadhyay, PHI Learning Pvt. Ltd. New Delhi 2019, ISBN-13: 978-81-203-3608-7. 2. Characterization of Materials Vol 1 &2, by Elton N. Kaufmann, John Wiley and Sons Publication, 2003. New Jersey. 3. Principles of instrumental analysis, Douglas A Skoog, Donald M West, Saunders College, Philadelphia. □ Publisher: Cengage; 6 edition (1 November 2014) ISBN-13: 978-81-315-25579. 4. NANO: The Essentials- Understanding Nanoscience and Nanotechnology, by T Pradeep, Tata McGraw Hill Education Pvt. Ltd. New Delhi)ISBN-13: 978-0-07-061788-9 5. X-Ray Diffraction Procedures: For Polycrystalline and Amorphous Materials, 2nd Edition - Harold P. Klug, Leroy E. Alexander,Publisher: Wiley-Blackwell; 2nd Revised edition edition (1 January 1974) ISBN-13: 978-0471493693 6. Transmission Electron Microscopy: A Textbook for Materials Science (4-Vol Set)- David B. Williams and C. Barry Carter, Publisher: Springer; 1st ed. 1996. Corr.6thprinting edition (15 April 2005) ISBN-13: 978-0306453243 7. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM - Ray F. Egerton ,Publisher: Springer; Softcover reprint of hardcover 1st ed. 2005 edition (12 October 2010) ISBN-13: 978-1441938374 8. Springer handbook of Nanotechnology ed. Bharat Bhushan (Springer), Publisher: Springer-Verlag (15 May 2006) ISBN-13: 978-3540343660. | | |

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| Course Code | NSC2P 02 | PRACTICAL -II | L | T | P | C |
| Core | | | 0 | 0 | 2 | 2 |
| Pre-requisite | Basic knowledge in general Physics and Chemistry | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ul style="list-style-type: none"> • To experimentally realize the concepts in Physics, Chemistry and nanoscience • To expose students to common topics in Physics and Chemistry to understand nanoscience | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Gain practical knowledge by applying the experimental methods to correlate with the theory – K4 2. Apply and understand the various procedures and techniques for the experiments in physics and chemistry experiments – K2, K3 3. Apply the analytical techniques and graphical analysis to interpret the experimental data – K3, K5 4. Develop intellectual communication skills and discuss the basic principles of scientific concepts in a group – K3 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate, K6- Create | | | | | | |
| List of Experiments: | | | | | | |
| <ol style="list-style-type: none"> 1. Solving chemical problems computationally. 2. Determination of partition coefficient of a mixture. 3. Study of kinetics of acid-catalyzed ester hydrolysis. 4. Evaluation of Langmuir adsorption isotherm. 5. Preparation and characterization of complexes using IR, NMR and electronic spectra and investigation of ligand field spectra of Cu(II) complexes 6. Construction of phase diagram for the two-component system. 7. Determination of Equivalent conductance of strong electrolytes (KCl) and verification of Onsagar equation. 8. Conductometry titrations of displacement and precipitation reactions - HCl vs NaOH | | | | | | |

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| Course Code | NSC3C 11 | ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY | L | T | P | C |
| Core | | | 3 | 0 | 0 | 3 |
| Pre-requisite | Basic knowledge in general inorganic Chemistry. | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| The main objectives of the course are to: <ul style="list-style-type: none"> • Understand the importance of organometallic compounds. • Learn the importance of elements in biological systems. • Learn different kinds of metallic and non-metallic clusters. • Learn basics of organometallic compounds. | | | | | | |
| Course Outcomes | | | | | | |
| 5. Remember the fundamentals of organometallic compounds – K1 2. Understand some organometallic compounds – K2, K3 3. Understand and evaluate different metallic and non-metallic clusters – K2, K5 4. Understand the importance of elements in biological systems – K1, K4 | | | | | | |
| K1– Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate, K6-Create | | | | | | |
| UNIT-I | Metallic & Non-metallic Clusters | | | | 15 Hours | |
| General electronic aspects and bonding in metal-metal single, double, triple and quadruple bonded complexes of non-carbonyl clusters. Carbonyl clusters. Carbonyl clusters-LNCCS and HNCCS. Capping rule. Reactions of metal carbonyl clusters, Wade-Mingos rules. IR spectral studies of bridging and non-bridging CO ligands, Isoelectronic and isolobal analogy. Non-Metallic Clusters. Boron hydrides and borazine. styx numbers. closo, nido, arachno polyhedral structures. Wade's rule. structure and bonding of carboranes. Medical applications of boron clusters. Structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Structure and bonding in sulphur and phosphorous compounds. General features of Silicates, alumino-silicates, zeolites, Silicones, Carbides and silicides. | | | | | | |
| UNIT - II | Organometallic Compounds I | | | | 16 Hours | |
| Organometallic compounds. 16 and 18 electron rules, Main group organometallics with alkyl and aryl ligands Groups 1, 2, 11, 12, 13, 14 and 15 (general features), σ -bonded complexes, cyclopentadienyl complexes and bis (arene) complexes. metal carbenes –Fischer and Schrock Carbenes (synthesis and properties), Tebbe's reagent. Transition metal complexes with chain π ligands (ethylene, acetylene, allyl and butadiene ligands). Complexes of ring π donor ligands (cyclobutadiene, C ₅ H ₅ , C ₆ H ₆). Fluxional organometallic compounds. | | | | | | |
| UNIT - III | Organometallic Compounds II | | | | 16 Hours | |
| Applications of organometallic compounds. Oxidative addition, reductive elimination and insertion reactions. Carbonylation by Collman's reagent. Hydrozirconation of alkenes and | | | | | | |

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| alkynes. Hydrogenation, hydrosilation, isomerization of alkenes, alkyne, cycloadditions, Zeigler-Natta catalysis, hydroformylation of alkenes, Monsanto acetic acid process and Wacker process. | | |
| UNIT- IV | Bio-inorganic Chemistry | 20 Hours |
| Bulk and trace metal ions, Role of metal ions in biological functions. Biological role of some trace nonmetals. (B, Si, S, Se, As, Cl, Br, I). Biological importance of nitric oxide. Ion transport across membranes - The sodium/potassium pump, structural role of calcium. Storage and transport of metal ions - ferritin, transferrin and siderophores. Oxygen transport by heme proteins - hemoglobin and myoglobin, structure of the O ₂ binding site, nature of heme-dioxygen binding, cooperativity. Hemerythrin and hemocyanin. A brief idea on structure and function of copper proteins in electron transport process, cytochromes, iron-sulphur proteins, tyrosinase, superoxide, dismutase. Lewis acid role of Zn(II) and Mn(II) containing enzymes, carboxy peptidase, vitamin B12 and coenzymes. Chlorophyll Photosystems I and II. Nitrogen fixation – Nitrogenase, Anticancer drugs. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Fourth edn. 2005, Wiley Interscience. 2. B. D. Gupta, A .J. Elias, Basic Organometallic Chemistry - Concepts, Synthesis and Applications, Second edition, University Press, 2013. 3. D.E. Fenton, Bioinorganic Chemistry. 5. S.J. Lippard and J.M. berg, Principles of Bioinorganic Chemistry. 4. J.E. Huheey, Inorganic Chemistry-Principles, Structure and Reactivity. 5. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, Affiliated east west press, 1993. 6. Robert W. Hay, Bioinorganic Chemistry, Ellis Horwood Limited, UK, 1984. 7. P. Powell, Principles of Organometallic Chemistry, 2nd edition, Chapman and Hall, London, 1998. 9. S.F.A. Kettle, Concise co-ordination chemistry, Nelson, 1969. 8. D.E. Fenton, Bioinorganic Chemistry. 5. S.J. Lippard and J.M. berg, Principles of Bioinorganic Chemistry. 9. Rosette M. Roat-Malone, Bioinorganic Chemistry | | |

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| Course Code | NSC3C 12 | SPECTROSCOPY | L | T | P | C |
| Core | | | 3 | 0 | 0 | 3 |
| Pre-requisite | Basic knowledge in general spectroscopy. | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ul style="list-style-type: none"> • Understand the fundamental concepts and principles in molecular spectroscopy. • Learn the method of solving problems for different molecular systems. • Understand the concepts of different types of spectra. • Learn the method of evaluation of chemical problems spectroscopically. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Remember the fundamentals of concepts and principles in molecular spectroscopy – K1 2. Understand concepts of different types of spectra – K2 3. Understand different chemical systems with different types of spectra and solving problems based on it – K2, K3 4. Problem solving, evaluation and analysis capacity – K3, K4, K5 | | | | | | |
| K1 – Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate, K6- Create | | | | | | |
| UNIT-I | Microwave Spectroscopy | 16 hours | | | | |
| Rotation spectra of diatomic and poly atomic molecules, Rigid and non-rigid rotator models, Asymmetric, symmetric and spherical tops. Isotope effect on rotation spectra, Stark effect, Nuclear and electron spin interactions. Rotational transitions and selection rules. Microwave spectrometer -Principles & Applications. | | | | | | |
| UNIT-II | Lower & Higher Energy Excitation Spectroscopy | 16 Hours | | | | |
| Basic principles, Beer-Lambert's Law, Molar extinction coefficient, intensity of electronic transitions. Types of electronic transitions. Franck- Condon principle, Ground and excited electronic states of diatomic molecules. Electronic spectra of polyatomic molecules. The fate of electronically excited state species - Vibrational relaxation, External conversion, Internal conversion, Fluorescence, Phosphorescence, Jablonski diagram. Electronic spectra of conjugated molecules - Dissociation and predissociation spectra. UV-Visible spectrophotometer – Principles & Applications. Fluorescence spectroscopy, Photoelectron spectroscopy (X-ray and Ultraviolet), X-ray Fluorescence, Augur electron spectroscopy, Electron energy loss spectroscopy. | | | | | | |
| UNIT-III | IR and Raman Spectroscopy | 15 Hours | | | | |
| Vibrational spectra of diatomic and poly atomic molecules, Harmonic oscillator model, Anharmonicity. Vibrational transitions and selection rules. Morse potential, Fundamentals, Overtones, Hot bands, Combination hands, Difference bands. Vibrational spectra of diatomic and polyatomic molecules, P, Q, R branches. IR and FTIR spectrophotometer - Principles - Instrumentation, Applications. Pure rotational, pure vibrational Raman spectra, Vibrational, rotational Raman spectra, Selection rules, Mutual exclusion principle. Raman spectrophotometer - Principles – Instrumentation, Laser Raman spectroscopy, Applications. | | | | | | |

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| UNIT-IV | Resonance Spectroscopy | 20 Hours |
| Interaction between nuclear spin and magnetic field, Level population, Larmour Precession, Resonance condition, Bloch equations, Relaxation times, Spin-Spin and spin-lattice relaxation, The Chemical shift, Instrumentation for NMR spectroscopy, CWNMR and FTNMR, Imaging, Electron Spin Spectroscopy of the unpaired electron, Total Hamiltonian, Fine structure, Electron-Nucleus coupling and hyperfine structure, ESR spectrometer, Mossbauer Spectroscopy : Resonance Fluorescence of gamma - rays, Recoilless emission of gamma - rays and Mossbauer Effect, Chemical shift, Effect of electric and magnetic fields, Example of Fe57, Experimental techniques. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Straughan & Walker; For Mossbauer Effect : Aruldas and G.K. Wertheim 2. Gunther K. Wertheim : "Mossbauer Effect : Principles and applications, (Academic Press) 3. Straughan and Walker (Eds): " Spectroscopy"- Vol. I and II (Chapman and Hall) 4. G.M. Barrow : "Introduction to molecular Spectroscopy", (McGraw Hill). 5. Long D.A : "Raman spectroscopy " (Mc Graw Hill (1977) 6. C.N.Banwell&E.N.McCash,Fundamentals of Molecular Spectroscopy,Tata, McGraw Hill 7. Aruldhass,MolecularStructure&Spectroscopy, Prentice Hall ,India 8. F.W.Atkins,PhysiclChemistry,Oxford University Press 9. Silverstein, Bassler, Monill - Spectroscopic Identification of Organic Compound- John Wiley & Sons, 1991. 10. Kemp - Organic Spectroscopy - McMillan, 1996. 11. Drago R S, Physical Methods for Chemists, W. B. Saunders (1992) 12. Pavia, Spectroscopy of Organic Compounds, Sounde Publications. 13. J.B. Lambert, H.F., Shurvell, D.A. Lightner and R.G Cooks, Organic Structured Spectroscopy, Prentice Hall. 14. Handbook of Analytical Techniques by Helmut Gunzler and Alex Williams, Publisher: Wiley-VCH, 2001; ISBN: 9783527301652. 15. Surface Analysis Methods in Materials Science by J. O'Connor, B. Sexton, R. Smart, Publisher: Springer, 2003; ISBN: 9783540413301. 16. Modern Techniques of Surface Science by D.P. Woodruff, Publisher: Cambridge University Press, 2016; ISBN: 9781139149716. 17. Mass spectrometry- Principles and applications by Edmond de Hoffmann and Vincent Stroobant, Publisher: John Wiley & Sons, 2007; ISBN: 9780470033104. 18. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry by Harald Gunther, Publisher: John Wiley & Sons, 2013; ISBN: 9783527330003. 19. Modern Spectroscopy by J. Mixhael Hollas, Publisher: John Wiley & Sons, 2004, ISBN: 9780470844168. | | |

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| Course Code | NSC3C 13 | DESIGN, SYNTHESIS AND PROPERTIES OF NANOMATERIALS | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in physics, chemistry and nanoscience | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ol style="list-style-type: none"> 1. Understand different top-down and bottom-up approaches available for nanomaterials synthesis. 2. Apply the knowledge on synthesis to properly design an experiment for tuning the size, shape and properties of the nanostructures 3. Understand and apply different lithographic techniques for the fabrication of nanostructures 4. Understand the fundamental principles and concepts related to the optical, electrical, magnetic, thermal and mechanical properties | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand physical, chemical, and lithographic techniques available for the preparation of nanoparticles or nanostructures and apply the knowledge to select a proper synthetic approach for a specific application (K2, K5) 2. Create experimental design to control the size, shape, distribution and properties of nanoparticles (K6) 3. Apply and analyze the design criteria for the fabrication of nanostructures by lithography (K3,K4) 4. Evaluate and correlate the structure-property optimization using the data collected from different analysis (K5,K6) 5. Apply the size and shape dependence of materials properties for tuning the material for various applications (K3) 6. Review the advantages of using nanostructured materials for various applications and the challenges that will face while using nanomaterials (K5) | | | | | | |
| K1 – Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate, K6- Create | | | | | | |
| UNIT-I | Physical and Chemical Methods | | 20 Hours | | | |
| <p>Introduction- Spontaneous growth, Vapor –Liquid-Solid (VLS) growth, and SWCNT and MWCNT growth mechanisms. Physical Vapour deposition techniques (PVD): Sputtering & e-beam Evaporation. Atomic layer deposition, Chemical vapour deposition method (CVD), Molecular beam epitaxy(MBE), & Electrospinning, Ball Milling. Chemical Methods: Nanoparticles through homogeneous & heterogenous nucleation in solution:-Co-precipitation method, Hydrothermal/ Solvothermal synthesis, Template based synthesis, Electrochemical synthesis, Sonochemical routes, Sol- gel, Micelles and microemulsions. Self-assembly methods and Langmuir Blodgett (LB) method.</p> | | | | | | |

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| UNIT-II | Lithographic Techniques | 10 hours |
| Lithography- Photolithography- Laser lithography and SPM based lithography (AFM & STM), Dip pen lithography and nanomanipulation. E-beam/SEM lithography. X-ray Lithography, Focused Ion beam lithography, Microcontact printing, nanoimprint. | | |
| UNIT-III | Optical, Electrical & Magnetic Properties of Nanostructures | 20 Hours |
| Interaction of light with matter. The nano perspective. The surface plasmon resonance-applications of nano plasmonics. Quantum dots – Optical properties related to quantum confinement. Special luminescent materials - electroluminescence- photochromic and electrochromic nanomaterials. Electrical conductivity in nanotubes and nanorods and nanocomposites. Electronic transport in nanostructures, single electron transfer devices (SETs), Electron spin transistor – resonant tunnel devices - quantum interference transistors (QUITs). | | |
| Introduction – magnetic phenomena and their classical interpretation- Magnetization and nanostructures. Superparamagnetic particles- susceptibility and related phenomena in superparamagnets- Magnetism in reduced dimensional systems- Two, one and zero dimensional systems. Physical properties of magnetic nanostructures - exchange coupled magnetic nanomaterials- spin –polarized tunneling- magneto-resistivity, GMR. Spintronics, Magneto electrical effects, ferrofluids, molecular nanomagnets, data storage applications of magnetic nanoparticles, Spintronic devices and applications. | | |
| UNIT-IV | Mechanical & Thermal properties of Nanostructures | 17 Hours |
| Nano-mechanics- Introduction- three atom chain- lattice mechanics- linear elasticity relations – molecular dynamics. Structure and mechanical properties of carbon nanotubes- nanomechanical measurement techniques- AFM – Nanoindentation. Nano-thermodynamics:- Thermodynamics the nano perspective – Background- application of classical thermodynamics to nanomaterials- small system thermodynamics. Modern nano-thermodynamics- Non-extensivity and nonintensity – nano-thermodynamics of a single molecule – modeling nanomaterials. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| Total Lecture Hours | | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Nanostructures and Nanomaterials- Synthesis, Properties & applications by GuozhongCao , Imperial college Press, (2006). Publisher: World Scientific Publishing Company; 2 edition (4 January 2011) ISBN-13: 978-9814324557 2. An introduction to Electrospinning and Nanofibers by Seeram Ramakrishna, KazutoshiFujihara, Wee Eong Tee, Teck Cheng Lim, Zaveri Ma, World Sci. Pub. Ltd. Singapore, 2005, Publisher: World Scientific Publishing Co Pte Ltd (8 May 2005) ISBN-13: 978-9812564542 3. Springer Handbook of Nanotechnology - Bharat Bhusan, Publisher: Springer-Verlag (15 May 2006) ISBN-13: 978-3540343660 4. Introduction to Nanoscience & Nanotechnology by Gabor L. Hornyak, Harry F. Tibbals, Joydeep Dutta, John J. Moore, CRC Press, Tylor & Francis Group New | | |

York, 2009. **Publisher:** CRC Press (15 December 2008) **ISBN-13:** 978-1420047790

5. Introduction to Nanoscale Science & Technology, Di Ventra, Evoy, Heflin, Springer Science, NY, 2004, **Publisher:** Springer; 1 edition (30 June 2004)
Sold by: Amazon Asia-Pacific Holdings Private Limited
6. Nanofabrication- Fundamentals and Applications, By Ampere A Tseng, World Scientific, Singapore 2008. □ **Publisher:** World Scientific Publishing Co Pte Ltd (18 March 2008) **ISBN-13:** 978-9812705426
7. Nanoparticles and Nanostructured Films- Preparation Characterization and Applications by Janos H. Fendler, WILEY-VCH Verlag GmbH. D-69469 Weinheim (Federal Republic of Germany), 1998, **Publisher:** Wiley VCH (28 May 1998) **ISBN-13:** 978-3527294435
8. Introduction to Nanotechnology - Charles P. Poole Jr. and Franks. J. Qwens, **Publisher:** Wiley-Interscience; 1 edition (30 May 2003) **Sold by:** Amazon Asia-Pacific Holdings Private Limited.
9. Nanomaterials – An Introduction to synthesis, Properties and Applications, by Dieter Vollath, Wiley – VCH Verlag GmbH & Co. Germany, 2008.
10. Properties of nanomaterials by Charles P. Poole.
11. The Physics & Chemistry of Nanosolids by Frank J. Owens and Charles P. Poole Jr. , John Wiley & Sons, Inc. New Jersey 2008.
1. Introduction to Nanoelectronics, by V. Mitin, V. Kochelap, M. Stroscio, **Cambridge University Press (2008).**
2. Nanoelectronics and Photonics: From Atoms to Materials, Devices, and Architectures by Anatoli Korokin I Federico Rosei, **2008 Springer Science, Business Media, LLC.**
3. Nanoelectronics and Information Technology: Advanced Electronic Materials and Novel Devices, by Rainer Waser, **Wiley-VCH (2003).**
4. Nanoelectronics and Nanosystems, by Karl Gosser, Peter Glosekotter, Jan Dienstuhl, **Springer (2004).**
5. Nanotechnology & Nanoelectronics, Materials, devices, measurement techniques, by W. R. Fahrner(Editor), **Springer, 2005**
6. Principles of Nanophotonics, by Motoichi Ohtsu, Kiyoshi Kobayashi, Tadashi Kawazoe, Takashi Yatsui, Makoto Naruse, **CRC press 2008 by Taylor & Francis Group**
7. Semiconductor Quantum Dots, L. Banyai and S.W.Koch, **World Scientific (1993).**
8. NanoBiophotonics, H. Masuhara, S. Kawata and F. Tokunga, **Elsevier Science, (2007).**
9. Fundamentals of Photonics, B. E. A. Saleh and A. C. Teich, John Wiley and Sons, New York, (1993).
10. Introduction to Biophotonics, P. N. Prasad **John Wiley and Sons, (2003).**
11. Molecular Nanomagnets, Dante Gatteschi, Roberta Sessoli, Jacques Villain, Oxford **University Press 2006, USA.**
12. Concepts in Spin Electronics, Sadamichi Maekawa, **Oxford University Press (2006).**
13. Nanomagnetism and Spintronics: Fabrication, Materials, Characterization and Applications
14. Farzad Nasirpouri , Alain Nogaret □ **Publisher:** World Scientific Publishing Company;
edition (December 21, 2010) **ISBN-10:** 9814273058

15. Nanophysics and Nanotechnology: An Introduction to Modern Concepts in Nanoscience, Edward L. **Wolf Wiley-VCH (2006).**
16. Biomineralization: Principles and Concepts in Bioinorganic Materials Chemistry. Mann, S., **2001. New York, Oxford University Press.**
17. Nanoscale Technology in Biological Systems, Edited by Ralph S. Greco, Fritz B. Prinz, R. Lane Smith, **CRC Press, USA, 2005.**
18. Nanoparticle Technology for Drug delivery, Ram B.Gupta, Uday, B.Compella, **2006 Taylor & Francis Group, LLC, NY.**
19. Nanoparticulates as Drug Carriers, Vladimir Ptorchilin, **Imperial College Press, London, 2006.**
20. Hybrid Nanocomposites for Nanotechnology, Electronic, Magnetic, Optical and Biomedical Applications,byLhadiMerhari, **Springer USA 2009.**

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|---|--|-------------------------------------|-------------------------|----------|-------------|----------|
| Course Code | NSC3C 14 | COMPUTATIONAL NANOTECHNOLOGY | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in general physics, Chemistry and mathematics. | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| The main objectives of the course are to: <ul style="list-style-type: none"> • Understand different computational tools. • Learn the building up of z-matrix. • Understand different kinds of modelling and simulations. • Evaluate different computed results through various methods. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Introduction to different computational tools – K2 2. Understand the need and importance of computational studies in supporting scientific results – K1, K4 3. Learn to write z-matrix – K2, K3, K6 4. Understand different simulations and applications in nano technology – K2, K3 | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Introduction to Computational Calculations | 20 Hours | | | | |
| Potential energy scanning, saddle points, local and global minima. Geometry optimization, Molecular orbital, charges, electron density. Frequency calculation Interaction energy. ESP map. Global reactive descriptors. Fukui descriptors. Koopmans's theorem. Different (freeware and commercial)- Excel, Origin, chem. Draw/Chem Sketch, Gaussian 09, Gaussview5, SPSS, VASP, material studio. | | | | | | |
| UNIT-II | Introduction to Computational Methods | 20 Hours | | | | |
| Basis sets- different types. Basis set truncation error. Electron correlation. Correlation energy. Basis set limit. Slater type orbitals and Gaussian type orbitals; z-matrix- basic idea and construction. Z-matrix of small molecules like H ₂ O, HCHO, CH ₃ OH and H ₂ O ₂ . Molecular mechanics. Semi-Empirical method. Ab initio method. Density functional theory method. Molecular dynamics. ONIOM method. | | | | | | |
| UNIT-III | Introduction to Python | 12 Hours | | | | |
| Variables and Data Types, python strings and lists, Operators and their Precedence, Iteration: while and for loops, Python Syntax, Colon & Indentation, Syntax of 'for loops, Conditional Execution: if, elif and else, functions, Python modules and packages, File Input/Output, Exception Handling, The NumPy Module, Vectorized Functions. | | | | | | |
| UNIT - IV | Computational Nanotechnology | 15 Hours | | | | |

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| Quantum confinement; change in properties with size. Applications of computational studies in nanotechnology. Simulations-different types-Monte Carlo Methods (Detailed treatment).Nano-computing and modelling. Computing transport in materials. Nano-design Nano-CAD. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. D. Frenkel and B. Smith, —Understanding molecular simulation from algorithm to applicationsII, Kluwar Academic Press, 1999. 2. K. Ohno, K. Esfarjani and Y. Kawazoe, —Introduction to Computational Materials Science from ab initio to Monte Carlo MethodsII, Springer-Verlag, 1999. 3. Jenson F, Introduction to Computational Chemistry – John Wiley 4. Cramer C.J., Essentials of Computational Chemistry – John Wiley 5. Young, Computational Chemistry – Wiley Inter Science 6. Andrews R. Leach, Molecular Modeling – Pearson 7. Ramachandran K.I et al computational Chemistry and Molecular Modeling Springer. 8. Schlick. T., Molecular Modeling and Simulations, Springer. 9. Python for Education, Ajith Kumar B.P. IUAC, New Delhi; free e-book. 10. Introduction to Python for Engineers and Scientists by Dr.Sandeep Nagar, Apress publications | | |

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|---|---|-----------------------|-------------------------|----------|-------------|----------|
| Course Code | NSC3P 03 | PRACTICAL -III | L | T | P | C |
| Core | | | 0 | 0 | 2 | 2 |
| Pre-requisite | Basic knowledge on different nanomaterials and their interesting properties | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Understand and develop practical skill on different synthetic approaches for nanomaterials 2. Apply the physical and chemical phenomenon associated with nanomaterials by choosing suitable synthetic method 3. Develop data collection skill and analyze the data components using analysis software 4. Evaluate the experimental results with the theory associated with nanosystems 5. Hands on experience on using various sophisticated instruments for analysis | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand and apply chemical and physical methods for the synthesis of nanomaterials (K2,K3) 2. Understand the advantages and disadvantages choosing a particular method for nanomaterial synthesis (K2) 3. Create awareness on the importance of data collection statistics and analysis of different types of data for proving the concepts studied (K4,K6) 4. Recognize different advanced tools available for data generation and analysis.(K2) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| List of Experiments: (Only selected experiments will do:Maximum 10 experiments) | | | | | | |
| <ol style="list-style-type: none"> 1. Synthesis of different sized Ag nanoparticles by aqueous method, Size distribution studies using DLS 2. Synthesis of different sized Au nanoparticles by aqueous method, Size distribution studies using DLS 3. Green Synthesis of Nanoparticles. 4. Sol-gel synthesis of ZnO nanoparticles. 5. Analysis of optical properties of ZnO nanoparticles 6. Geometry optimization and frequency calculation using Gaussian program. 7. Introduction to Origin software for data analysis 8. Structure and physical property elucidation of small molecules using Chem Draw/Chem Sketch. 9. Chemical synthesis of CdSe Quantum dots with different sizes. 10. Band gap estimation of CdSe quantum dots by using optical spectroscopy 11. Exciton and plasmon interaction studies of Au-CdSe system by using optical spectroscopy | | | | | | |

12. Operation of Electrochemical Workstation
13. Deposition of Polyaniline on ITO/FTO using Electrochemical Workstation.
14. Structural elucidation of Electrodeposited polyaniline using FTIR
15. Chemical Synthesis of Magnetic nanoparticles and size determination.
16. Electrochemical synthesis of TiO₂ Nanostructures. Optical Studies by using UV-VIS spectrophotometer. Electronic structure analysis by using Cyclic Voltammetry.
17. Electrochemical Synthesis of ZnO nanorods - Optical Studies by using UV-VIS spectrophotometer. Electronic structure analysis by using Cyclic Voltammetry.
18. Thin film deposition of TiO₂ and ZnO by Electrochemical method – Study the optical and electronic properties.
19. Compare the results of 1D structure with 2D thin films of both TiO₂ and ZnO.
20. Thin film preparation using spin coating method and thickness measurement using Profilometer.
21. Hall measurements of electrodeposited TiO₂ thin films
22. Performing Potential energy scanning and geometry optimization
23. Frequency calculation and interpretations
24. Prediction of electronic transitions and analysis of MOs
25. Calculation of global reactive parameters through Koopmans's theorem
26. Prediction of possible conformers and interactions
27. Prediction of correlation coefficient
28. Calculation of global reactive parameters through orbital energy method
29. Calculation of binding/stabilization energy
30. Prediction of donor-acceptor interactions
31. Calculation with periodic boundary conditions

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| Course Code | NSC4PR 01 | PROJECT | L | T | P | C |
| Project | | | 0 | 0 | 8 | 8 |
| Pre-requisite | Basic knowledge on nanoscience and nanomaterials | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Inculcate and improve the research attitude of the student 2. To understand the process of literature review and use of online research resources 3. Train to design a research problem and to understand how to fix the objectives and methodologies to solve the problem 4. Documentation practices and improvement of communication and presentation skills | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Apply the scientific concepts to identify and design a research problem in the area of nanoscience (K3) 2. Understand and analyze the results or data obtained from experiments or simulation using data analysis softwares (K2,K4) 3. Apply the theoretical knowledge to explain the data collected from different advanced characterization techniques (K3) 4. Understand the importance of documentation procedure and research publication. (K2) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
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SYLLABUS
of
ELECTIVE COURSES

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| Course Code | NSC4E 01 | NANOSTRUCTURED SOLAR CELLS | L | T | P | C |
| Elective | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in Nanoscience | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Conscious of energy crisis, its reason, current status and possible solutions 2. Recognize renewable and non-renewable energy resources and their contribution towards global energy production 3. Importance of re-newable energy resources and tapping such energies 4. Role of Nanoscience or nanotechnology in producing novel materials and designs for efficient production of energy using renewable resources | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Analyze the reasons for energy crisis and understand the importance of sustainable energy development (K4,K2) 2. Understand Hydrogen economy and advantages and challenges of Hydrogen fuel and its production (K2) 3. Understand the possibilities of solar energy production using nanostructured materials and create awareness on using solar panels for house hold and other energy usages. (K2,K6) 4. Analyze the importance of different design architectures for efficient tapping of solar energy using nanoscience (K4) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Primary Perspective in Energy Conversion | | 14 Hours | | | |
| Current energy scenario; Energy and climate: - Greenhouse effect, conventional energy sources Vs non-conventional energy sources. Outline of alternative energy schemes – solar, wind, biomass, hydro, and nuclear. Clean low cost, sustainable energy development, prospects of renewable energy. | | | | | | |
| UNIT-II | Photovoltaic Solar Energy Conversion | | 16 Hours | | | |
| Properties of sunlight: Solar radiation at earth's surface- Air Mass. Semiconductors and junctions, carrier generation, Recombination, Carrier Transport, Solar cell operation, Principles of photovoltaic energy conversion (PV), Solar cell parameters, Factors affecting the solar cell efficiency, Types of photovoltaic Cells. | | | | | | |
| UNIT-III | Silicon Solar Cells | | 20 Hours | | | |
| Si solar cells- Structure, and working. Optical properties, optical losses, antireflection coating, light trapping. Reducing recombination, Silicon solar cell manufacturing, Silicon wafers, processing technologies, solar cell fabrication technologies, Modules and arrays, inter connection issues, temperature effects and other effects. Efficiency | | | | | | |

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| measurements, IV Characterization, Life time etc. General materials properties of silicon. Types of silicon solar cells. | | |
| UNIT-IV | Nanostructured Solar Cells | 17 Hours |
| Fundamentals of nanostructured solar cells, nanostructures in conventional thin film solar cells. Dye sensitized solar cells (DSSC), Design and working. Quantum dot sensitized solar cells (QDSSC), Design, working and charge transfer kinetics. Organic solar cell, Organic-Inorganic Hybrid Bulk Hetero Junction (BHJ-SC) Solar cells, Nanostructured ETA solar cells, Current status and future direction. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Nanostructured Materials for Solar Energy Conversion, By Tetsuo Soga, 2006 Elsevier B.V. All rights reserved. 2. PVCDROM, "www.pveducation.org", 3. Aldo V. da Rosa, <i>Fundamentals of Renewable Energy Processes, 2nd Edition</i> (Elsevier Academic Press, 2009). 4. Fuel cells- principals and Applications, by B.Viswanathan, M.AuliceScibioh, Universities Press, India, 2006. 5. Green Chemistry and Chemical Engineering, Proton Exchange Membrane Fuel Cells Contamination and Mitigation Strategies, By hui Li, Shanna Knights, Zheng Shi, John W. Van Zee, Jin Jun Zhang, Taylor and Francis Group, 2010, USA. 6. Martin A. Green, <i>Solar Cells: Operating Principles, Technology, and System Approaches</i> (Prentice-Hall, 1998) 7. Jenny Nelson, <i>The Physics of Solar Cells</i> (Imperial College Press, 2003) 8. D. Linden Ed., <i>Handbook of Batteries</i>, 2nd edition, McGraw-Hill, New York (1995) 9. G.A. Nazri and G. Pistoia, <i>Lithium Batteries: Science and Technology</i>, KulwerAcademic Publishers, Dordrecht, Netherlands (2004). 10. J. Larminie and A. Dicks, <i>Fuel Cell System Explained</i>, John Wiley, New York (2000). | | |

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| Course Code | NSC4E 02 | NANOMATERIALS FOR PHOTOCATALYSIS AND SOLAR FUEL GENERATION | L | T | P | C |
| Elective | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in nanomaterials and their synthesis | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Familiarize students the importance of nanomaterials for sustainable development. 2. Enhancing the student's knowledge on nanomaterials for environmental remediation. 3. Understand the photocatalysis reactions for solar fuel generation. 4. Apply the knowledge gained for developing efficient nanostructured photocatalysts. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand the benefits of nanomaterials for sustainable development (K2) 2. Analyze the concepts of photocatalysis and its technological significance. (K4) 3. Apply the photocatalysis reaction mechanisms towards contaminant degradation, hydrogen evolution and carbon dioxide reduction. (K3) 4. Create strategies for developing efficient nanostructured photocatalysts.(K6) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Photocatalysis | | 20 Hours | | | |
| Introduction; Light and matter interaction; Principles of Photocatalysis; Electronic band structure of semiconductors; Mechanisms of charge formation, separation and transfer; Basic principles of photocatalytic water splitting for hydrogen generation; Basic principles of photocatalytic reduction of CO ₂ ; Photocatalysis surface and active species. | | | | | | |
| UNIT-II | Environmental Remediation | | 16 Hours | | | |
| Introduction; Fabrication of nanostructured photocatalysts; Methods of improving photocatalytic activity: Design parameters; Photodegradation of dyes; Photodegradation of persistent organic pollutants; Photodegradation of Inorganic pollutants; Photodegradation of emerging contaminants; Photodegradation of gaseous pollutants; Characterization and analysis of acquired data. | | | | | | |
| UNIT-III | Hydrogen Evolution and Carbondioxide Reduction | | 16 Hours | | | |
| Introduction; Electronic band structure considerations; Photocatalytic reaction mechanism and charge transfer; Fabrication of nanostructured photocatalysts and design parameters: H ₂ generation and CO ₂ reduction; Z-scheme heterojunction photocatalysts; Quantification and calculation of efficiency; Characterization | | | | | | |

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| UNIT-IV | Strategies for Improving Performance of Photocatalysts | 15 Hours |
| Introduction; Issues related to single-component photocatalysts; Microstructure modulation; Influence of facet and defects; Integration of noble metal nanostructures; Carbonaceous materials compounding – rGO, CNTs, CQDs; Integration with other semiconductor nanostructures. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Gianluca Li Puma, Detlef W. Bahnemann, Dionysios D. Dionysiou, Jinhua Ye and Jenny Schneider, Photocatalysis: Fundamentals and Perspectives, Publisher: Royal Society of Chemistry, ISBN: 9781782620419, 1782620419. 2. Umar Ibrahim Gaya, Heterogeneous Photocatalysis Using Inorganic Semiconductor Solids, Publisher: Springer Netherlands, ISBN: 9789400777750, 9400777752 3. Kazuya Nakata and Akira Fujishima, TiO₂ photocatalysis: Design and applications, Journal of Photochemistry and Photobiology C: Photochemistry Reviews 2012, 13, 169-189, https://doi.org/10.1016/j.jphotochemrev.2012.06.001 4. Chunping Xu, Prasaanth Ravi Anusuyadevi, Cyril Aymonier, Rafael Luque and Samuel Marre, Nanostructured materials for photocatalysis, Chemical Society Reviews, 2019,48, 3868-3902, https://doi.org/10.1039/C9CS00102F | | |

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| Course Code | NSC4E 03 | MICRO/NANO ELECTRO MECHANICAL SYSTEMS (MEMS/NEMS) | L | T | P | C |
| Elective | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in nanoscience and nanodevices | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Understand an overview of MEMS and NEMS 2. Understand different fabrication methods of MEMS/NEMS 3. Identify the applications of MEMS/NEMS 4. Understand different characterization tools of MEMS/NEMS | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand the basics and working principles of MEMS/NEMS (K2) 2. Recognize different application potential of MEMS/NEMS (K2) 3. Evaluate the quality of MEMS/NEMS using different characterization tools (K5) 4. Understand the Cross-disciplinary application of MEMS and NEMS (K2) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | MEMS Fabrication | | 18 Hours | | | |
| Overview of micro electro mechanical devices and technologies. Introduction to architecture design, Process flow, Fabrication, Packaging and testing. MEMS Fabrication, Deposition, lithography, and etching, Surface micromachining, Bulk micromachining, Bonding technologies, LIGA technology and related fabrication methods | | | | | | |
| UNIT-II | Applications of MEMS | | 18 Hours | | | |
| MEMS device concepts (micro sensors/actuators), Use of capacitive, Inductive, Optical, piezoresistive, Piezoelectric methods for sensing. MEMS Applications, Accelerometers and gyros, Pressure sensors, Micro optics, etc. Microsystems Packaging | | | | | | |
| UNIT-III | MEMS/NEMS Characterization | | 15 Hours | | | |
| Introduction to existing and next-generation metrology tools for MEMS and NEMS inspection and qualification. Theoretical principles of metrology and experimental work on characterization of prototype MEMS and NEMS devices. | | | | | | |
| UNIT-IV | Biological Applications of MEMS/NEMS | | 16 Hours | | | |
| Cross-disciplinary application of MEMS and NEMS to the biological sciences. Interaction of living cells/tissues with nanofabricated structures, Microfluidics for the movement and control of solutions - the development of I/O architectures for efficient readout of bioreactions. | | | | | | |
| UNIT-V | Contemporary Issues | | 5 Hrs. | | | |
| Expert lectures, General Seminars, online seminars – webinars | | | | | | |
| | | | Total Lecture Hours | | 72 Hours | |

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| Text Books/References |
| <ol style="list-style-type: none">1. Mohamed Gad – el – Hak, “The MEMS Handbook”, Second Edition, CRC Press, 2005.2. James J. Allen, “Micro Electro Mechanical System Design”, CRC, 2005.3. K. Subramanian, “Micro Electro Mechanical Systems: A Design Approach”, Springer, 2008.4. Tai-Ran Hsu, MEMS and Microsystems- Design, Manufacture and Nanoscale Engineering, John Wiley & Sons, INC. 2008. ISBN: 978-0-470-08301-7. |

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| Course Code | NSC4E 04 | SUSTAINABLE NANOMATERIALS | L | T | P | C |
| Elective | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge on nanomaterials | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Understand the toxicity of nanomaterials 2. Aware of environmental pollution act and importance of Green Chemistry 3. Understand different green synthetic approaches for the nanomaterial 4. Understand the environmental applications of nanomaterials | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand the environmental pollution and could recognize the nanomaterial toxicity (K2,K1) 2. Understand the importance of Green Chemistry (K2) 3. Apply different green synthesis approach for the materials preparation (K3) 4. Apply the nanomaterials for environmental protection (K3) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Nanomaterials Toxicity | | 18 Hours | | | |
| Environmental pollution and hazards: Toxicity of chemicals and their characterization, R&S Numbers, material safety data sheet (MSDS), highly toxic nanomaterials. | | | | | | |
| UNIT-II | Principle of Green Chemistry | | 18 Hours | | | |
| Environmental Pollution content Act (USEPA) 1990, Green chemistry, 12 principle of green chemistry, atom economy, alternative solvents, renewable materials, etc. | | | | | | |
| UNIT-III | Green Synthesis of Nanomaterials | | 15 Hours | | | |
| Green methods for nanomaterial synthesis, use of supercritical carbon dioxide, ionic liquids, RESS process, use of green reagents (citrate and glucose based synthesis of metal nanoparticles) biosynthesis of nanostructures, template-free synthesis of mesoporous silica and metal oxide | | | | | | |
| UNIT-IV | Environmental Applications of Nanomaterials | | 16 Hours | | | |
| Environmental application of nanomaterials. Water purification system, systems for harvesting solar energy, mesoporous materials for naked eye detection of toxic metal ions in water (mesoporous silica) self –cleaning materials, non-wetting glasses, super hydrophobic coatings etc. | | | | | | |
| UNIT-V | Contemporary Issues | | 5 Hrs. | | | |
| Expert lectures, General Seminars, online seminars – webinars | | | | | | |
| | | | Total Lecture Hours | | 72 Hours | |

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| Text Books/References |
| <ol style="list-style-type: none">1. Paul T. Anastas and John C. Warner, Green Chemistry : Theory and Practice, Oxford University Press (2000)2. Paul M. Matlack, Introduction to Green Chemistry, CRC Press, 2nd ed. (2010)3. Geoffrey B. Smith, Green Nanotechnology: Solutions for Sustainability and Energy in the Built Environment, CRC Press (2010)4. P. Raveendran, Jie Fu & S.L. Wallen. Completely “green” synthesis and stabilization of metal nanoparticles. J.Am.Chem.Soc.(2003), 125, 13940-41. |

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| Course Code | NSC4E 05 | NANOMATERIALS FOR SUPERCAPACITOR APPLICATIONS | L | T | P | C |
| Elective | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in Nanoscience | | Syllabus Version | 2022 | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Conscious of energy crisis, its reason, current status and possible solutions 2. Recognize the significance of energy storage 3. Importance of efficient storage and release of energy 4. Role of Nanoscience or nanotechnology in producing novel materials and designs for efficient storage of energy using renewable resources | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Analyze the performance of electric capacitors and understand their advantages and disadvantages (K4,K2) 2. Understand different electrochemical techniques to know better the electrode-electrolyte interface (K2) 3. Understand the possibilities of electrochemical double layer supercapacitors for efficient energy storage and create awareness on using such advanced technologies (K2,K6) 4. Analyze the importance of novel energy storage devices with improved performance using nanoscience (K4) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Fundamentals of Electric Capacitors | | 14 Hours | | | |
| Introduction, energy storage in capacitor, types and structures of capacitors. General principles of electrochemistry, equilibrium electrochemistry, dynamic electrochemistry. General properties of electrochemical capacitors. Electrochemical cell, electrochemical interfaces, different electrochemical techniques. | | | | | | |
| UNIT-II | Electrochemical Double-Layer Supercapacitors | | 16 Hours | | | |
| Introduction, Electrode-Electrolyte interfaces, Electrode Potential and double layer potential windows. Electrochemical double layer supercapacitors: structure and capacitance, equivalent series resistance, leakage resistance, supercapacitor charging and discharging, energy and power densities of EDL supercapacitors. EDLC electrode Materials. | | | | | | |
| UNIT-III | Electrochemical Pseudo capacitors | | 20 Hours | | | |
| Introduction, Electrochemical pseudo capacitors, interfaces of electrode and electrolyte. Electrochemical Impedance spectroscopy and equivalent circuits. Electrode materials and Cell Designs. Pseudo capacitive materials, Asymmetric structures. Electrolyte structures and materials. | | | | | | |

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| UNIT-IV | Characterization & Applications of Electrochemical Supercapacitors | 17 Hours |
| Electrochemical cell design and fabrication. Cyclic voltammetry, Charging Discharging curve, electrochemical impedance spectroscopy, Physical Characterization methods. Applications of Electrochemical supercapacitors: power electronics, portable energy systems, hybrid electric vehicle etc. Perspectives and challenges of electrochemical super capacitors | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| 11. Electrochemical Supercapacitors for Energy Storage and Delivery: Fundamentals and Applications, by Aiping Yu, Victor Chabot and Jiujun Zhang, CRC Press, Tylor & Francis Group, New York (2013). 12. Supercapacitors: Materials, Systems and Applications, Max Lu, Francois Beguin, Elzbieta Frackowiak, | | |

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|---|---|--|-----------------|----------|----------|----------|
| Course Code | NSC4E 06 | COMPUTATIONAL STUDIES ON BIO-ACTIVE COMPOUNDS | L | T | P | C |
| Elective | | | 4 | 0 | 0 | 4 |
| Pre-requisite | Basic knowledge in general Chemistry and mathematics. | Syllabus Version | 2022 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| The main objectives of the course are to: <ul style="list-style-type: none"> • Understand different computational tools. • Learn different bio-active compounds. • Learn drug likeness. • Learn about computational study of bio-active compounds. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand different bio-active compounds – K2 2. Understand the need and importance of computational studies in supporting scientific results – K1, K4 3. Learn drug likeness and related parameters – K2, K3, K6 4. Understand different drug-target interactions– K2, K3 | | | | | | |
| K2 – Understand K3 – Apply K4 – Analyze K6 - Create | | | | | | |
| UNIT-I | Errors and Statistical Tools in Data Analysis | | 15 Hours | | | |
| Significant figures. Errors and classification; accuracy and precision; significant figures and rules; selection of data- T-test; F-test; Q-test; Euler's theorem- exact and inexact differentials; Cartesian-polar-spherical coordinates. | | | | | | |
| UNIT-II | Bio-active Compounds & Metals in Medicine | | 16 hours | | | |
| Natural products. Classification: flavonoids, terpenoids, steroids, alkaloids. Structure and general characteristics. Proteins. DNA. RNA. Biological interactions. Medicinal importance of bio-active compounds. Some examples. Bio-activities. Metal toxicity and homeostasis. Metal deficiency and diseases. Toxic effects of metals. Effect of deficiency and excess of essential metal ions. Toxicity due to non-essential elements. Speciation of metal ions. Detoxification mechanism. Role of lithium and aluminium in biological systems. Chelation therapy and chemotherapy. Metal complexes as drugs. Anticancer drugs and Vanadium based diabetics drugs. Inorganic pollutants in natural water. Plants as accumulators of elements. Indicator plants and biominerals. | | | | | | |
| UNIT-III | Introduction to Medicinal Chemistry | | 20 Hours | | | |
| Features of Drug like molecules. Drug classification: synthetic, semi-synthetic and non-synthetic drugs. Drug classification according to medicinal use: pharmacodynamic medicinal use. Pharmacodynamic agents and chemotherapeutic agents. Lipinski's rule of 5. Examples of receptors and discussion about drug-receptor interaction. Physicochemical properties determining biological activity such as solubility, acidity and reactivity. Importance of liphophilicity constant (logP) for predicting solubility. Calculation of | | | | | | |

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| logP value for medicinal compounds. Factors determining stability and bioavailability of medicinal compounds. Isosterism and bio-isosterism. Influence of structural features of drugs (such as optical and geometrical isomerism) on biological activities. ED50, IC50, TD50 and LD50. A brief introduction on the following terms: Pharmacology, Pharmacodynamics, Pharmacokinetics and ADME, pharmacotherapeutics, pharmacogeny, toxicology, Basic steps in drug discovery: from lead discovery to commercialization (a brief introduction only) structural activity relationship (SAR) studies in lead discovery and optimization. Modern synthetic methods of lead synthesis and lead optimization. | | |
| UNIT-IV | Computation of Bio-active Compounds | 16 Hours |
| Combinatorial chemistry. General computational methodology and evaluation of computed results. QSAR/QSPR study. Developing 2D and 3D QSAR/QSPR models. Molecular docking and drug-target interactions. Statistical analysis of computed results. Donor-acceptor interactions. Different biological assays: Antioxidant; DPPH, TEAC. Merits and demerits of experimental studies on antioxidant activities. Importance of computational studies on evaluating antioxidant capacities. theoretical antioxidant mechanisms and their computational evaluation. Evaluation of UV filtering and metal chelation capacity. Multi target interactions. | | |
| UNIT-V | Contemporary Issues | 5 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007. 2. Jenson F, Introduction to Computational Chemistry – John Wiley 3. Cramer C.J., Essentials of Computational Chemistry – John Wiley 4. Young, Computational Chemistry – Wiley Inter Science 5. S.S. Sastry (SS), Introductory Methods of Numerical Analysis, PHI 6. J.B. Scarborough (SB), Numerical Mathematical Analysis, Oxford & IBH 7. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry. Author(s): John M Beale Jr., PhD, John Block, ISBN/ISSN: 9780781779296, Edition: Twelfth, 2010 8. Gareth Thomas, Fundamentals of Medicinal Chemistry, ISBN: 9780470 84307-9, WileyBlackwell | | |

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| Course Code | NSC4E 07 | PRECISION NANOCLUSTERS: ORIGIN AND APPLICATIONS | L | T | P | C |
| Core | | | 4 | 0 | 0 | 4 |
| Pre-requisite | | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <p>The main objectives of the course are to:</p> <ol style="list-style-type: none"> 1. To understand the applications of various precision nanomaterials in different aspects of Science 2. To analyse the potentials of precision nanoprobe in cancer therapeutics. 3. To evaluate the uses of different nanoprobe in catalysis, sensing, fabrication of solar cells and light-emitting devices. 4. To create new functional nanoprobe for advanced applications. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. This course is designed to understand (K1) the applications of precision nanomaterials in different aspects of Science, including catalysis, sensing, fabrication of solar cells and light-emitting devices, and biology (K3, K6). 2. This particular course module will help students to analyse (K2) each precision nanoprobe at the laboratory level. 3. Towards the end of this course, students could evaluate (K3) which precision nanoprobe will be ideal for specific applications. 4. Such experience will help to create (K4) novel precision materials during their Ph.D. career. | | | | | | |
| K1 – Remember K2 – Understand K3 – Apply K4 – Analyze K5 – Evaluate, K6-Create | | | | | | |
| UNIT-I | Precision Nanoclusters: Origin, Synthesis, & Characterization | | | | 17 Hours | |
| <p>Polydisperse nanoparticles to monodisperse nanoparticles and monodisperse nanoparticles to atomically precise nanoclusters – Brust synthesis and beyond. Electronic and geometric stability of nanoclusters (Magic numbers). Size-focused synthesis of gold, silver, and copper nanoclusters – Chemical reduction method, LEIST methodology, carbon monoxide reduction method. Different isolation techniques – Fractionated precipitation, recrystallization, solvent extraction, polyacrylamide gel electrophoresis, Size exclusion chromatography, High – performance liquid chromatography, Thin – layer chromatography. Synthesis and separation of highly stable gold and silver nanoclusters (eg: Au₂₅(SR)₁₈, Au₃₈(SR)₂₄, Au₁₀₂(SR)₄₄, and Ag₂₉(BDT)₁₂(TPP)₄). Understanding composition and structure of nanoclusters using advanced mass spectrometry (ESI-MS and MALDI-TOF), Single crystal studies, Transmission electron microscopy, and other spectroscopic and microscopic techniques (XPS, absorption and photoluminescence spectroscopy). Theoretical models of structures of gold nanoclusters – “Divide and protect model” concept, Inherent structure rule, Superatom complex model, Superatom network model, Grand unified model (Brief). Precision nanoclusters protected with ligands other than thiols.</p> | | | | | | |

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| UNIT-II | Optical Properties of Nanoclusters | 15 hours |
| Optical properties – Optical absorption and Photoluminescence – Capping the gold core with different ligands, Tailoring core size and doping, Aggregation-induced emission. Nonlinear properties – Two-photon absorption/emission, Second harmonic generation. Ultrafast electron dynamics – Metallic or nonmetallic state of gold nanoparticles, Electron and energy transfer. Electrochemical properties (Brief). | | |
| UNIT-III | Chemistry of Nanoclusters | 18 Hours |
| Chemistry of metallic core – Modification by doping and formation of heterometallic nanoclusters (bimetallic, trimetallic, etc). Chemical reactivity – Intercluster reactions. Chemistry of ligands – Role of ligands in the size and structure of nanoclusters, Energy/Electron transfer, Isomerization, photosensitization. Ligand exchange, Ligand conjugation – coupling (EDC or DCC) reaction, and Click reaction. Stability of nanoclusters – Optical stability, thermal stability. Self-assembly of nanoclusters using various molecular driving forces (eg: Hydrogen bonding, Electrostatic interactions, Van der Waals interactions, Dipolar interactions, C-H \cdots π / $\pi\cdots\pi$ interactions, Amphiphilicity, Metal chelation, Metal-metal interactions, Light-triggered dipole – induced attractions, and external Templates). | | |
| UNIT-IV | Applications of Nanoclusters | 17 Hours |
| Catalysis – Oxidation (eg: CO, styrene, alcohol, cyclohexane), Hydrogenation (selective, alkyne, nitro compounds), C–C coupling reactions, Electron – transfer catalysis, Hydrolysis, Electrocatalysis, Photocatalysis. Sensors – Cation or anion sensing, Molecular sensing, Biosensing (glucose, biothiols, ATP, protein, and nucleic Acid). Applications in Solar cells and Light-emitting devices. Biological applications – Antimicrobial, Biolabelling, Bioimaging, Biomedical targeting, and Cancer Therapeutics – photodynamic, and photothermal Therapy. | | |
| UNIT-V | Contemporary Issues | 5 Hours |
| Expert lectures, General Seminars, online seminars – webinars | | |
| | Total Lecture Hours | 72 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Atomically Precise Nanoclusters, Yan Zhu and RongchaoJin, Jenny Stanford Publishing Pte. Ltd., (2021) 2. Atomically Precise Metal Nanoclusters, Zhikun Wu and RongchaoJin, Morgan & Claypool, (2020) 3. Protected Metal Clusters From Fundamentals to Applications, Tatsuya Tsukuda, HannuHäkkinen, Elseveir, (2015) 4. Precision Nanoclusters, Pradeep <i>et al.</i>Elseveir (2022, In press). 5. Chakraborty, I.; Pradeep, T. Atomically Precise Clusters of Noble Metals: Emerging Link between Atoms and Nanoparticles. <i>Chem. Rev.</i>2017, <i>117</i>, 8208-8271. https://doi.org/10.1021/acs.chemrev.6b00769. 6. Jin, R.; Zeng, C.; Zhou, M.; Chen, Y. Atomically Precise Colloidal Metal Nanoclusters and Nanoparticles: Fundamentals and Opportunities. <i>Chem. Rev.</i>2016, <i>116</i>, 10346-10413. https://doi.org/10.1021/acs.chemrev.5b00703. | | |

7. Kang, X.; Zhu, M. Tailoring the Photoluminescence of Atomically Precise Nanoclusters. *Chem. Soc. Rev.***2019**, *48*, 2422-2457.
<https://doi.org/10.1039/c8cs00800k>
8. Rival, J. V.; Mymoona, P.; Lakshmi, K. M.; Nonappa; Pradeep, T.; Shibu, E. S. Self-Assembly of Precision Noble Metal Nanoclusters: Hierarchical Structural Complexity, Colloidal Superstructures, and Applications. *Small***2021**, *17*, 2005718.
<https://doi.org/10.1002/smll.202005718>.

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| Course Code | NSC4E 08 | MATERIALS IN MEDICINE | L | T | P | C |
| Core Course | | | 60 | 4 | 4 | 4 |
| Pre-requisite | Basic knowledge in physical, chemical and biological sciences | Syllabus Version | 2022-2023 | | | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. To develop basic understanding about materials in medicine. 2. To introduce the concepts of biomaterials and their evaluation. 3. To learn the various structure and forms of biomaterials including the 'nano-biomaterials'. 4. To familiarize with the clinical importance of biomaterials. | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. This course is designed to develop basic knowledge (K1) related to materials used in medical field. 2. The detailed description of course module will help students to understand (K2) the physico-chemical and biological characterization methods of materials at the laboratory level. 3. Introduce the concept of nano-biomaterials and their potential applications (K3). 4. The course will help the students to analyze (K4) the scope of tissue engineering scaffolds, so that they would be able to evaluate (K5) and choose biomaterials for specific applications. 5. Such experience will create (K6) interest in students to pursue a career in biomedical research. | | | | | | |
| K1= Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Introduction to Materials in Medicine | 15 Hours | | | | |
| Introduction to biomaterials, functionally active materials and other materials used in medical devices and implants, Various classes of biomaterials including nano-biomaterials, Properties of Biomaterials. | | | | | | |
| UNIT-II | Characterization of Biomaterials | 15 Hours | | | | |
| Physico-chemical, morphological, thermal and mechanical characterisation of biomaterials, Surface and bulk analysis, Identification of phase and structure, Essentials of spectroscopic techniques used in materials characterization. | | | | | | |
| UNIT-III | Biocompatibility | 15 Hours | | | | |
| Essentials of biocompatibility. <i>In vivo</i> host responses to materials. Wound healing principles. Methods of biological safety evaluation. Biological evaluation of nanomaterials. Pre-clinical testing for safety and efficacy of biomaterials. | | | | | | |
| UNIT-IV | Applications of Biomaterials | 15 Hours | | | | |
| Use of biomaterial-based products in various specialities of medicine, Medical device translation, Standards and Regulations. | | | | | | |

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| UNIT-V | Expert Lectures on Advances in Biomedical Research | 12 Hrs. |
| Expert lectures, General Seminars, online seminars – webinars. Tissue engineering, scaffold fabrication, additive manufacturing, Regenerative medicine and state-of-the-art topics in biomedical technology. | | |
| | Total Lecture Hours | 72 Hours |
| Tutorials (1 per Unit) = 4 Practicals/Hands on training = 4 Credits (1 credit for 15 hours lecture) = 4 | | |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. Biocompatibility and Performance of Medical Devices 2nd Ed, Ed: Jean-Pierre Boutrand, Woodhead Publishing Limited, Cambridge CB22 3HJ, UK 2. Biomaterials Science and Biocompatibility, Eds Frederick H. Silver, David L. Christiansen, Springer-Verlag New York in 1999 3. Biomaterials Science: An Introduction to Materials in Medicine, Eds Buddy D. Ratner, Allan S. Hoffman, Frederick J. Schoen, Jack E. Lemons, Elsevier Academic Press, California, USA 4. Nanofabrication towards biomedical application: Techniques, tools, Application and impact by Challa S., Kumar, S. R.; Carola. Publisher: J. H. John Wiley & Sons, 2005; ISBN: 9783527311156. 5. Tissue Engineering, Palsson, B. O.; Bhatia, S. N. Publisher: Prentice Hall, 2003; ISBN: 6. Lanza, R.; Langer, R.; Joseph, P. Principles of Tissue Engineering. Publisher: Academic Press. 2013; ISBN-10: 0130416967. | | |

**SYLLABUS
of
AUDIT COURSES**

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|---|--|---|-------------------------|----------|-----------------|----------|
| Course Code | NSC1A 01 | ABILITY ENHANCEMENT COURSE (AEC) | L | T | P | C |
| Audit Course | | | 1 | 1 | 0 | 2 |
| Pre-requisite | None | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Skill identification for students in their respective field of study. 2. Recognize different research methodologies by introducing new research environments 3. Understand the basic concepts of research process 4. Make the student to work in a group by sharing knowledge | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Recognize the skills associated with each student (with academic or industry) (K1) 2. Create research attitude suitable for academia or industry (K6) 3. Understand the process of defining a research problem and the importance of data analysis (K2) 4. Create better communication skill (K6) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | RESEARCH METHODOLOGY | | | | 6 Hours | |
| Research- what is research, need of research, types of research, application of research in business. Research process- selection of topic of interest, formulation of a research problem, design a research, construct instrument for data collection, reliability and validity of instrument, sample, data collection, data processing and analysis, displaying results, repeatability, questionnaire designing, research report. | | | | | | |
| UNIT-II | INDUSTRIAL/RESEARCH INSTITUTION VISIT | | | | 6 Hours | |
| Understanding basic concepts of research/research process, motivation and objective of research, research problem, familiarize with instruments for data collection. | | | | | | |
| UNIT-III | INTERNSHIP | | | | 25 Hours | |
| Experience in new environment, selection of a new topic, formulating a new research problem, data collection, data analysis, discussion of results, presentation of results, research report and publications. | | | | | | |
| UNIT-IV | RESEARCH PRESENTATION | | | | 5 Hours | |
| Importance of conferences, seminars, workshops, publications in peer reviewed national / international journals, patents. Power point preparation- Introduction/preamble, data display, discussion of results, conclusion, time management, communication. | | | | | | |
| Total Lecture Hours | | | | | 42 Hours | |
| Text Books/References | | | | | | |
| <ol style="list-style-type: none"> 1. Research methodology: (Concepts and Cases) Deepak Chawla, NeenaSondhi, 2. Research methodology (Methods and Techniques) CR Kothari, Gaurav Garg | | | | | | |

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| Course Code | NSC2A 02 | PROFESSIONAL COMPETENCY COURSE (PCC) | L | T | P | C |
| Audit Course | | | 1 | 1 | 0 | 2 |
| Pre-requisite | None | | Syllabus Version | | 2022 | |
| L= Lecture, T= Tutorial, P- Practical, C= Credits | | | | | | |
| Course Objectives | | | | | | |
| <ol style="list-style-type: none"> 1. Inculcate scientific writing and communication skill 2. Understand the basic ethical issues confronted by the scientist 3. Recognize the skill areas the student would like to develop 4. Create awareness on the fundamentals of technology transfer | | | | | | |
| Course Outcomes | | | | | | |
| <ol style="list-style-type: none"> 1. Understand the scientific paper or thesis writing skill (K2) 2. Realize the ethical issues associated with scientific research and capable to analyze and address unethical situations (K2,K4) 3. Able to evaluate their own values and interests as they relate to their professional careers. (K5) 4. Understand the fundamentals of technology transfer and issues related (K2) | | | | | | |
| K1=Remember, K2= Understand, K3= Apply, K4= Analyze, K5= Evaluate, K6= Create | | | | | | |
| UNIT-I | Scientific Writing and Communication Skill | | | | 12 Hours | |
| <p>Writing and communication skill is very much essential to express scientific ideas or results clearly to validate their significance. For the successful publication of a research work, development of scientific writing skill is essential. Writing Research report, research proposals. Every aspect of writing scientific grants from funding agencies. Introduction to every aspect of grant writing, including selecting funding mechanisms, writing individual grant sections and understanding administrative policies. Strategies for effective scientific writing-core elements of each sections- Principles of writing research manuscript by composing and editing the sections- Familiarization with reference manager- how to peer review an article from the perspective of a researcher- reviewer- journal editor – complete and submit a research manuscript (based on an abstract given). Patent filing.</p> | | | | | | |
| UNIT-II | Integrity in Scientific Research | | | | 10 Hours | |
| <p>Familiarize the graduate students with the basic ethical issues confronted by the scientist. To gain insight into how one can responsibly conduct research throughout their career - To know how to properly address unethical situations- To realize that new ethical issues/ concerns will arise and that the best way to tackle these will be to discuss ethical situations with colleagues, seek guidance from proper channels, and routinely participate in conduct of research training courses/ seminars. Importance of team work, group discussion and collaborative research (MOU etc.), Know about plagiarism.</p> | | | | | | |

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| UNIT-III | Individual Development Plan | 10 Hours |
| <p>Individual development plan is intended for the graduate students before they go on to job market. Give opportunity to the participants to evaluate their own values and interests as they relate to their professional careers. Introduce the students to three or four different career tracks such as industry (profit or non profit), government sector, academic, scientific institution, etc.. ask the student to identify the skill areas they would like to develop.</p> | | |
| UNIT-IV | Fundamentals of Technology Commercialization | 10 Hours |
| <p>Innovative transformation of scientific and technical knowledge into commercial products and services. Importance of cross-disciplinary teams of students to assess real technologies for commercial applications with a specific focus on developing an understanding of the commercialization process, and skills in licensing and new venture development. Introduce concepts that improve and accelerate the commercialization process. From decisions made by scientists at the research bench, through the development, patenting, and licensing of new technologies, to the formation of entrepreneurial enterprises and monetization of assets. Data sharing with stake holders.</p> | | |
| | Total Lecture Hours | 42 Hours |
| Text Books/References | | |
| <ol style="list-style-type: none"> 1. The Craft of Scientific Writing, Michael Alley, 4th Ed. Springer, New York, USA (2018) 2. A Guide to the Scientific Career: Virtues, Communication, Research and Academic Writing Edited by Mohammedali M Shoja et.al, Wiley Black well (2019). 3. Handbook of Science Communication by Anthony Wilson, Jane Gregory, Steve Miller, Shirley Earl, IOP Publishing (1999). | | |