



**Course Content of
Chemical Sciences**

AcSIR-Chemical Cluster

1. CSIR-CECRI
2. CSIR-CSMCRI
3. CSIR-IICT
4. CSIR-IIP
5. CSIR-NCL
6. CSIR-NIIST
7. CSIR-IMMT (New Course –Provisionally Approved)

100 level courses

101 and 102/103 compulsory

CHE-LAB-1-001

Research Methodology: 1-0-0-1

CHE-LAB-1-002

Analytical Tools and Instrumentation: 1-0-0-1

Or

CHE-LAB-1-003

Basic mathematics and numerical methods: 1-0-0-1

CHE-LAB-1-004* (*Optional course)

Basic Chemistry for Interdisciplinary sciences: 1-0-0-1

CHE-LAB-1-005* (*Optional course)

Introduction to Nanoscience and Nanotechnology: 1-0-0-1

CHE-LAB-1-006* (*Optional course)

Introduction to Chemical Biology: 1-0-0-1

*Optional courses, over and above minimum requirements

200 level courses

201/202/203 compulsory (Core)

CHE-LAB-2-001

Advanced Physical Chemistry: 2-0-0-2

CHE-LAB-2-002

Advanced Inorganic Chemistry: 2-0-0-2

CHE-LAB-2-203

Advanced Organic Chemistry: 2-0-0-2

CHE-LAB-2-004

Advanced Analytical Chemistry: 2-0-0-2

CHE-LAB-2-005

Advanced Quantum Mechanics: 2-0-0-2

CHE-LAB-2-006

Advanced Organometallic Chemistry: 2-0-0-2

CHE-LAB-2-007

Advanced Coordination Chemistry: 2-0-0-2

CHE-LAB-2-008

Advanced Photochemistry: 2-0-0-2

CHE-LAB-2-009

Advanced Polymer Chemistry: 2-0-0-2

CHE-LAB-2-010

Advanced Electrochemistry: 2-0-0-2

CHE-LAB-2-011
Advances in Bioinorganic chemistry: 2-0-0-2

CHE-LAB-2-012
Advances in hydrocarbon chemistry: 2-0-0-2

CHE-LAB-2-013
Advanced process chemistry: 2-0-0-2

CHE-LAB-2-014
Advanced Materials Science: 2-0-0-2

CHE-LAB-2-015
Advanced Catalysis: 2-0-0-2

CHE-LAB-2-016
Advanced Surface Science: 2-0-0-2

CHE-LAB-2-017
Advanced Separation Science and Technology: 2-0-0-2

CHE-LAB-2-018
Advanced Materials Characterization Techniques: 2-0-0-2

CHE-LAB-2-019
Advances in Nanoscience and Nanotechnology: 2-0-0-2

CHE-LAB-2-020
Advances in soft matter chemistry: 2-0-0-2

CHE-LAB-2-021
Advances in Chemical Biology: 2-0-0-2

CHE-LAB-2-022
Advanced Biomaterials: 2-0-0-2

CHE-LAB-2-023
Rare Earth Chemistry: 2-0-0-2

CHE-LAB-2-024
Sol-gel chemistry: 2-0-0-2

CHE-LAB-2-025
Combinatorial chemistry: 1-0-0-1

CHE-LAB-2-026
Green chemistry: 1-0-0-1

CHE-LAB-2-027
Coal chemistry: 2-0-0-2

CHE-LAB-2-028
Alternative feedstock options for petrochemicals: 2-0-0-2

CHE-LAB-2-029
Natural products: 2-0-0-2

CHE-LAB-2-030
Ionic liquids: 1-0-0-1

CHE-LAB-2-031
Synthetic methods for organic chemists: 2-0-0-2

CHE-LAB-2-032
Organic reaction mechanisms: 2-0-0-2

CHE-LAB-2-033
Dyes and pigments: 1-0-0-1

CHE-LAB-2-034
Physical organic chemistry: 2-0-0-2

CHE-LAB-2-035
Thermodynamics and Statistical Mechanics: 2-0-0-2

CHE-LAB-2-036
Composite materials: 2-0-0-2

CHE-LAB-2-037
Carbon allotropes: 1-0-0-1

CHE-LAB-2-038
Organic spectroscopy applications: 2-0-0-2

CHE-LAB-2-039
Surface characterization techniques: 2-0-0-2

300 Level courses

CHE-LAB-3-001
Mathematical Methods: 2-0-0-2

CHE-LAB-3-002
Numerical Methods: 2-0-0-2

CHE-LAB-3-003
Electronic structure theory: 2-0-0-2

CHE-LAB-3-004
Molecular modeling and simulation: 2-0-0-2

CHE-LAB-3-005
Computer aided drug design: 2-0-0-2

CHE-LAB-3-006
Computational materials design: 2-0-0-2

CHE-LAB-3-007
Multiphase reaction kinetics: 1-0-0-1

CHE-LAB-3-008
Carbohydrate chemistry: 2-0-0-2

CHE-LAB-3-009
Biophysical chemistry: 2-0-0-2

CHE-LAB-3-010
Physics and chemistry of collagen: 2-0-0-2

CHE-LAB-3-011
Marine Natural products: 2-0-0-2

CHE-LAB-3-012
Supramolecular chemistry : 2-0-0-2

CHE-LAB-3-013
Total Synthesis: 1-0-0-1

CHE-LAB-3-014
Asymmetric Synthesis: 1-0-0-1

CHE-LAB-3-015
Chemistry and biology of Heterocycles: 2-0-0-2

CHE-LAB-3-016
Agrochemicals: 2-0-0-2

CHE-LAB-3-017
Fluoro organic chemistry: 2-0-0-2

CHE-LAB-3-018
Corrosion science: 2-0-0-2

CHE-LAB-3-019
Nutraceuticals: 2-0-0-2

CHE-LAB-3-020
Salts from marine resources: 2-0-0-2

CHE-LAB-3-021
Ionic liquids for lubricants: 1-0-0-1

CHE-LAB-3-022
Applications of ionic liquids: 1-0-0-1

CHE-LAB-3-023
Homogeneous Catalysis: 1-0-0-1

CHE-LAB-3-024
Catalysis in petroleum refining: 2-0-0-2

CHE-LAB-3-025
Catalysis for organic synthesis: 1-0-0-1

CHE-LAB-3-026
Catalysis for biomass refining: 1-0-0-1

CHE-LAB-3-027
Biocatalysis in petroleum refining: 1-0-0-1

CHE-LAB-3-028
Materials and devices for energy conversion: 2-0-0-2

CHE-LAB-3-029
Functional Ceramics: 1-0-0-1

CHE-LAB-3-030
Modern Magnetic Materials: 1-0-0-1

CHE-LAB-3-031

Porous structures: 2-0-0-2

CHE-LAB-3-032

Biomaterials for targeted therapeutics : 2-0-0-2

CHE-LAB-3-033

Organic electrochemistry: 2-0-0-2

CHE-LAB-3-034

Electrochemical power sources: 2-0-0-2

CHE-LAB-3-035

Alternate energy materials: 2-0-0-2

CHE-LAB-3-036

Photoinduced electron and Energy transfer: 2-0-0-2

CHE-LAB-3-037

Hydrogen generation and storage: 2-0-0-2

CHE-LAB-3-038

Thermochemical Conversion of Biomass: 1-0-0-1

CHE-LAB-3-039

CO₂ sequestration and conversion: 2-0-0-2

CHE-LAB-3-040

Natural gas to liquid fuels: 2-0-0-2

CHE-LAB-3-041

Gasoline reformulation techniques: 2-0-0-2

CHE-LAB-3-042

Block copolymers: 2-0-0-2

CHE-LAB-3-043

Polymers for membrane applications: 2-0-0-2

CHE-LAB-3-044

Ion exchange polymers: 1-0-0-1

CHE-LAB-3-045

Conducting polymers: 1-0-0-1

CHE-LAB-3-046

Polymers and Colloidal Solutions: 2-0-0-2

CHE-LAB-3-047

Biodegradable polymers: 2-0-0-2

CHE-LAB-3-048

Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2

CHE-LAB-3-049

Pi-conjugated polymers: 2-0-0-2

CHE-LAB-3-050

Liquid Crystals: 2-0-0-2

CHE-LAB-3-051
X-Ray Diffraction and Structure of Solids: 2-0-0-2

CHE-LAB-3-052
NMR spectroscopy: 2-0-0-2

CHE-LAB-3-053
Mass spectrometry applications: 2-0-0-2

CHE-LAB-3-054
Ultrafast processes and spectroscopy: 2-0-0-2

CHE-LAB-3-055
Small Angle Scattering Techniques: 2-0-0-2

CHE-LAB-3-056
Natural products and drug discovery: 2-0-0-2

CHE-LAB-3-057
Lipid science & technology: 2-0-0-2

CHE-LAB-3-058
Photobiology: 2-0-0-2

CHE-LAB-3-059
Nanobiotechnology: 1-0-0-1

400 level courses

Compulsory courses

CHE-LAB-4-001
Project proposal writing & presentation: 0-0-4-2

CHE-LAB-4-002
Project proposal writing & presentation: 0-0-4-2

CHE-LAB-4-003
CSIR-800: 0-0-8-4

CSIR-CENTRAL ELECTROCHEMICAL RESEARCH INSTITUTE, KARAIKUDI

100 Level Courses

CHE-CECRI-1-001

Research Methodology: 1-0-0-1

CHE-CECRI-1-003

Basic mathematics and numerical methods: 1-0-0-1

CHE-CECRI-1-005* (*Optional course)

Introduction to Nanoscience and Nanotechnology: 1-0-0-1

CHE-CECRI-1-006* (*Optional course)

Introduction to Chemical Biology: 1-0-0-1

*Optional courses, over and above minimum requirements

200 Level Courses

CHE-CECRI-2-001

Advanced Physical Chemistry: 2-0-0-2

CHE-CECRI-2-004

Advanced Analytical Chemistry: 2-0-0-2

CHE-CECRI-2-010

Advanced Electrochemistry: 2-0-0-2

CHE-CECRI-2-014

Advanced Materials Science: 2-0-0-2

CHE-CECRI-2-016

Advanced Surface Science: 2-0-0-2

CHE-CECRI-2-018

Advanced Materials Characterization Techniques: 2-0-0-2

CHE-CECRI-2-019

Advances in Nanoscience and Nanotechnology: 2-0-0-2

CHE-CECRI-2-022

Advanced Biomaterials: 2-0-0-2

CHE-CECRI-2-030

Ionic liquids: 1-0-0-1

CHE-CECRI-2-034

Physical organic chemistry: 2-0-0-2

CHE-CECRI-2-039

Surface characterization techniques: 2-0-0-2

300 Level Courses

CHE-CECRI-3-006

Computational materials design: 2-0-0-2

CHE-CECRI-3-012

Supramolecular chemistry : 2-0-0-2

CHE-CECRI-3-018

Corrosion science: 2-0-0-2

CHE-CECRI-3-028

Materials and devices for energy conversion: 2-0-0-2

CHE-CECRI-3-033

Organic electrochemistry: 2-0-0-2

CHE-CECRI-3-034

Electrochemical power sources: 2-0-0-2

CHE-CECRI-3-035

Alternate energy materials: 2-0-0-2

CHE-CECRI-3-036

Photoinduced electron and Energy transfer: 2-0-0-2

CHE-CECRI-3-037

Hydrogen generation and storage: 2-0-0-2

CHE-CECRI-3-043

Polymers for membrane applications: 2-0-0-2

CHE-CECRI-3-045

Conducting polymers: 1-0-0-1

CHE-CECRI-3-059

Nanobiotechnology: 1-0-0-1

Additional Courses suggested by CECRI

Polymer Electrolyte Fuel Cell 2-0-0-2

Advanced Lithium Batteries 2-0-0-2

Functional Materials 2-0-0-2

Electrochemical Technology 2-0-0-2

Advanced Corrosion Technology 2-0-0-2

Electrochemical Remediation 2-0-0-2

400 Level Courses

CHE-CECRI-4-001

Project proposal writing & presentation: 0-0-4-2

CHE-CECRI-4-002

Project proposal writing & presentation: 0-0-4-2

CHE-CECRI-4-003

CSIR-800: 0-0-8-4

CSIR IIP List of Courses for Chemical Sciences

100 level courses

001 and 002/003 compulsory

CHE-IIP-1-001

Research Methodology: 1-0-0-1

CHE-IIP-1-002

Analytical Tools and Instrumentation: 1-0-0-1

200 level courses

CHE-IIP-2-003

Advanced Organic Chemistry: 2-0-0-2

CHE-IIP-2-004

Advanced Analytical Chemistry: 2-0-0-2

CHE-IIP-2-012

Advances in hydrocarbon chemistry: 2-0-0-2

CHE-IIP-2-015

Advanced Catalysis: 2-0-0-2

CHE-IIP-2-028

Alternative feedstock options for petrochemicals: 2-0-0-2

300 Level courses

CHE-IIP-3-007

Multiphase reaction kinetics: 1-0-0-1

CHE-IIP-3-021

Ionic liquids for lubricants: 1-0-0-1

CHE-IIP-3-024

Catalysis in petroleum refining: 2-0-0-2

CHE-IIP-3-027

Biocatalysis in petroleum refining: 1-0-0-1

CHE-IIP-3-038

Thermochemical Conversion of Biomass: 1-0-0-1

CHE-IIP-3-039

CO₂ sequestration and conversion: 2-0-0-2

CHE-IIP-3-040

Natural gas to liquid fuels: 2-0-0-2

CHE-IIP-3-041

Gasoline reformulation techniques: 2-0-0-2

400 level courses

Compulsory courses

CHE-IIP-4-001

Project proposal writing & presentation: 0-0-4-2

CHE-IIP-4-002

Project proposal writing & presentation: 0-0-4-2

CHE-IIP-4-003

CSIR-800: 0-0-8-4

CSIR-CSMCRI

100 level courses

001 and 002/003 are compulsory

- i) CHE- CSMCRI-: 1-001: Research Methodology: 1-0-0-1
- ii) CHE- CSMCRI-: 1-002: Analytical Tools and Instrumentation: 1-0-0-1
- iii) CHE- CSMCRI-: 1-003: Basic mathematics and numerical methods: 1-0-0-1
- iv) CHE- CSMCRI-: 1-004* Basic Chemistry for Interdisciplinary sciences: 1-0-0-1
- v) CHE- CSMCRI-: 1-005* Introduction to Nanoscience and Nanotechnology: 1-0-0-1

(*Optional course)

200 level courses

001/002/003 compulsory (Core)

- i) CHE-CSMCRI-: 2-001: Advanced Physical Chemistry: 2-0-0-2
- ii) CHE-CSMCRI-:2-002: Advanced Inorganic Chemistry: 2-0-0-2
- iii) CHE-CSMCRI-: 2-003: Advanced Organic Chemistry: 2-0-0-2
- iv) CHE-CSMCRI-: 2-004: Advanced Analytical Chemistry: 2-0-0-2
- v) CHE-CSMCRI-:2-005: Advanced Quantum Mechanics: 2-0-0-2
- vi) CHE-CSMCRI-:2-007: Advanced Coordination Chemistry: 2-0-0-2
- vii) CHE-CSMCRI-: 2-009: Advanced Polymer Chemistry: 2-0-0-2
- viii) CHE-CSMCRI-: 2-010: Advanced Electrochemistry: 2-0-0-2
- ix) CHE-CSMCRI-:2-013: Advanced process chemistry: 2-0-0-2
- x) CHE-CSMCRI-:2-014: Advanced Materials Science: 2-0-0-2
- xi) CHE-CSMCRI-: 2-015: Advanced Catalysis: 2-0-0-2
- xii) CHE-CSMCRI-: 2-016: Advanced Surface Science: 2-0-0-2
- xiii) CHE-CSMCRI-:2-017: Advanced Separation Science and Technology: 2-0-0-2
- xiv) CHE-CSMCRI-: 2-018: Advanced Materials Characterization Techniques: 2-0-0-2
- xv) CHE-CSMCRI-:2-019: Advances in Nanoscience and Nanotechnology: 2-0-0-2
- xvi) CHE-CSMCRI-: 2-026: Green chemistry: 1-0-0-1
- xvii) CHE-CSMCRI-: 2-029: Natural products: 2-0-0-2
- xviii) CHE-CSMCRI-:2-030: Ionic liquids: 1-0-0-1
- xix) CHE-CSMCRI-:2-032: Organic reaction mechanisms: 2-0-0-2

300 Level courses

- i) CHE-CSMCRI-3-004: Molecular modeling and simulation: 2-0-0-2
- ii) CHE-CSMCRI-3-011: Marine Natural products: 2-0-0-2
- iii) CHE-CSMCRI-3-012: Supramolecular chemistry : 2-0-0-2
- iv) CHE-CSMCRI-3-014: Asymmetric Synthesis: 1-0-0-1
- v) CHE-CSMCRI-3-020: Salts from marine resources: 2-0-0-2
- vi) CHE-CSMCRI-3-022: Applications of ionic liquids: 1-0-0-1
- vii) CHE-CSMCRI-3-023: Homogeneous Catalysis: 1-0-0-1
- viii) CHE-CSMCRI-3-025: Catalysis for organic synthesis: 1-0-0-1
- ix) CHE-CSMCRI-3-026: Catalysis for biomass refining: 1-0-0-1
- x) CHE-CSMCRI-3-031: Porous structures: 2-0-0-2
- xi) CHE-CSMCRI-3-034: Electrochemical power sources: 2-0-0-2
- xii) CHE-CSMCRI-3-035: Alternate energy materials: 2-0-0-2
- xiii) CHE-CSMCRI-3-036: Photoinduced electron and Energy transfer: 2-0-0-2
- xiv) CHE-CSMCRI-3-038: Thermochemical Conversion of Biomass: 1-0-0-1
- xv) CHE-CSMCRI-3-039: CO₂ sequestration and conversion: 2-0-0-2
- xvi) CHE-CSMCRI-3-042: Block copolymers: 2-0-0-2
- xvii) CHE-CSMCRI-3-043: Polymers for membrane applications: 2-0-0-2
- xviii) CHE-CSMCRI-3-044: Ion exchange polymers: 1-0-0-1
- xix) CHE-CSMCRI-3-045: Conducting polymers: 1-0-0-1
- xx) CHE-CSMCRI-3-051: X-Ray Diffraction and Structure of Solids: 2-0-0-2

xxi) CHE-CSMCRI-3-052: NMR spectroscopy: 2-0-0-2

400 level courses

Compulsory courses

- i) CHE-CSMCRI-4-001: Project proposal writing & presentation: 0-0-4-2
- ii) CHE-CSMCRI-4-002: Project proposal writing & presentation: 0-0-4-2
- iii) CHE-CSMCRI-4-003: CSIR-800: 0-0-8-4



**CSIR-IICT AcSIR PhD Program - 2011
Academic Session: August-December - 2011**

Courses Offered in Academic Session: August-December – 2011

100 level courses

1. AcSIR-IICT-CS-101: Communication and Writing Skill: 2-0-0-2
2. AcSIR-IICT-CS-102: Analytical Techniques : 2-0-0-2

200 level courses

- 1 AcSIR-IICT-CS-201: Frontier Organic Chemistry: 4-0-0-4
- 2 AcSIR-IICT-CS-202: Frontier Inorganic Chemistry: 4-0-0-4
- 3 AcSIR-IICT-CS-203: Frontier Physical Chemistry: 4-0-0-4

CSIR-IICT AcSIR PhD Program - 2012
Academic Session: February-July - 2012
List of Courses Academic Session: February-July - 2012

Chemical Sciences

CHE (IICT) - 100 level courses

1. CHE-IICT-1-002: Analytical Tools and Instrumentation: 1-0-0-1
2. CHE-IICT-1-005 (optional): Introduction to Nanoscience and Nanotechnology: 1-0-0-1

CHE (IICT) - 200 level courses

1. CHE-IICT-2-001: Advanced Physical Chemistry: 2-0-0-2
2. CHE-IICT-2-003: Advanced Organic Chemistry: 2-0-0-2
3. CHE-IICT-2-004: Advanced Analytical Chemistry: 2-0-0-2
4. CHE-IICT-2-009: Advanced Polymer Chemistry: 2-0-0-2
5. CHE-IICT-2-015: Advanced Catalysis: 2-0-0-2 .
6. CHE-IICT-2-017: Advanced Separation Science and Technology: 2-0-0-2
7. CHE-IICT-2-019: Advances in Nanoscience and Nanotechnology: 2-0-0-2
8. CHE-IICT-2-020: Advances in soft matter chemistry: 2-0-0-2
9. CHE-IICT-2-026: Green chemistry: 2-0-0-2
10. CHE-IICT-2-033: Dyes and pigments: 1-0-0-1
11. CHE-IICT-2-036: Composite materials: 2-0-0-2

CHE (IICT) - 300 level courses

1. CHE-IICT-3-012: Supramolecular chemistry : 2-0-0-2
2. CHE-IICT-3-013: Total Synthesis: 1-0-0-1
3. CHE-IICT-3-014: Asymmetric Synthesis: 1-0-0-1
4. CHE-IICT-3-016: Agrochemicals: 2-0-0-2
5. CHE-IICT-3-017: Fluoro Organic Chemistry: 2-0-0-2
6. CHE-IICT-3-018: Corrosion science: 2-0-0-2
7. CHE-IICT-3-026: Catalysis for biomass refining: 1-0-0-1
8. CHE-IICT-3-028: Materials and devices for energy conversion: 2-0-0-2
9. CHE-IICT-3-034: Electrochemical power sources: 2-0-0-2
10. CHE-IICT-3-037: Hydrogen generation and storage: 2-0-0-2

11. CHE-IICT-3-039: CO₂ sequestration and conversion: 2-0-0-2
12. CHE-IICT-3-042: Block copolymers: 2-0-0-2
13. CHE-IICT-3-045: Conducting polymers: 1-0-0-1
14. CHE-IICT-3-046: Polymers and Colloidal Solutions: 2-0-0-2
15. CHE-IICT-3-048: Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2
16. CHE-IICT-3-049: Pi-conjugated polymers: 2-0-0-2
17. CHE-IICT-3-050: Liquid Crystals: 2-0-0-2
18. CHE-IICT-3-051: X-Ray Diffraction and Structure of Solids: 2-0-0-2
19. CHE-IICT-3-052: NMR spectroscopy: 2-0-0-2:
20. CHE-IICT-3-053: Mass spectrometry applications: 2-0-0-2

CSIR-National Chemical Laboratory

100 level courses

001 and 002/003 compulsory

CHE(NCL):1-001: Research Methodology: 2-0-0-2

CHE(NCL):1-002: Analytical Tools and Instrumentation: 2-0-0-2

Or

CHE(NCL):1-003: Basic mathematics and numerical methods: 2-0-0-2

CHE(NCL):1-004: Basic Chemistry for Interdisciplinary sciences: 1-0-0-1

CHE(NCL):1-005: Introduction to Nanoscience and Nanotechnology: 1-0-0-1

CHE(NCL):1-006: Introduction to Chemical Biology: 1-0-0-1

200 level courses

001/002/003 compulsory (Core)

CHE(NCL):2-001: Advanced Physical Chemistry: 3-0-0-3

CHE(NCL):2-002: Advanced Inorganic Chemistry: 3-0-0-3

CHE(NCL):2-003: Advanced Organic Chemistry: 3-0-0-3

CHE(NCL):2-004: Advanced Analytical Chemistry: 3-0-0-3

CHE(NCL):2-005: Advanced Quantum Mechanics: 3-0-0-3

CHE(NCL):2-006: Advanced Organometallic Chemistry: 3-0-0-3

CHE(NCL):2-008: Advanced Photochemistry: 2-0-0-2

CHE(NCL):2-009: Advanced Polymer Chemistry: 3-0-0-3

CHE(NCL):2-010: Advanced Electrochemistry: 2-0-0-2

CHE(NCL):2-014: Advanced Materials Science: 3-0-0-3

CHE(NCL):2-015: Advanced Catalysis: 3-0-0-3

CHE(NCL):2-016: Advanced Surface Science: 2-0-0-2

CHE(NCL):2-017: Advanced Separation Science and Technology: 2-0-0-2

CHE(NCL):2-018: Advanced Materials Characterization Techniques: 3-0-0-3

CHE(NCL):2-019: Advances in Nanoscience and Nanotechnology: 3-0-0-3

CHE(NCL):2-021: Advances in Chemical Biology: 3-0-0-3

CHE(NCL):2-022: Advanced Biomaterials: 3-0-0-3

CHE(NCL):2-026: Green chemistry: 3-0-0-3

CHE(NCL):2-032: Organic reaction mechanisms: 3-0-0-3

CHE(NCL):2-035: Thermodynamics and Statistical Mechanics: 3-0-0-3

CHE(NCL):2-036: Composite materials: 2-0-0-2

CHE(NCL):2-037: Carbon allotropes: 1-0-0-1

CHE(NCL):2-038: Organic spectroscopy applications: 3-0-0-3

CHE(NCL):2-039: Surface characterization techniques: 2-0-0-2

300 Level courses

CHE(NCL):3-001: Mathematical Methods: 2-0-0-2

CHE(NCL):3-002: Numerical Methods: 2-0-0-2

CHE(NCL):3-003: Electronic structure theory: 2-0-0-2

CHE(NCL):3-004: Molecular modeling and simulation: 2-0-0-2

CHE(NCL):3-006: Computational materials design: 2-0-0-2

CHE(NCL):3-008: Carbohydrate chemistry: 2-0-0-2

CHE(NCL):3-015: Chemistry and biology of Heterocycles: 2-0-0-2

CHE(NCL):3-023: Homogeneous Catalysis: 1-0-0-1

CHE(NCL):3-028: Materials and devices for energy conversion: 2-0-0-2

CHE(NCL):3-029: Functional Ceramics: 1-0-0-1

CHE(NCL):3-030: Modern Magnetic Materials: 1-0-0-1

CHE(NCL):3-031: Porous structures: 2-0-0-2

CHE(NCL):3-034: Electrochemical power sources: 2-0-0-2

CHE(NCL):3-035: Alternate energy materials: 2-0-0-2

CHE(NCL):3-037: Hydrogen generation and storage: 2-0-0-2

CHE(NCL):3-046: Polymers and Colloidal Solutions: 3-0-0-3

CHE(NCL):3-048: Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2

CHE(NCL):3-051: X-Ray Diffraction and Structure of Solids: 3-0-0-3

CHE(NCL):3-052: NMR spectroscopy: 3-0-0-3

CHE(NCL):3-053: Mass spectrometry applications: 2-0-0-2

CHE(NCL):3-055: Small Angle Scattering Techniques: 3-0-0-3

400 level courses

Compulsory courses

CHE(NCL):4-001: Project proposal writing & presentation: 0-0-4-2

CHE(NCL):4-002: Project proposal writing & presentation: 0-0-4-2

CHE(NCL):4-003: CSIR-800: 0-0-8-4

**National Institute for Interdisciplinary Science & Technology (NIIST)
Thiruvananthapuram.**

Chemistry Courses.

CHE(NIIST)- 100 Level Courses

- 1) CHE(NIIST): 1-001: Research Methodology: 1-0-0-1
- 2) CHE(NIIST): 1-002: Analytical Tools and Instrumentation: 1-0-0-1
- 3) CHE(NIIST): 1-003: Basic Mathematics and Numerical Methods: 1-0-0-1
- 4) CHE(NIIST): 1- 004: Basic Chemistry for Interdisciplinary sciences: 1-0-0-1
- 5) CHE(NIIST): 1-005: Introduction to Nanoscience and Nanotechnology: 1-0-0-1
- 6) CHE(NIIST): 1-006: Introduction to Chemical Biology: 1-0-0-1

CHE(NIIST) -200 Level Courses

- 1) CHE(NIIST): 2-002: Advanced Inorganic Chemistry: 2-0-0-2
- 2) CHE(NIIST): 2-003: Advanced Organic Chemistry : 2-0-0-2
- 3) CHE(NIIST): 2-005 : Advanced Quantum Mechanics: 2-0-0-2
- 4) CHE(NIIST): 2-006 : Advanced Organometallic Chemistry: 2-0-0-2
- 5) CHE(NIIST): 2-007 : Advanced Co-ordination Chemistry : 2-0-0-2
- 6) CHE(NIIST): 2-008: Advanced Photochemistry : 2-0-0-2
- 7) CHE(NIIST): 2-009: Advanced Polymer Chemistry: 2-0-0-2
- 8) CHE(NIIST): 2-014: Advanced Material Science : 2-0-0-2
- 9) CHE(NIIST): 2-018: advanced Materials Characterization Techniques: 2-0-0-2
- 10)CHE(NIIST): 2-019 : Advances in Nanoscience nanotechnology : 2-0-0-2
- 11)CHE(NIIST): 2-023: Rare Earth Chemistry: 2-0-0-2
- 12)CHE(NIIST): 2 -024: Sol-Gel Chemistry :2-0-0-2
- 13)CHE(NIIST): 2-026: Green Chemistry Concepts: 1-0-0-1
- 14)CHE(NIIST): 2-029: Natural Products: 2-0-0-2
- 15)CHE(NIIST): 2- 031: Synthetic Methods for Organic Chemists: 2-0-0-2
- 16)CHE(NIIST): 2-032: Organic Reaction Mechanisms: 2-0-0-2
- 17)CHE(NIIST): 2-036: Composite Materials: 2-0-0-2
- 18)CHE(NIIST): 2-038: Organic Spectroscopy applications: 2-0-0-2
- 19)CHE(NIIST): 2-039: Surface Characterization Techniques: 2-0-0-2

CHE(NIIST)- 300 Level Courses

- 1) CHE(NIIST): 3- 003: Electronic structure Theory: 2-0-0-2
- 2) CHE(NIIST): 3-004: Molecular Modeling and simulation: 2-0-0-2
- 3) CHE(NIIST): 3- 008: Carbohydrate Chemistry: 2-0-0-2
- 4) CHE(NIIST): 3-012: Supramolecular Chemistry: 2-0-0-2
- 5) CHE(NIIST): 3-013: Total Synthesis : 1-0-0-1
- 6) CHE(NIIST): 3- 014: Asymmetric synthesis: 1-0-0-1
- 7) CHE(NIIST): 3- 015: Chemistry and Biology of heterocycles: 2-0-0-2
- 8) CHE(NIIST): 3- 023: Homogenous Catalysis: 1-0-0-1

- 9) CHE(NIIIST): 3-025 : Catalysis for Organic Synthesis: 1-0-0-1
- 10)CHE(NIIIST): 3-028: Materials and Devices for energy conversion: 2-0-0-2
- 11)CHE(NIIIST): 3- 029: Functional ceramics: 1-0-0-1
- 12)CHE(NIIIST): 3-036: Photoinduced electron and Energy Transfer: 2-0-0-2
- 13)CHE(NIIIST): 3- 042: Block Copolymers: 2-0-0-2
- 14)CHE(NIIIST): 3-049: Pi-conjugated Polymers: 2-0-0-2
- 15)CHE(NIIIST): 3- 050: Liquid Crystals: 2-0-0-2
- 16)CHE(NIIIST): 3-054: Ultrafast processes and Spectroscopy: 2-0-0-2
- 17)CHE(NIIIST): 3- 056: Natural Products and drug discovery: 2-0-0-2
- 18)CHE(NIIIST): 3- 058: Photobiology: 2-0-0-2

100 level courses

101 and 102/103 are compulsory

CHE-LAB-1-101

Research Methodology: 1-0-0-1

Good laboratory practices, Safety in the laboratory, First Aid in the laboratory, Maintenance of laboratory records, Scientific literature management, Communication skills (scientific writing and presentation), Intellectual property management & planning, Ethics in Science, Computer applications and tools, Statistical methods & Data analysis

CHE-LAB-1-102

Analytical Tools and Instrumentation: 1-0-0-1

Thermal methods (TG, DTG, DTA, TMA, DSC), X-ray methods (XRD, XRF, SAXS), NMR (^1H , ^{13}C) and other Spectroscopic methods (EPR, IR, UV, Fluorescence), Chromatographic methods (TLC, GC, LC), Mass spectroscopy, Electron Microscopy (SEM, TEM), Electron Probe Micro Analysis (EDS, WDS), Quantitative Analysis (AAS, ICP, CHN)

CHE-LAB-1-103

Basic mathematics and numerical methods: 1-0-0-1

Determinants and Matrices, Complex Variables, Vector analysis, Infinite Series, Special Functions, Differential Equations, Interpolation and Approximation, Numerical differentiation and Integration, Basic Linux, Introduction to Algorithms, basic programming, Shell and Shell Scripting, Network Computing and Parallel Computing, Matlab/Scilab/Octave/Gnuplot

CHE-LAB-1-104* (*Optional course)

Basic Chemistry for Interdisciplinary sciences: 1-0-0-1

Basics of inorganic, organic, physical and biochemistry, Nomenclature (IUPAC), molarity, molality and normality, types of bonding, Ionic, covalent and non-bonding interactions, Acids and bases, Atomic structure, periodic table and periodic properties, stoichiometry, chemical reactions and kinetics, solvent effects, functional groups in organic compounds, general named reactions and reaction mechanisms, carbohydrates, lipids, proteins, nucleotides, enzymes, photosynthesis

CHE-LAB-1-105* (*Optional course)

Introduction to Nanoscience and Nanotechnology: 1-0-0-1

General considerations, Introduction, definitions, consequences of size reduction, Properties: structural, thermodynamic, optical, electrical and magnetic properties, Methods of synthesis, Surface modifications, factors governing the stability and assembly, Characterization of nanomaterials, Applications of Nanomaterials

CHE-LAB-1-106* (*Optional course)

Introduction to Chemical Biology: 1-0-0-1

chemical biology/synthetic biology, Structure, function and chemistry of biological macromolecules including amino acids, proteins, nucleic acids and carbohydrates, Chemical kinetics and thermodynamics in biology, Chemical reactions and chemical diversity in Biology The Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Drugs from Nature, Drug interaction

*Optional courses, over and above minimum requirements if required

200 level courses

201/202/203 compulsory (Core)

CHE-LAB-2-201

Advanced Physical Chemistry: 2-0-0-2

Thermodynamics and chemical kinetics, Quantum Mechanics, Atomic structure and spectroscopy, Chemical bonding in diatomics, Chemical applications of group theory, Colloids and Surface science, surfactants, Interface and Interfacial properties, Electrochemistry.

CHE-LAB-2-202

Advanced Inorganic Chemistry: 2-0-0-2

Structure & Bonding in Inorganic Compounds, Chemistry of Coordination Compounds, Symmetry in Chemistry & Group Theory, Main group chemistry, Organometallic chemistry, Electronic Spectra of Transition Metal Compounds, Magneto Chemistry, Metal Cluster Compounds, Inorganic Reaction Mechanism, Electron Transfer Reactions in Metal Complexes, Bioinorganic Chemistry (Metalloenzymes, Metal complexes as oxygen carriers, Photosynthesis), Metal Complexes in Medicinal Chemistry, Catalysis by Inorganic Complexes.

CHE-LAB-2-203

Advanced Organic Chemistry: 2-0-0-2

Stereochemistry, reaction mechanism, C-C and C-X bond formations, Retrosynthetic analysis, photochemistry, pericyclic reactions, reactive intermediates, Methods of asymmetric synthesis and their application in total synthesis, oxidation-reduction reactions, organocatalysis, metathesis reactions.

CHE-LAB-2-204

Advanced Analytical Chemistry: 2-0-0-2

Analytical instrumentation, signal and noise, Overview of optical methods of analysis: Components of optical instruments, atomic and molecular spectrometry based on absorption, emission and scattering, Electroanalytical techniques (basic electrochemistry, voltammetry, potentiometry), Analytical separations and introduction to chromatographic methods, GC, LC, Mass spectrometry, electromigration techniques, hyphenated techniques, detectors, Analytical tools for petroleum refining.

CHE-LAB-2-205

Advanced Quantum Mechanics: 2-0-0-2

Revision of Hydrogen atom and particle in box (1D and 3D), Approximate methods in quantum mechanics; Non degenerate perturbation; Perturbation treatment of the Helium atom ground state and first excited state; Variation method for helium atom ground state; Comparison of perturbation and variation method, Structure of many electron wave function, Antisymmetry, Valence bond theory for homo and hetero nuclear diatomic molecules; Molecular orbital theory Comparison of MO and VB theory; Introduction to density functional theory; Hartree Fock theory, Overview of methods beyond Hartree Fock theory; Configuration Interaction; Many body perturbation; Coupled cluster

CHE-LAB-2-206

Advanced Organometallic Chemistry: 2-0-0-2

Fundamentals, The 18 Valence Electron Rule; Structure and bonding of organometallic complexes using molecular orbital theory.

σ -Donor Ligands: Transition-Metal-Alkyl and -Aryl compounds; σ -Donor/ π -Acceptor Ligands: Transition-Metal-Alkenyl, -Aryl and -Alkynyl Complexes, Transition-Metal-Carbenes (Fischer and Schrock Carbenes); Metal Carbonyl; Structure, properties and principal reaction types of the above complexes; σ , π -Donor/ π -Acceptor Ligands: Olefin Complexes; Alkyne, Allyl and Enyl Complexes, Complexes of the cyclic C_nH_n
Fundamental Mechanism of Organometallic Transformations: Oxidative addition, Migratory Insertion, β -hydride elimination and reductive elimination; Interaction of C-C and C-H σ -bonds with Transition Metals

CHE-LAB-2-207

Advanced Coordination Chemistry: 2-0-0-2

Naming of coordination compounds, classification of ligands, chelate and macrocyclic effect, Theories dealing with the formation of Coordination Compounds, Spectrochemical Series; Splitting of d-orbitals, Jahn–Teller Effect; Stability constants of Transition metal complexes and their determination by Job's Method. Spin–Orbit Coupling, Electronic states and term symbols, Selection rules (Laporte and spin selection rule), Interpretation of electronic spectra of Transition metal complexes, Orgel and Tanabe Sugano diagrams. Charge Transfer spectra, Magnetic Properties of Transition elements, Chemistry of Inner Transition Elements.

CHE-LAB-2-208

Advanced Photochemistry: 2-0-0-2

Introduction to photochemistry, excited state processes, fluorescence and phosphorescence, quantum yields, charge-transfer spectra, solvatochromism, photochromism, transient absorption techniques, Luminescence emission lifetimes, two- and multiphoton processes, photoinduced energy and electron transfer, FRET, fluorescence polarization, excimers, exciplexes, delayed fluorescence, Photochemistry of Organic chromophores. Photochemistry in organized and confined media.

CHE-LAB-2-209

Advanced Polymer Chemistry: 2-0-0-2

Techniques of polymerization, polymer characterization techniques, Stereochemistry of Polymers, polymer nano-architectures, random and block copolymers, Liquid Crystalline Polymers, Conducting Polymers, Non-linear Polymers, Polymer Blends and Composites, polymer rheology, inorganic, bio and supramolecular polymers

CHE-LAB-2-210

Advanced Electrochemistry: 2-0-0-2

Basic electrochemistry concepts, Reference electrodes, Electrochemical Thermodynamics, Kinetics of electron transfer, the Taft equation, Diffusion, Double Layers, electrode Kinetics, the Gibbs adsorption isotherm, the Lippmann equation, infinitely dilute solutions and thermal balance, Electro capillary phenomena, Faradaic vs. capacitive currents, transport properties, potential theory, Electrochemical Techniques, Voltammetry, Reversible and irreversible reactions, Mass transport by convection, rotating electrodes, Equivalent circuits, A.C. voltammetry, Electrolysis methods, Adsorption, Thin layer cells, Electrochemistry of polymers and inorganic solids, Spectroelectrochemistry, Applications.

CHE-LAB-2-211

Advances in Bioinorganic chemistry: 2-0-0-2

Metal ions in biology, structure and function of metallo-proteins and enzymes, Communication role for metals in biology. Heme and non-heme systems with one-, two- or multi-metal, photosynthesis and photosystem II; O_2 -binding, reduction to O_2^- , O_2^{2-} , and O^{2-} species their utilization in hydroxylation and epoxidation; nitrogen fixation, water-oxidation reactions. Synthetic models, Correlation with structure and function of the natural enzymes,

design and synthesis, mechanisms. Metal based drugs, Porphyrins, Corrins, hydroporphyrins.

CHE-LAB-2-212

Advances in hydrocarbon chemistry: 2-0-0-2

Chemistry of crude oil, thermal cracking, visbreaking and coking processes, catalytic cracking, hydro cracking and hydrogen production processes, catalytic reforming process, Chemistry and industrial processes for alkylates, isomerisation processes, Petrochemicals, Basic Building blocks; C₁-Chemistry; Petrochemicals from n-paraffins; Petrochemicals from olefins and aromatics; Refinery-Petrochemical Integration, Future Prospects

CHE-LAB-2-213

Advanced process chemistry: 2-0-0-2

Integral and Differential analysis; Evaluation of rate equations, unit processes, mass transfer, mass balance, energy balance, fluid flow, Design of homogeneous systems, different types of reactors, green chemistry

CHE-LAB-2-214

Advanced Materials Science: 2-0-0-2

Crystal systems and space groups, Close packing and various simple structure types like AB, AB₂, AB₃ and complex structural types ABX₃, AB₂X₄, etc. Factors affecting crystal structures, Common preparative methods; X-ray diffraction and Electron microscopy, Defect structures, colour centers, reciprocal lattices, Properties of solids – Band theory, metals, insulators, semiconductors, dielectric and ferroelectric properties, magnetic properties, optical properties, ionic conduction; structure-processing-property correlations.

CHE-LAB-2-215

Advanced Catalysis: 2-0-0-2

Homogeneous and heterogeneous catalysis, adsorption, diffusion, kinetics, equilibrium and rate expressions; chiral catalysis, Surface Science in Catalysis, Catalytic Materials; Supports; Active Components, Classes of reactions and types of reactors; Catalyst preparation methods; Characterization of catalysts; Catalysis in super critical media; Brief introduction of organo and electrocatalysis; Structure-activity-property-stability of catalysts, Catalysts in chemical industry, Catalysis in petroleum refining and petrochemicals; Catalysis in the utilization of renewable feed stocks and concepts of sustainable chemistry.

CHE-LAB-2-216

Advanced Surface Science: 2-0-0-2

Introduction to Surface Science - Surface phenomena - Adsorption, Desorption, Adsorption Models, Special properties of surfaces and interfaces, Electronic structure of surfaces, Surface modification and its applications, Nanoscale catalysis and applications, Surface spectroscopy and microscopy tools for nanocatalysis

CHE-LAB-2-217

Advanced Separation Science and Technology: 2-0-0-2

Resins and membranes for separations, Classification of membranes; electromembrane Processes; Ion-exchange membranes and their applications, Electrodialysis and related processes. Polymer electrolyte membrane and their applications for fuel cells; Water electrolyzer for hydrogen production; Reverse electrodialysis for non-renewable energy from concentration gradient, reverse osmosis, nanofiltration, ultrafiltration, pervaporation and gas separation: Membrane fouling, concentration polarization and other limitations of Pressure-driven membrane technologies.

CHE-LAB-2-218

Advanced Materials Characterization Techniques: 2-0-0-2

Optical Microscopy, Electron microscopy: TEM, HRTEM, SEM, STEM, EDX, FIB, e-beam lithography, Scanning probe microscopy: AFM, STM, MFM, confocal, etc, Raman spectroscopy/microscopy, Thermal analysis techniques, Magnetic measurements, Electrical measurements, Spectroscopic ellipsometry.

CHE-LAB-2-219

Advances in Nanoscience and Nanotechnology: 2-0-0-2

Low-dimensional structures: Quantum wells, Quantum wires, and Quantum dots, Nano clusters & Nano crystals, fullerenes, carbon nano tubes and graphene, Nano Composites, synthesis and characterization techniques, Properties at Nano Scales and comparison with bulk materials, fabrication techniques, general applications, nanomaterials in biology.

CHE-LAB-2-220

Advances in soft matter chemistry: 2-0-0-2

Condensed Matter, Colloids, Characterization of colloids by light scattering and electric-field based techniques, Micelles, Self-assembled systems, Molecular gels, Lyotropic liquid crystalline phases, One-, Two- and Three-dimensionally ordered phases, Thermotropic Liquid crystals textures and their identification, characterization of mesophases, Description of order parameter, Phase transitions.

CHE-LAB-2-221

Advances in Chemical Biology: 2-0-0-2

Amino Acids, Peptides & Proteins, Design of poly peptides, Peptide hormones and their pharmaceutical significance, Peptide mimetics as therapeutics, Chemistry of Carbohydrates, Nucleic acids, Structure & function of DNA and RNA, Nucleic acid mimetics & their therapeutic applications, Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Basic principles of medicinal chemistry, Drugs from Nature, Natural products based drug discovery, Kinetics and thermodynamics of biological process, Enzyme Catalysis, consecutive, parallel and competitive reactions in biological systems, Thermodynamics, allosteric effect in biology, types of bonds, hydration and their specific contribution towards specific thermodynamic parameters, enthalpy or entropy, Scatchard analysis, hill plot analysis.

CHE-LAB-2-222

Advanced Biomaterials: 2-0-0-2

Definition of biomaterials, Surface property requirements of biomaterials, Types of materials used in medicine, Synthesis and surface characterization, Biology of wound healing, foreign body response and tissue remodeling, Molecular and cellular interactions of materials with biological environment, Degradation and long term fate of materials used in medicine, Requirements of biomaterials for biomedical implants, surface coatings, wound dressings, sutures, cardiovascular devices, ophthalmology, dentistry, orthopedics and cosmetic surgeries, Applications in drug delivery and tissue engineering, Standard protocols for testing the efficacy and efficiency of biomaterials, The regulatory environment for biomaterials, Some concepts for design development of common biomaterials.

CHE-LAB-2-223

Rare Earth Chemistry: 2-0-0-2

Lanthanides and actinides, Electronic structure, periodic properties, extraction, separation, solution chemistry, coordination compounds, spectroscopy, luminescence, magnetism, dyes and pigments, trans-uranium elements, nuclear technology, displays and energy related applications.

CHE-LAB-2-224**Sol-gel chemistry: 2-0-0-2**

Introduction, Hydrolysis and condensation reactions, Solution chemistry and physics of intermediates, Role of the anion on the hydrolysis and condensation reactions, Kinetics of Hydrolysis and Condensation, Non-Hydrolytic Sol-Gel Processing, Gelation, Ageing, Drying, Densification, Characterization, Chemistry of Sol-Gel Silicates, Solution chemistry of transition metal alkoxide precursors, Sol-gel synthesis and characterization of important materials, structure-property relationships

CHE-LAB-2-225**Combinatorial chemistry: 1-0-0-1**

Principles and techniques of combinatorial chemistry, Popular organic reactions in combinatorial chemistry. solid-phase organic synthesis, Solution-phase parallel synthesis, mixture-based compound libraries, principles of compound library design, natural product and natural product-like libraries, case studies of combinatorial chemistry in drug discovery

CHE-LAB-2-226**Green chemistry: 1-0-0-1**

Green chemistry concepts: Basic understanding, scope and interdisciplinary nature of green chemistry; Environmental factors; Carbon credit, Energy efficiency and atom economy, Catalysis and green chemistry, Alternate reaction media and reaction systems, ionic liquids, supercritical fluids, solventless chemistry.

CHE-LAB-2-227**Coal chemistry: 2-0-0-2**

Mining processes, mine safety, Sampling methods of coal and its importance, Coal classification systems, Physical characterization, proximate analysis, Ultimate analysis, Sulphur analysis, Ash fusion temperature, Low temperature Carbonization, Swell Index, Cracking Index, Thermogravimetric analysis etc, Size Reduction and Size Classification of Coal, Structure of coal, Organic functionality of coal, aromatic Index, Mineral matter content, Mineralogy of coal, Geological origin of coal, petrographic analysis, geochemical processes during mining of coals, Coal Utilization, Coal Conversion processes, Other useful products from coal, Environmental Issues, CO₂ sequestration.

CHE-LAB-2-228**Alternative feedstock options for petrochemicals: 2-0-0-2**

Global scenario of Petrochemicals, Renewable resources; categorization of resources; chemicals from edible renewable resource; Chemicals from non-edible renewable resources; Catalytic reactions (mineral acid, bases; enzymes, homogeneous and heterogeneous catalysts); alternate fuels; fuels derived from renewable resources; biodiesel, bioethanol, biobutanol; Hydrogen generation from renewable feed stocks, Conversion of glycerol; Naphtha as a conventional source, Need for sustainability in production of Petrochemicals, Alternate Options; from Refineries sources, Natural Gas/Methane as an Option and other Non Refinery Sources, CO₂ utilization, Identification and Recommendations based on techno-economic analysis for India.

CHE-LAB-2-229**Natural products: 2-0-0-2**

Carbohydrates and polysaccharides, Structure and functions of important derivatives of monosaccharides, Classification and nomenclature and synthesis of some simple Alkaloids; Terpenoids and Steroids such as pinene; Camphor and Cadenine; α -vetinone; Hirsutene and Abietic acid (Terpenoids); Cholesterol; Testosterone and Andestrone (Steroids) etc. isolation and characterization, elucidation of structure-property relationships. Biosynthesis of steroids, terpenoids, fatty acids, alkaloids and polysaccharides, biosynthesis of natural products

CHE-LAB-2-230

Ionic liquids: 1-0-0-1

Introduction to ionic liquids, ionic liquids vs. molecular solvents/ionic salts (solids), ionic liquids vs. eutectic mixtures, solvent polarities using different spectral techniques (parameters), physicochemical properties of ionic liquids, effect of functional groups on the properties of ionic liquids, surface active ionic liquids, aggregation behavior of ionic liquids, interaction of ionic liquids with different molecular solvents, interaction of ionic liquids with biopolymers, thermodynamics of the binary mixtures of ionic liquids, structure property relationship in ionic liquids.

CHE-LAB-2-231

Synthetic methods for organic chemists: 2-0-0-2

Formation of carbon-carbon bond employing various kinds of organometallic reagents, C-C double bonds through different reactions, oxidation, reduction through various kinds of reagents, functional group interconversion, by substitution including protection and deprotection, alkylation of enolates, and other carbon nucleophiles, reaction of carbon nucleophiles with carbonyl compounds, electrophilic addition to C-C multiple bonds, reactions of C-C multiple bonds, Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

CHE-LAB-2-232

Organic reaction mechanisms: 2-0-0-2

Basics, The concept of Aromaticity, How to write an organic reaction mechanism?, Popular name reactions, Reactive intermediates: Generation, stability, structures and reactivity of carbocation, carbanion, carbene, radicals, benzyne, nitrene, Types of mechanism: classification, limitations examples of aliphatic nucleophilic substitution - aliphatic electrophilic substitution - aromatic nucleophilic substitution - aromatic electrophilic Substitution - types of radical reactions - molecular rearrangements oxidation and reduction; Electrophilic reactions-Friedel crafts reaction, Riemer Tiemann reaction, Beckmann rearrangements; nucleophilic reactions- aldol condensation, perkin reaction, benzoin condensation; free radical reaction-halogenation of alkane, addition of HBr on alkene in presence of peroxide; allylic halogenation - using N-Bromo Succinamide (NBS), thermal halogenation of alkene $\text{CH}_3 - \text{CH} = \text{CH}_2$

CHE-LAB-2-233

Dyes and pigments: 1-0-0-1

Colour and constitution, chromogen and chromophore. Classification of dyes based on structure and mode of dyeing, Chemistry of some important dyes, NIR reflecting dyes, Dyes for solar cells

CHE-LAB-2-234

Physical organic chemistry: 2-0-0-2

Hammett concepts-Quantitative structure activity relationships, linear free energy relationships, Molecular mechanics, Semi-empirical and *ab initio* molecular theory, Pericyclic Reactions; Substituent Effects; Frontier Molecular Orbitals, HOMO-LUMO Interactions, Aromaticity, Odd and Even Alternant Hydrocarbons, Pericyclic Reactions The Woodward-Hoffman Rules. Free Energy Changes, Transition State Theory, The Eyring Equation, The Mechanistic Significance of Kinetic versus Thermodynamic Control of Organic Reactions, The Hammond Postulate, The Curtin-Hammett Principle; Kinetic Isotope Effects, The Reactivity-Selectivity Principle, Substituent Effects, Absorption of Light by Organic Molecules, Jablonsky Diagrams, Morse Potential Energy Curves, Common Photochemical Reactions, Photocycloadditions.

CHE-LAB-2-235**Thermodynamics and Statistical Mechanics: 2-0-0-2**

Introduction: Thermodynamics – A Macroscopic Theory of Matter; Laws of Thermodynamics, Ideal Gas Laws, Specific Heat Capacities; Concept of Free Energy, Hamiltonian Mechanics, Equilibrium Distributions and Ergodic Hypothesis, Ensembles, Thermodynamic Functions and the Distribution Function, $g(r)$, Imperfect Gases, Kinetic Theory of Gases, Time Dependent Processes, Phase Transitions

CHE-LAB-2-236**Composite materials: 2-0-0-2**

Concept of Composite materials, Various types of composites, Classification based on Matrix Material: Organic Matrix composites, Polymer matrix composites (PMC), Carbon matrix Composites or Carbon-Carbon Composites, Metal matrix composites (MMC), Ceramic matrix composites (CMC); Classification based on reinforcements: Fiber Reinforced Composites, Fiber Reinforced Polymer (FRP) Composites, Laminar Composites, Particulate Composites, Reinforcements/Fibers, Types of fibres, Multiphase fibers, Whiskers and Flakes, Mechanical properties of fibres, Processing of Advanced composites, Metal Matrix Composites: Casting – Solid State diffusion technique, Cladding – Hot isostatic pressing; Ceramic Matrix Composites: Liquid Metal Infiltration – Liquid phase sintering; Carbon – Carbon composites: Knitting, Braiding, Weaving; Polymer matrix composites: Preparation of Moulding compounds and prepregs – hand lay up method – Autoclave method – Filament winding method – Compression moulding – Reaction injection moulding, Processing and characteristics of nanocomposites, hybrid composites, functionally graded composites, smart and functional composites.

CHE-LAB-2-237**Carbon allotropes: 1-0-0-1**

Synthesis, characterization, structure, properties and applications of: Diamond, Graphite, Amorphous carbon, Charcoals, Fullerene and related compounds, Carbon nanotubes, Graphene.

CHE-LAB-2-238**Organic spectroscopy applications: 2-0-0-2**

Mass spectroscopy, IR spectroscopy, Proton magnetic resonance spectroscopy, Structural assignment by employing NMR techniques, Carbon-13 NMR spectroscopy, Introduction COSY, HSQC, HMBC, NOESY, ROESY, Structural elucidation using 2D-NMR methods

CHE-LAB-2-239**Surface characterization techniques: 2-0-0-2**

XPS, LEED, XAS, SEM, AFM, TEM, NSOM, SPR, SERS, static and dynamic contact angle measurements, Ellipsometry.

300 Level courses

CHE-LAB-3-301

Mathematical Methods: 2-0-0-2

Determinants and Matrices : Orthogonal Matrices, Hermitian Matrices, Unitary Matrices, Diagonalisation of Matrices, Vector analysis : Scalar and Vector product, Triple scalar and vector product, Gradient, Divergence, Curl, Vector Integration, Gauss Theorem, Stokes Theorem. Vector Analysis in Curvilinear coordinates and Tensors, Infinite Series: Fundamental Concepts, Convergence tests, Taylors expansion, Power Series, Special Functions: Gamma Function, The Beta Function, Differential Equations: Series Solution-Frobenius Method, Bessel Functions, Legendre Functions, Hermite Functions, Laguerre Functions, Fourier Series, Applications of Fourier Series, Fourier Transforms

CHE-LAB-3-302

Numerical Methods: 2-0-0-2

Fortran and Linux basics, Solution to the linear algebraic equations, Eigen Values problems, Interpolation and extrapolation, Random number and sorting, Minimization and maximization of functions, Modeling of data

CHE-LAB-3-303

Electronic structure theory: 2-0-0-2

Post-Hartree-Fock methods: Moller-Plesset perturbation theory (MP2, MP3, and MP4), Configuration Interaction (CI), Coupled-Cluster single double (triple) (CCSD(T))—performance of various methods for the prediction of van der Waal and hydrogen bonding interactions, spectral properties. Density functional theory based methods: Hybrid and Minnesota functional – Application of DFT methods (excitation energy calculations). Density functional methods with Dispersion correction (Grimme's approaches). Car-Parrinello Molecular Dynamics (CPMD) and Born-Oppenheimer Molecular Dynamics (BOMD).

CHE-LAB-3-304

Molecular modeling and simulation: 2-0-0-2

Molecular Mechanics: Features of molecular mechanics - Force Fields: Bonds structure and bending angles, Electrostatic Vander Waals and non-bonded interactions, Hydrogen bonding - Derivatives of molecular mechanics energy function - Calculating thermodynamic properties - Force Field for inorganic systems - Energy minimization, Molecular Dynamics Simulation: Molecular Dynamics using simple models, Molecular Dynamics with continuous potentials, Solvent effects, Conformational changes, Thermostats, Barostats, Lincs and shake algorithms, Monte Carlo simulation Methods, sorption, Applications of Molecular Modeling

CHE-LAB-3-305

Computer aided drug design: 2-0-0-2

Definition of a drug molecule and factor affecting their biological activity, definition of chemotherapeutic index, therapeutic index, design of a drug molecule and relationship of functional groups, discovery of new drugs: drug discovery without a lead, lead discovery, random screen, non-random screen, concept of absorption, distribution, metabolism, and excretion (ADME), drug receptors, physicochemical properties, mechanism of a drug action, stereochemistry and drug action, synthetic and natural drugs and their modifications to increase oral bioavailability, chirality and drug action, bioisosterism, drug receptor-interactions, topographical and stereo-chemical considerations, concept of drug resistance, drug synergism, enzyme inhibition and activation, molecular modeling and *insilico* drug design, concept of structure-activity relationship(SAR) and quantitative structure-activity

relationship (QSAR), Lipinski rule of five, mechanism of action of some important drug molecules.

CHE-LAB-3-306

Computational materials design: 2-0-0-2

Solids, Drude and Sommerfield theories of metals, Kronig-Penning model, Tight-Binding approximation, band structure, density of states, prediction of electrical and magnetic properties, Prediction of properties of organic molecules and polymers, Introduction to Multiscale Modeling and Simulations and applications. Monte Carlo simulation in various ensembles, Gas sensing properties of various porous materials using grand canonical Monte Carlo method, Dissipative particle dynamics, Mesoscale dynamics and applications.

CHE-LAB-3-307

Multiphase reaction kinetics: 1-0-0-1

Mass transfer theories, Multi phase reactors, Multi phase reactors selection criteria; Mass transfer coupled with chemical reaction; measurement of gas-liquid parameters, Reaction in porous catalysts; effective diffusivity and structure of porous catalysts, Important design parameters for gas-liquid and solid reactors, Reactor modeling in petroleum refining industry, Modeling of catalytic sweetening, isomerisation, hydro treating, and FT synthesis.

CHE-LAB-3-308

Carbohydrate chemistry: 2-0-0-2

Mono and disaccharides, polysaccharides, Bacterial polysaccharides, starch and cellulose, derivatives of cellulose, Protecting groups, Glycosylation reactions, Dynamics and interactions, carboxy methyl cellulose and gun cotton, structure, Conformational analyses, glycoconjugates, Immunology of carbohydrates.

CHE-LAB-3-309

Biophysical chemistry: 2-0-0-2

Physico Chemical properties of Water, State of Water in biostructures & its significance, Lipids & Proteins, Membrane organization & stability, Protein lipid interactions, Phase properties of biological membranes, Transport across the membrane, Osmosis, molecular basis of aqueous channels, Structural level of proteins & stabilizing forces, Conformational analysis of polypeptides, Ramachandran plot, Double helical structure of DNA, Conformational parameters of Nucleic acids & their constituents, Types & structure of RNA, mRNA, rRNA, tRNA, Protein-ligand and DNA-protein interactions.

CHE-LAB-3-310

Physics and chemistry of collagen: 2-0-0-2

Molecular Structure of Collagen, Native collagen fibrils, X-ray Diffraction studies of collagen, Electron microscopic appearance of collagen, synthetic collagen-like polypeptides, Chemistry of Collagen and its Distribution, Biosynthesis of Collagen, Crosslinking, Degradation, Isolation and Characterization of Collagen, Physico-Chemical Techniques for Collagenous Matrices, Microscopy and other Non-invasive methods.

CHE-LAB-3-311

Marine Natural products: 2-0-0-2

Polysaccharide contents of various seaweeds, Phaeophyceae and Rhodophyceae, Bioactive compounds from halophytic plants and marine algae/seaweeds, Gelling polysaccharides, extraction from natural sources, characterization and properties. Preparation of polysaccharide based biodegradable materials, hybrid composites, stimuli responsive materials. Applications of polysaccharide based materials. Biosynthesis of bioactive polysaccharides, steroids, fatty acid derivatives and alkaloids.

CHE-LAB-3-312

Supramolecular chemistry : 2-0-0-2

Nature of supramolecular interactions, role of various non-covalent interactions, multiple hydrogen bonding motifs, Stability of H-bonds, Jorgensen model for H-bonding, supramolecular synthons, dimensions of supramolecular chemistry, Janus molecules. Photoresponsive molecules and self-assembly, Molecular recognition, classification of supramolecular host-guest complexes, supramolecular self-assembly, supramolecular polymers, molecular capsules, self-assembled dendrimers, self-assembled nanotubes, low molecular weight organogels. Characterization techniques of self-assemblies, supramolecular sensors.

CHE-LAB-3-313

Total Synthesis: 1-0-0-1

Synthesis of complex organic molecules – planning and execution; Concepts of Retrosynthetic Analysis and Total synthesis of Natural products; Retrosynthesis; Disconnection; Synthons; Linear and Convergent Synthesis; Photochemistry in total synthesis; MCRs in total synthesis; Breakthrough synthesis – past and present.

CHE-LAB-3-314

Asymmetric Synthesis: 1-0-0-1

Strategies for the preparation of optically pure compounds; Stereoselective, Enantioselective and Diastereoselective reactions; Stoichiometric asymmetric synthesis-chiral auxiliaries, Evans Aldol and modified versions; Catalytic asymmetric synthesis; Asymmetric Dihydroxylation; Asymmetric Aminohydroxylation; Asymmetric Hydrogenation; Asymmetric allylation, propargylation, and alkylation; Chiral Organocatalysis; Cascade reactions by organocatalysis; Transition Metal based catalysis; Asymmetric amplification and autocatalysis.

CHE-LAB-3-315

Chemistry and biology of Heterocycles: 2-0-0-2

Privileged heterocycles, Electronic properties, reactivity (electrophilicity and nucleophilicity), Synthetic methodologies, Biological properties of Natural products and drug candidates, Biosynthesis, Dimeric compounds and related stereochemistry

CHE-LAB-3-316

Agrochemicals: 2-0-0-2

Biochemistry in agriculture, Carbohydrates, Proteins, Lipids, Vitamins and Minerals and Enzymes, Soil science, guidelines on agricultural crops micronutrients and fertilizers, Chemistry of pesticides, synthesis, formulations, mode of action, toxicology, resistance and residual analysis, Methodologies for the synthesis of agrochemicals and other relevant organic molecules, chemistry in Integrated Pest Management, Semiochemicals, insect growth regulators, botanical pesticides and other biotechnological approaches, Analysis of agrochemicals and residues - Botanical pesticides, hormones, pheromone, kairomones and plant volatiles

CHE-LAB-3-317

Fluoro organic chemistry: 2-0-0-2

Importance of fluorine in organic compounds, Strategies to introduce fluorine/ trifluoromethyl group into organic molecules, Preparation of fluorinated reagents, Preparation of fluorinated carbon materials and their uses, Known fluorinated drugs and their mode of action, Overview on CFCs, HCFCs, HFCs, their preparation and applications, Halon substitutes, Harmful effects of fluorine and inorganic fluorides

CHE-LAB-3-318

Corrosion science: 2-0-0-2

Basic aspects, Forms of corrosion, Atmospheric corrosion and protective coatings, Immersion corrosion and electrochemical protection, Corrosion monitoring, impedance spectroscopy, harmonics and NDT techniques.

CHE-LAB-3-319

Nutraceuticals: 2-0-0-2

Raw material preparation, and characterization, extraction of valuable biomolecules, characterization of these molecules with stability study, preparation and formulations for functional foods. Characterization and stability study of nutraceuticals, properties and stability packaging of nutraceuticals.

CHE-LAB-3-320

Salts from marine resources: 2-0-0-2

Physicochemical properties of NaCl crystals, Chemistry of salt manufacture, Influence of other dissolved salts in the salt purity, Survey of site for solar salt production, Scientific design and layout of solar salt works, Solar Salt manufacture, Mechanization of solar salt industries, Preparation of ultra pure salt through innovative methods, Fortification of salt with essential nutrients, Application of phase equilibrium for recovery of marine chemicals, Recovery of valuable marine chemicals from bittern, High purity magnesium chemicals from bittern

CHE-LAB-3-321

Ionic liquids for lubricants: 1-0-0-1

Lubrication by Ionic liquids and its structural correlation, Ionic liquids interaction with surfaces, synthetic oil lubricants, synthesis of lubricating ionic liquids, effect of alkyl chain length and anions, IL lubrication oils at variable temperatures, thin films, heat capacity and thermal properties, viscosity and wetting properties, ionic liquids as additives for lubricants, comparison with conventional hydrocarbon oils, Case studies.

CHE-LAB-3-322

Applications of ionic liquids: 1-0-0-1

Introduction to task specific ionic liquids, self-assembly of ionic liquids in aqueous/non aqueous media and synthesis of nanomaterials therein, ionic liquids in catalysis, extraction of metal ions, ionic liquids and biopolymers: dissolution, regeneration and ionic-gel formation, processing of lignocellulosic biomass using ionic liquids, clean separation of various fractions of biomass and recovery of valuable chemicals using ionic liquids, application of ionic liquids in electrochemistry, separation of azeotropic mixtures using ionic liquids, organic reactions in ionic liquids.

CHE-LAB-3-323

Homogeneous Catalysis: 1-0-0-1

Organometallic Catalysis, Applications in organic synthesis: Olefin Isomerization, C-C Coupling reactions: Heck, Suzuki, Stille and Sonogashira reactions, Alkene and Alkyne Metathesis, C-Heteroatom coupling: Hydroamination, Olefin Oxidation, C-H activation, Oxidation reactions, hydrogenation of Alkenes, Industrial Applications.

CHE-LAB-3-324

Catalysis in petroleum refining: 2-0-0-2

Deactivation in Catalysts and its Consequences, Regeneration and Rejuvenation in Catalysis, Industrial Catalytic Processes; Hydro cracking; Hydro treating; Reforming; Isomerization and Alkylation; Fluid Catalytic Cracking and Deep Catalytic Cracking, Catalysis for Clean Fuels; Gas to Liquid Technology; Catalysis for Hydrogen Production,

Catalysis beyond Petroleum; Electro catalysis; Photo catalysis, Laboratory Training in Catalysis.

CHE-LAB-3-325

Catalysis for organic synthesis: 1-0-0-1

A background on fine and specialty chemicals in chemical industry; Concept of atom economy; Homogeneous and heterogeneous catalytic reactions: hydrogenation, hydrogenolysis, dehydrogenation, selective oxidation, alkylation & acylation, isomerization and C-C bond forming reactions, Enzyme catalysis in organic synthesis; Reaction mechanisms

CHE-LAB-3-326

Catalysis for biomass refining: 1-0-0-1

Classification of biomass; Catalytic processing of cellulosic and lignocellulosic materials for monomers or oligomers; Catalytic transformation biomass to fuels; Value addition of biomass/monomers to fine and specialty chemicals; Value addition of glycerol and their derivatives; Concept of bio-refinery – Role of catalysis

CHE-LAB-3-327

Biocatalysis in petroleum refining: 1-0-0-1

Scope of Biocatalysis in Petroleum Refining, Thermophilic microorganisms and the thermozymes, Structure and function of proteins, Non-aqueous Biocatalysis, Protein Engineering and rate improvement, Enzyme kinetics and models, Challenges and opportunities on Bioprocess development on: Bio-desulphurization of crude oil and petroleum fractions; Bio-cracking and Bio-vis breaking; Bio-desulphurization of waste gases; Biocatalysts for renewable hydrocarbons and petrochemicals.

CHE-LAB-3-328

Materials and devices for energy conversion: 2-0-0-2

Design of organic and Inorganic semiconductors, Approaches to process organic semiconductors by covalent and non covalent modifications, band edges and band gaps, Modulation of charge transport properties, kinetics of electron transfer, Design of small molecule dyes for DSSC, Electron transfer at interfaces, Transistors and solar cells, Fabrication of Devices, Device characterisation using dark current, IV curves under illumination, IPCE, Calculation of Voc, Jsc, Vpp, Ipp, FF and Pmax. hybrid solar cells

CHE-LAB-3-329

Functional Ceramics: 1-0-0-1

Advanced Electronic Ceramics, high temperature ceramic super conductors, Dielectric ceramics, microwave ceramics, low k materials, SOFC materials, solid-ionic conductors, phosphor materials, Impedance analysis, varistors, sensors, ceramic magnets, thermal shock resistance and super plastic ceramics.

CHE-LAB-3-330

Modern Magnetic Materials: 1-0-0-1

Types of magnetism, molecular field theory, measurement techniques, magnetoresistance (AMR, GMR, CMR, TMR), hard and soft magnets, New magnetic materials, applications.

CHE-LAB-3-331

Porous structures: 2-0-0-2

Definitions, Micro-Porous and Mesoporous Solids, Structural Chemistry of Zeolite Framework Types, MOFs, COFs, Synthesis, Structure Determination, Role of the Structure-directing Agents, The Chemistry of Microporous Framework Solids, Adsorption and Diffusion, Catalytic Applications, hydrogen storage, separation, CO₂ sequestration, sensors,

CHE-LAB-3-332

Biomaterials for targeted therapeutics : 2-0-0-2

Rational design and engineering of lipid-based targeted drug delivery vehicles and their therapeutic applications - Design of polymeric micelles as nano drug carriers - Design of polymer-based nanometric targeted delivery systems and their therapeutic applications - Set-backs and unmet challenges – Cancer and its Hall Marks - Principles of designing anti-cancer therapeutics – Molecular basis of lung, breast, melanoma and prostate cancers – Rationale for selecting leading pathways in cancer therapy – Nuclear hormone receptors as targets in cancer therapy – Rationale for design of cancer therapy against multiple pathways – Concept of designing hybrid molecules as a dual strategy – Use of nanotechnology in cancer therapy – Concept of cancer stem cells and design of cancer stem cell therapeutics.

CHE-LAB-3-333

Organic electrochemistry: 2-0-0-2

Cathodic reactions of organic compounds, Anodic reactions of organic compounds, Classifications of electrode reactions, Stereochemistry of electrochemical processes, Applications of organic electrochemistry.

CHE-LAB-3-334

Electrochemical power sources: 2-0-0-2

Energy scenario, emissions and global warming, fuel cells, Thermodynamic potentials, electrochemical processes and electrode kinetics, Proton exchange membranes, proton conducting mechanisms, recent advances, Operating conditions, overview of characterization techniques, technical aspects, advantages, materials, significances and challenges, Materials for supercapacitor applications, recent advances in the system development, battery vs. supercapacitor, modern technologies, challenges and prospects.

CHE-LAB-3-335

Alternate energy materials: 2-0-0-2

Energy scenario, Non-renewable and renewable energy sources; description of renewable sources and their importance. Technologies for biomass energy conversion, Solar energy, Wind Turbines, Geothermal Technologies; Applications; Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.

CHE-LAB-3-336

Photoinduced electron and Energy transfer: 2-0-0-2

Thermodynamic aspects, Calculation of free energy change from redox potentials, Weller equation, Kinetic aspects, concept of reorganization energy, Marcus theory, Inverted region kinetics, Back electron transfer, circumventing back electron transfer, Applications of photoinduced electron and energy transfer, Reaction centre and photoinduced electron transfer processes in photosynthetic bacteria, Solar water splitting, Dye-sensitized solar cells, Organic photovoltaics, Few organic reactions initiated by PET, Photo-remediation of organic waste materials, Mechanisms and dynamics of fluorescence quenching, Fluorescence anisotropy, Energy transfer to single and multiple acceptors, Resonance energy transfer and its implication, Sensors based on photoinduced processes.

CHE-LAB-3-337

Hydrogen generation and storage: 2-0-0-2

Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.

CHE-LAB-3-338

Thermochemical Conversion of Biomass: 1-0-0-1

Thermochemical conversion technologies for biomass pyrolysis, gasification, combustion, thermal and catalytic conversion of biomass; upgradation of pyrolysis products; bio-refining products and applications; biorefinery concept; Hybrid methods of conversion and effective utilization; Alternative and/or clean fuels, functional and bulk chemicals from biomass; life cycle analysis; carbon and water foot prints; Utilization of products and feasibility assessment; Science, technology and policy of biomass energy; Strategies for Enhancing role of renewable energy and Indian scenario.

CHE-LAB-3-339

CO₂ sequestration and conversion: 2-0-0-2

CO₂ Sequestration; Capture techniques; overview of transportation and storage techniques, Basic properties of CO₂, Reactivity of CO₂, Utilization of CO₂ as chemical feedstock, Utilization of CO₂ as inert solvent for chemical synthesis, Coordination chemistry of CO₂ and reactivity of coordinated CO₂, Transition metal promoted reactions of CO₂, The chemistry of N-CO₂ bonds, Applications of CO₂ for the synthesis of polymers, photochemical reduction of CO₂, utilization of CO₂ for the production of hydrocarbon fuels.

CHE-LAB-3-340

Natural gas to liquid fuels: 2-0-0-2

generation processes; SMR; POx; ATR; DMR and Tri reforming, Syngas conversion processes; FT Synthesis, LTFT, HTFT, Low Pressure versus high pressure FT, Syn-crude up gradation by hydrocracking, methanol synthesis, chemistry of the processes; catalysts, development in reactors; tubular; multitubular; fixed bed; fluidized bed; FFB; CFB, SBCR, variables affecting SCBR, Commercial Processes; MTO; UOP/Hydro MTO; Exxon Mobil MTO; Lurgi MTP, DME Synthesis, status and prospects of DME production; Challenges for DME commercialization, commercialization activities of GTL plants, SSPD, SMDS, AGC- 21 and Gasel Processes.

CHE-LAB-3-341

Gasoline reformulation techniques: 2-0-0-2

Environmental regulations on Fuel quality, Gasoline specifications and concept of reformulated gasoline, Gasoline production routes; Gasoline from Crude oil; General Properties of gasoline; Gasoline quality improvement drivers ; Chronological development in gasoline composition; Gasoline additives, Gasoline blending unit in a refinery; Dealing with aromatics, olefins and sulfur concentrations; Integration techniques to obtain reformulated gasoline, Refining processes; Reforming; Isomerisation, FCC Gasoline, Alkylation, Technologies for Alkylation.

CHE-LAB-3-342

Block copolymers: 2-0-0-2

Chain and controlled block copolymerization, monomer reactivity ratios, Copolymer compositions, molecular architecture, blends, grafts, melts, self assembly and phase separation, phase diagram, range of applicability of copolymerization equation; types of copolymerization; Block copolymers with controlled molecular weight, Living Polymerization, block copolymer synthesis, characterization techniques, block copolymers for biomedical and industrial applications, Amphiphilic block copolymer micelles, Block copolymer thin films.

CHE-LAB-3-343

Polymers for membrane applications: 2-0-0-2

Polymers as membrane materials, functional polymers containing styrene and its derivatives; Functionalized poly(arylene ether)s, Nafion and other Poly(perfluorosulfonic acid) Membranes, Post functionalized polymeric membranes, random and block copolymers; functional poly(imide)s; functional polyphosphazene; functionalized bio-

polymers, design of new functional polymers; Glassy and rubbery polymers, characterization of polymer membranes, transport phenomena, polymer nanocomposites for membranes in the separation of gases and liquids, membrane fouling.

CHE-LAB-3-344

Ion exchange polymers: 1-0-0-1

Adsorbents and ion exchange resins, Classification of ion exchange resins, Synthesis and characterization of ion-exchange resins and polymers, Water treatment and other applications, fouling, regeneration.

CHE-LAB-3-345

Conducting polymers: 1-0-0-1

Synthesis and characterization, electrical transport properties, theory of conductivity, doping, electrochromic properties, Classification and types of organic conductors, Structure and properties of conducting charge-transfer salts, Conducting polymers based on organometallic compounds, Applications of conducting polymers, EMI shielding, supercapacitors, sensors

CHE-LAB-3-346

Polymers and Colloidal Solutions: 2-0-0-2

Intermolecular forces and potentials, Overview of Statistical physics, DLVO theory, charged colloids, Poisson Boltzmann theory, Debye radius, Bjerrum length, electrophoresis, zeta potential, diffusion, Hydrodynamic interactions. Brief overview of Phase transitions in hard sphere colloids, Random walk, self avoiding random walk, flexible polymers, persistence length, Excluded volume interactions, Polymer solutions in the dilute limit/semi-dilute limit, Entropy of mixing, theta temperature, rubber elasticity, Polyelectrolytes, polymer at surfaces: Brushes, polymer dynamics.

CHE-LAB-3-347

Biodegradable polymers: 2-0-0-2

Polymers from biomass, microbial production, synthetic polymers, structure and properties, Biodegradation mechanism, measurement techniques, processing techniques, sterilization and storage, global standards, market potential, applications.

CHE-LAB-3-348

Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2

Controlled or Living Radical Polymerization, TEMPO-mediated polymerization and atom Transfer radical Polymerization (ATRP), Kinetics of ATRP, Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide mediated polymerization (NMP), Ring opening Metathesis polymerization (ROMP), living ROP, Macromolecular architectures using controlled living polymerizations

CHE-LAB-3-349

Pi-conjugated polymers: 2-0-0-2

Synthesis and characterization, electronic and optical properties, energy band structure, Display Materials: Organic Light Emitting Diodes, Organic thin film transistors, device preparation, working principle, advantages, drawbacks; Organic photovoltaics, OFETs, device preparation and characterization, factors influencing efficiency, stability.

CHE-LAB-3-350

Liquid Crystals: 2-0-0-2

Liquid crystal phases, classification, Chiral liquid crystalline phases, Ferroelectric liquid crystalline phases, discotic liquid crystalline phases, Characterization techniques, Surface Alignment of Liquid Crystals, Dichroic LCs, Polycatenar mesogenes, Display and photovoltaic applications.

CHE-LAB-3-351

X-Ray Diffraction and Structure of Solids: 2-0-0-2

Introduction to X-ray crystallography, Crystal growth, evaluation and mounting, Symmetry and space group determination, Background theory for data collection, Data collection using four-circle diffractometers, Area detectors, Crystal lattices, Structure factors, Crystal symmetry, Structure solutions, Structure refinement, An introduction to maximum entropy, Least squares fitting of parameters, Practical aspects of structure refinement, Crystallographic Database, Structure solution from Powder Diffraction Data

CHE-LAB-3-352

NMR spectroscopy: 2-0-0-2

Quantum Mechanics of NMR, Multinuclear NMR spectroscopy, Periodic table of NMR, Heteronuclear double resonance experiments, Magnetization transfer and signal enhancement, NMR of diamagnetic and paramagnetic compounds, Multidimensional NMR: 2D NMR, 1H-1H correlations, Heteronuclear Correlation Spectroscopy, 2D Exchange (EXSY), 2D NOESY, ROESY, DOSY Structure elucidation of small molecules, NMR of macromolecules, Multidimensional NMR Spectra, NMR Spectroscopy of Solids, 2D experiments in solids, semi rigid systems: HR MAS, Magnetic Resonance Imaging: In Vivo NMR, Imaging, MRI, functional MRI, NMR imaging of materials.

CHE-LAB-3-353

Mass spectrometry applications: 2-0-0-2

Applications to analyze molecular, macromolecular and biological samples, Sample Preparation Protocols, Drug Metabolism and Pharmacokinetics (DMPK), Development of Quantitative analytical methods using mass spectrometry, Application to some model drugs, Metabolomics, Proteomics, GC-MS, LC-MS, MALDI-TOF, GC-TOF, TOF/TOF MS, LC-ESI-MS, Protein Database search (MASCOT), Clinical Mass Spectrometry,

CHE-LAB-3-354

Ultrafast processes and spectroscopy: 2-0-0-2

Different types of lasers, components and building of lasers and generation of ultrafast lasers. Principles, instrumentation and applications of different types of ultrafast spectroscopy, Conventional and laser flash Photolysis, and Pump-Probe spectroscopy, Steady state and time resolved Raman spectroscopy, Coherent anti-Stokes resonance Raman Spectroscopy, Femtosecond stimulated Raman Spectroscopy Femtosecond vibrational coherence spectroscopy, Transient grating Spectroscopy, Fluorescence up-conversion, Time correlated single photon counting, ultrafast physical, chemical and biological systems.

CHE-LAB-3-355

Small Angle Scattering Techniques: 2-0-0-2

SAXS and Fourier Transforms, General Theorems in Small Angle Scattering: Particulate systems: Porod and Guinier regimes, Pair density distribution functions, Single particle form factor for spheres, rods and plates, polydispersity, Structure factors for equilibrium concentrated particulate systems, measured structure factors for systems exhibiting polydispersity, Two phase systems: General Theorems, Detailed analysis of scattering from lamellar systems, relevance to semicrystalline polymers.

CHE-LAB-3-356

Natural products and drug discovery: 2-0-0-2

Natural products: Importance, lead, clinical trials in drug discovery research, Case studies of marketed natural product drugs, Synthetic Biology and Genetic engineering in the production of natural product, A brief overview of drug discovery approach, Cause of diseases, Target identification, Target validation, Modeling, Synthesis and SAR, Drug

Delivery, Clinical Trials, Etiology, pathogenesis, prevention, drug targets and chemotherapy, drug resistance and remedies of tropical infectious diseases, Etiology and remedies of diseases developed through metabolic disorders.

CHE-LAB-3-357

Lipid science & technology: 2-0-0-2

Chemistry and Biochemistry of Lipids, Lipid Modification for Surfactant Preparation and Oleochemicals, Analytical Techniques for Lipids and Allied Products, Processing, Degumming, Bleaching, Dewaxing, Neutralization & Deodorization, Hydrogenation, By-products of lipids and their Value Addition,

CHE-LAB-3-358

Photobiology: 2-0-0-2

Primary processes in photosynthesis, antenna effect, reaction center, primary processes in vision, bio and chemiluminescence and environmental photobiology and UV effects, Phototherapy and photodynamic therapy, sensitizers, structures of porphyrinic and non-porphyrinic sensitizers, type I and type II mechanisms, advantages and disadvantages of light in medicine.

CHE-LAB-3-359

Nanobiotechnology: 1-0-0-1

Concept of hybrid systems, signaling and signaling responses; biological systems as transducers, Biology at the nano-interface, fluorescent nanoparticles for life sciences, applications, DNA based particles used as building blocks, micelles, Nucleic Acid Engineering using DNA as Nano materials, Cells & Microfabricated Devices, Nanomaterials for drug delivery, imaging, diagnostics, therapy, separation, Biosensors

400 level courses

Compulsory courses

CHE-LAB-4-401

Project proposal writing & presentation: 0-0-4-2

CHE-LAB-4-402

Project proposal writing & presentation: 0-0-4-2

CHE-LAB-4-403

CSIR-800: 0-0-8-4

100 level courses

CHE-IIP-1-001

Research Methodology: 1-0-0-1

Good laboratory practices, Safety in the laboratory, First Aid in the laboratory, Maintenance of laboratory records, Scientific literature management, Communication skills (scientific writing and presentation), Intellectual property management & planning, Ethics in Science, Computer applications and tools, Statistical methods & Data analysis

CHE-IIP-1-002

Analytical Tools and Instrumentation: 1-0-0-1

Thermal methods (TG, DTG, DTA, TMA, DSC), X-ray methods (XRD, XRF, SAXS), NMR (^1H , ^{13}C) and other Spectroscopic methods (EPR, IR, UV, Fluorescence), Chromatographic methods (TLC, GC, LC), Mass spectroscopy, Electron Microscopy (SEM, TEM), Electron Probe Micro Analysis (EDS, WDS), Quantitative Analysis (AAS, ICP, CHN)

200 level courses

CHE-IIP-2-003

Advanced Organic Chemistry: 2-0-0-2

Stereochemistry, reaction mechanism, C-C and C-X bond formations, Retrosynthetic analysis, photochemistry, pericyclic reactions, reactive intermediates, Methods of asymmetric synthesis and their application in total synthesis, oxidation-reduction reactions, organocatalysis, metathesis reactions.

CHE-IIP-2-004

Advanced Analytical Chemistry: 2-0-0-2

Analytical instrumentation, signal and noise, Overview of optical methods of analysis: Components of optical instruments, atomic and molecular spectrometry based on absorption, emission and scattering, Electroanalytical techniques (basic electrochemistry, voltammetry, potentiometry), Analytical separations and introduction to chromatographic methods, GC, LC, Mass spectrometry, electromigration techniques, hyphenated techniques, detectors, Analytical tools for petroleum refining.

CHE-IIP-2-012

Advances in hydrocarbon chemistry: 2-0-0-2

Chemistry of crude oil, thermal cracking, visbreaking and coking processes, catalytic cracking, hydro cracking and hydrogen production processes, catalytic reforming process, Chemistry and industrial processes for alkylates, isomerisation processes, Petrochemicals, Basic Building blocks; C₁-Chemistry; Petrochemicals from n-paraffins; Petrochemicals from olefins and aromatics; Refinery-Petrochemical Integration, Future Prospects

CHE-IIP-2-015

Advanced Catalysis: 2-0-0-2

Homogeneous and heterogeneous catalysis, adsorption, diffusion, kinetics, equilibrium and rate expressions; chiral catalysis, Surface Science in Catalysis, Catalytic Materials; Supports; Active Components, Classes of reactions and types of reactors; Catalyst preparation methods; Characterization of catalysts; Catalysis in super critical media; Brief introduction of organo and electrocatalysis; Structure-activity-property-stability of catalysts, Catalysts in chemical industry, Catalysis in petroleum refining and petrochemicals; Catalysis in the utilization of renewable feed stocks and concepts of sustainable chemistry.

CHE-IIP-2-028

Alternative feedstock options for petrochemicals: 2-0-0-2

Global scenario of Petrochemicals, Renewable resources; categorization of resources; chemicals from edible renewable resource; Chemicals from non-edible renewable resources; Catalytic reactions (mineral acid, bases; enzymes, homogeneous and heterogeneous catalysts); alternate fuels; fuels derived from renewable resources; biodiesel, bioethanol, biobutanol; Hydrogen generation from renewable feed stocks, Conversion of glycerol; Naphtha as a conventional source, Need for sustainability in production of Petrochemicals, Alternate Options; from Refineries sources, Natural Gas/Methane as an Option and other Non Refinery Sources, CO₂ utilization, Identification and Recommendations based on techno-economic analysis for India.

300 Level courses

CHE-IIP-3-007

Multiphase reaction kinetics: 1-0-0-1

Mass transfer theories, Multi phase reactors, Multi phase reactors selection criteria; Mass transfer coupled with chemical reaction; measurement of gas-liquid parameters, Reaction in porous catalysts; effective diffusivity and structure of porous catalysts, Important design parameters for gas-liquid and solid reactors, Reactor modeling in petroleum refining industry, Modeling of catalytic sweetening, isomerisation, hydro treating, and FT synthesis.

CHE-IIP-3-021

Ionic liquids for lubricants: 1-0-0-1

Lubrication by Ionic liquids and its structural correlation, Ionic liquids interaction with surfaces, synthetic oil lubricants, synthesis of lubricating ionic liquids, effect of alkyl chain length and anions, IL lubrication oils at variable temperatures, thin films, heat capacity and thermal properties, viscosity and wetting properties, ionic liquids as additives for lubricants, comparison with conventional hydrocarbon oils, Case studies.

CHE-IIP-3-024

Catalysis in petroleum refining: 2-0-0-2

Deactivation in Catalysts and its Consequences, Regeneration and Rejuvenation in Catalysis, Industrial Catalytic Processes; Hydro cracking; Hydro treating; Reforming; Isomerization and Alkylation; Fluid Catalytic Cracking and Deep Catalytic Cracking, Catalysis for Clean Fuels; Gas to Liquid Technology; Catalysis for Hydrogen Production, Catalysis beyond Petroleum; Electro catalysis; Photo catalysis, Laboratory Training in Catalysis.

CHE-IIP-3-027

Biocatalysis in petroleum refining: 1-0-0-1

Scope of Biocatalysis in Petroleum Refining, Thermophilic microorganisms and the thermozymes, Structure and function of proteins, Non-aqueous Biocatalysis, Protein Engineering and rate improvement, Enzyme kinetics and models, Challenges and opportunities on Bioprocess development on: Bio-desulphurization of crude oil and petroleum fractions; Bio-cracking and Bio-vis breaking; Bio-desulphurization of waste gases; Biocatalysts for renewable hydrocarbons and petrochemicals.

CHE-IIP-3-038

Thermochemical Conversion of Biomass: 1-0-0-1

Thermochemical conversion technologies for biomass pyrolysis, gasification, combustion, thermal and catalytic conversion of biomass; upgradation of pyrolysis products; bio-refining products and applications; biorefinery concept; Hybrid methods of conversion and effective utilization; Alternative and/or clean fuels, functional and bulk chemicals from biomass; life cycle analysis; carbon and water foot prints; Utilization of products and feasibility assessment; Science, technology and policy of biomass energy; Strategies for Enhancing role of renewable energy and Indian scenario.

CHE-IIP-3-039**CO₂ sequestration and conversion: 2-0-0-2**

CO₂ Sequestration; Capture techniques; overview of transportation and storage techniques, Basic properties of CO₂, Reactivity of CO₂, Utilization of CO₂ as chemical feedstock, Utilization of CO₂ as inert solvent for chemical synthesis, Coordination chemistry of CO₂ and reactivity of coordinated CO₂, Transition metal promoted reactions of CO₂, The chemistry of N-CO₂ bonds, Applications of CO₂ for the synthesis of polymers, photochemical reduction of CO₂, utilization of CO₂ for the production of hydrocarbon fuels.

CHE-IIP-3-040**Natural gas to Liquid fuels: 2-0-0-2**

generation processes; SMR; POx; ATR; DMR and Tri reforming, Syngas conversion processes; FT Synthesis, LTFT, HTFT, Low Pressure versus high pressure FT, Syn-crude up gradation by hydrocracking, methanol synthesis, chemistry of the processes; catalysts, development in reactors; tubular; multitubular; fixed bed; fluidized bed; FFB; CFB, SBCR, variables affecting SCBR, Commercial Processes; MTO; UOP/Hydro MTO; Exxon Mobil MTO; Lurgi MTP, DME Synthesis, status and prospects of DME production; Challenges for DME commercialization, commercialization activities of GTL plants, SSPD, SMDS, AGC- 21 and Gasel Processes.

CHE-IIP-3-041**Gasoline reformulation techniques: 2-0-0-2**

Environmental regulations on Fuel quality, Gasoline specifications and concept of reformulated gasoline, Gasoline production routes; Gasoline from Crude oil; General Properties of gasoline; Gasoline quality improvement drivers ; Chronological development in gasoline composition; Gasoline additives, Gasoline blending unit in a refinery; Dealing with aromatics, olefins and sulfur concentrations; Integration techniques to obtain reformulated gasoline, Refining processes; Reforming; Isomerisation, FCC Gasoline, Alkylation, Technologies for Alkylation.

400 level courses

Compulsory courses

CHE-IIP-4-001

Project proposal writing & presentation: 0-0-4-2

CHE-IIP-4-002

Project proposal writing & presentation: 0-0-4-2

CHE-IIP-4-003

CSIR-800: 0-0-8-4

CSIR-National Chemical Laboratory

100 level courses

001 and 002/003 are compulsory

CHE(NCL):1-001: Research Methodology: 1-0-0-1

Good laboratory practices, Safety in the laboratory, First Aid in the laboratory, Maintenance of laboratory records, Scientific literature management, Communication skills (scientific writing and presentation), Intellectual property management & planning, Ethics in Science, Computer applications and tools, Statistical methods & Data analysis

CHE(NCL):1-002: Analytical Tools and Instrumentation: 1-0-0-1

Thermal methods (TG, DTG, DTA, TMA, DSC), X-ray methods (XRD, XRF, SAXS), NMR (^1H , ^{13}C) and other Spectroscopic methods (EPR, IR, UV, Fluorescence), Chromatographic methods (TLC, GC, LC), Mass spectroscopy, Electron Microscopy (SEM, TEM), Electron Probe Micro Analysis (EDS, WDS), Quantitative Analysis (AAS, ICP, CHN)

CHE(NCL):1-003: Basic mathematics and numerical methods: 1-0-0-1

Determinants and Matrices, Complex Variables, Vector analysis, Infinite Series, Special Functions, Differential Equations, Interpolation and Approximation, Numerical differentiation and Integration, Basic Linux, Introduction to Algorithms, basic programming, Shell and Shell Scripting, Network Computing and Parallel Computing, Matlab/Scilab/Octave/Gnuplot

CHE(NCL):1-004: Basic Chemistry for Interdisciplinary sciences: 1-0-0-1

Basics of inorganic, organic, physical and biochemistry, Nomenclature (IUPAC), molarity, molality and normality, types of bonding, Ionic, covalent and non-bonding interactions, Acids and bases, Atomic structure, periodic table and periodic properties, stoichiometry, chemical reactions and kinetics, solvent effects, functional groups in organic compounds, general named reactions and reaction mechanisms, carbohydrates, lipids, proteins, nucleotides, enzymes, photosynthesis

CHE(NCL):1-005: Introduction to Nanoscience and Nanotechnology: 1-0-0-1

General considerations, Introduction, definitions, consequences of size reduction, Properties: structural, thermodynamic, optical, electrical and magnetic properties, Methods of synthesis, Surface modifications, factors governing the stability and assembly, Characterization of nanomaterials, Applications of Nanomaterials

CHE(NCL):1-006: Introduction to Chemical Biology: 1-0-0-1

chemical biology/synthetic biology, Structure, function and chemistry of biological macromolecules including amino acids, proteins, nucleic acids and carbohydrates, Chemical kinetics and thermodynamics in biology, Chemical reactions and chemical diversity in Biology The Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Drugs from Nature, Drug interaction

200 level courses

001/002/003 compulsory (Core)

CHE(NCL):2-001: Advanced Physical Chemistry: 2-0-0-2

Thermodynamics and chemical kinetics, Quantum Mechanics, Atomic structure and spectroscopy, Chemical bonding in diatomics, Chemical applications of group theory, Colloids and Surface science, surfactants, Interface and Interfacial properties, Electrochemistry.

CHE(NCL):2-002: Advanced Inorganic Chemistry: 2-0-0-2

Structure & Bonding in Inorganic Compounds, Chemistry of Coordination Compounds, Symmetry in Chemistry & Group Theory, Main group chemistry, Organometallic chemistry, Electronic Spectra of Transition Metal Compounds, Magneto Chemistry, Metal Cluster Compounds, Inorganic Reaction Mechanism, Electron Transfer Reactions in Metal Complexes, Bioinorganic Chemistry (Metalloenzymes, Metal complexes as oxygen carriers, Photosynthesis), Metal Complexes in Medicinal Chemistry, Catalysis by Inorganic Complexes.

CHE(NCL):2-003: Advanced Organic Chemistry: 2-0-0-2

Stereochemistry, reaction mechanism, C-C and C-X bond formations, Retrosynthetic analysis, photochemistry, pericyclic reactions, reactive intermediates, Methods of asymmetric synthesis and their application in total synthesis, oxidation-reduction reactions, organocatalysis, metathesis reactions.

CHE(NCL):2-004: Advanced Analytical Chemistry: 2-0-0-2

Analytical instrumentation, signal and noise, Overview of optical methods of analysis: Components of optical instruments, atomic and molecular spectrometry based on absorption, emission and scattering, Electroanalytical techniques (basic electrochemistry, voltammetry, potentiometry), Analytical separations and introduction to chromatographic methods, GC, LC, Mass spectrometry, electromigration techniques, hyphenated techniques, detectors, Analytical tools for petroleum refining.

CHE(NCL):2-005: Advanced Quantum Mechanics: 2-0-0-2

Revision of Hydrogen atom and particle in box (1D and 3D), Approximate methods in quantum mechanics; Non degenerate perturbation; Perturbation treatment of the Helium atom ground state and first excited state; Variation method for helium atom ground state; Comparison of perturbation and variation method, Structure of many electron wave function, Antisymmetry, Valence bond theory for homo and hetero nuclear diatomic molecules; Molecular orbital theory Comparison of MO and VB theory; Introduction to density functional theory; Hartree Fock theory, Overview of methods beyond Hartree Fock theory; Configuration Interaction; Many body perturbation; Coupled cluster

CHE(NCL):2-006: Advanced Organometallic Chemistry: 2-0-0-2

Fundamentals, The 18 Valence Electron Rule; Structure and bonding of organometallic complexes using molecular orbital theory.

σ -Donor Ligands: Transition-Metal-Alkyl and -Aryl compounds; σ -Donor/ π -Acceptor Ligands: Transition-Metal-Alkenyl, -Aryl and -Alkynyl Complexes, Transition-Metal-Carbenes (Fischer and Schrock Carbenes); Metal Carbonyl; Structure, properties and principal reaction types of the above complexes; σ , π -Donor/ π -Acceptor Ligands: Olefin Complexes; Alkyne, Allyl and Enyl Complexes, Complexes of the cyclic C_nH_n

Fundamental Mechanism of Organometallic Transformations: Oxidative addition, Migratory Insertion, β -hydride elimination and reductive elimination; Interaction of C-C and C-H σ -bonds with Transition Metals

CHE(NCL):2-008: Advanced Photochemistry: 2-0-0-2

Introduction to photochemistry, excited state processes, fluorescence and phosphorescence, quantum yields, charge-transfer spectra, solvatochromism, photochromism, transient absorption techniques, Luminescence emission lifetimes, two- and multiphoton processes, photoinduced energy and electron transfer, FRET, fluorescence polarization, excimers, exciplexes, delayed fluorescence, Photochemistry of Organic chromophores. Photochemistry in organized and confined media.

CHE(NCL):2-009: Advanced Polymer Chemistry: 2-0-0-2

Techniques of polymerization, polymer characterization techniques, Stereochemistry of Polymers, polymer nano-architectures, random and block copolymers, Liquid Crystalline Polymers, Conducting Polymers, Non-linear Polymers, Polymer Blends and Composites, polymer rheology, inorganic, bio and supramolecular polymers

CHE(NCL):2-010: Advanced Electrochemistry: 2-0-0-2

Basic electrochemistry concepts, Reference electrodes, Electrochemical Thermodynamics, Kinetics of electron transfer, the Taft equation, Diffusion, Double Layers, electrode Kinetics, the Gibbs adsorption isotherm, the Lippmann equation, infinitely dilute solutions and thermal balance, Electro capillary phenomena, Faradaic vs. capacitive currents, transport properties, potential theory, Electrochemical Techniques, Voltammetry, Reversible and irreversible reactions, Mass transport by convection, rotating electrodes, Equivalent circuits, A.C. voltammetry, Electrolysis methods, Adsorption, Thin layer cells, Electrochemistry of polymers and inorganic solids, Spectroelectrochemistry, Applications.

CHE(NCL):2-014: Advanced Materials Science: 2-0-0-2

Crystal systems and space groups, Close packing and various simple structure types like AB, AB₂, AB₃ and complex structural types ABX₃, AB₂X₄, etc. Factors affecting crystal structures, Common preparative methods; X-ray diffraction and Electron microscopy, Defect structures, colour centers, reciprocal lattices, Properties of solids – Band theory, metals, insulators, semiconductors, dielectric and ferroelectric properties, magnetic properties, optical properties, ionic conduction; structure-processing-property correlations.

CHE(NCL):2-015: Advanced Catalysis: 2-0-0-2

Homogeneous and heterogeneous catalysis, adsorption, diffusion, kinetics, equilibrium and rate expressions; chiral catalysis, Surface Science in Catalysis, Catalytic Materials; Supports; Active Components, Classes of reactions and types of reactors; Catalyst preparation methods; Characterization of catalysts; Catalysis in super critical media; Brief introduction of organo and electrocatalysis; Structure-activity-property-stability of catalysts, Catalysts in chemical industry, Catalysis in petroleum refining and petrochemicals; Catalysis in the utilization of renewable feed stocks and concepts of sustainable chemistry.

CHE(NCL):2-016: Advanced Surface Science: 2-0-0-2

Introduction to Surface Science - Surface phenomena - Adsorption, Desorption, Adsorption Models, Special properties of surfaces and interfaces, Electronic structure of surfaces, Surface modification and its applications, Nanoscale catalysis and applications, Surface spectroscopy and microscopy tools for nanocatalysis

CHE(NCL):2-017: Advanced Separation Science and Technology: 2-0-0-2

Resins and membranes for separations, Classification of membranes; electromembrane Processes; Ion-exchange membranes and their applications, Electrodialysis and related

processes. Polymer electrolyte membrane and their applications for fuel cells; Water electrolyzer for hydrogen production; Reverse electro dialysis for non-renewable energy from concentration gradient, reverse osmosis, nanofiltration, ultrafiltration, pervaporation and gas separation: Membrane fouling, concentration polarization and other limitations of Pressure-driven membrane technologies.

CHE(NCL):2-018: Advanced Materials Characterization Techniques: 2-0-0-2

Optical Microscopy, Electron microscopy: TEM, HRTEM, SEM, STEM, EDX, FIB, e-beam lithography, Scanning probe microscopy: AFM, STM, MFM, confocal, etc, Raman spectroscopy/microscopy, Thermal analysis techniques, Magnetic measurements, Electrical measurements, Spectroscopic ellipsometry.

CHE(NCL):2-019: Advances in Nanoscience and Nanotechnology: 2-0-0-2

Low-dimensional structures: Quantum wells, Quantum wires, and Quantum dots, Nano clusters & Nano crystals, fullerenes, carbon nano tubes and graphene, Nano Composites, synthesis and characterization techniques, Properties at Nano Scales and comparison with bulk materials, fabrication techniques, general applications, nanomaterials in biology.

CHE(NCL):2-021: Advances in Chemical Biology: 2-0-0-2

Amino Acids, Peptides & Proteins, Design of poly peptides, Peptide hormones and their pharmaceutical significance, Peptide mimetics as therapeutics, Chemistry of Carbohydrates, Nucleic acids, Structure & function of DNA and RNA, Nucleic acid mimetics & their therapeutic applications, Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Basic principles of medicinal chemistry, Drugs from Nature, Natural products based drug discovery, Kinetics and thermodynamics of biological process, Enzyme Catalysis, consecutive, parallel and competitive reactions in biological systems, Thermodynamics, allosteric effect in biology, types of bonds, hydration and their specific contribution towards specific thermodynamic parameters, enthalpy or entropy, Scatchard analysis, hill plot analysis.

CHE(NCL):2-022: Advanced Biomaterials: 2-0-0-2

Definition of biomaterials, Surface property requirements of biomaterials, Types of materials used in medicine, Synthesis and surface characterization, Biology of wound healing, foreign body response and tissue remodeling, Molecular and cellular interactions of materials with biological environment, Degradation and long term fate of materials used in medicine, Requirements of biomaterials for biomedical implants, surface coatings, wound dressings, sutures, cardiovascular devices, ophthalmology, dentistry, orthopedics and cosmetic surgeries, Applications in drug delivery and tissue engineering, Standard protocols for testing the efficacy and efficiency of biomaterials, The regulatory environment for biomaterials, Some concepts for design development of common biomaterials.

CHE(NCL):2-026: Green chemistry: 1-0-0-1

Green chemistry concepts: Basic understanding, scope and interdisciplinary nature of green chemistry; Environmental factors; Carbon credit, Energy efficiency and atom economy, Catalysis and green chemistry, Alternate reaction media and reaction systems, ionic liquids, supercritical fluids, solventless chemistry.

CHE(NCL):2-032: Organic reaction mechanisms: 2-0-0-2

Basics, The concept of Aromaticity, How to write an organic reaction mechanism?, Popular name reactions, Reactive intermediates: Generation, stability, structures and reactivity of carbocation, carbanion, carbene, radicals, benzyne, nitrene, Types of mechanism: classification, limitations examples of aliphatic nucleophilic substitution - aliphatic electrophilic substitution - aromatic nucleophilic substitution - aromatic electrophilic Substitution - types of radical reactions - molecular rearrangements oxidation and reduction; Electrophilic reactions-Friedel crafts reaction, Reimer Tiemann reaction, Beckmann

rearrangements; nucleophilic reactions- aldol condensation, perkin reaction, benzoin condensation; free radical reaction-halogenation of alkane, addition of HBr on alkene in presence of peroxide; allylic halogenation - using N-Bromo Succinamide (NBS), thermal halogenation of alkene $\text{CH}_3 - \text{CH} = \text{CH}_2$

CHE(NCL):2-035: Thermodynamics and Statistical Mechanics: 2-0-0-2

Introduction: Thermodynamics – A Macroscopic Theory of Matter; Laws of Thermodynamics, Ideal Gas Laws, Specific Heat Capacities; Concept of Free Energy, Hamiltonian Mechanics, Equilibrium Distributions and Ergodic Hypothesis, Ensembles, Thermodynamic Functions and the Distribution Function, $g(r)$, Imperfect Gases, Kinetic Theory of Gases, Time Dependent Processes, Phase Transitions

CHE(NCL):2-036: Composite materials: 2-0-0-2

Concept of Composite materials, Various types of composites, Classification based on Matrix Material: Organic Matrix composites, Polymer matrix composites (PMC), Carbon matrix Composites or Carbon-Carbon Composites, Metal matrix composites (MMC), Ceramic matrix composites (CMC); Classification based on reinforcements: Fiber Reinforced Composites, Fiber Reinforced Polymer (FRP) Composites, Laminar Composites, Particulate Composites, Reinforcements/Fibres, Types of fibres, Multiphase fibers, Whiskers and Flakes, Mechanical properties of fibres, Processing of Advanced composites, Metal Matrix Composites: Casting – Solid State diffusion technique, Cladding – Hot isostatic pressing; Ceramic Matrix Composites: Liquid Metal Infiltration – Liquid phase sintering; Carbon – Carbon composites: Knitting, Braiding, Weaving; Polymer matrix composites: Preparation of Moulding compounds and prepregs – hand lay up method – Autoclave method – Filament winding method – Compression moulding – Reaction injection moulding, Processing and characteristics of nanocomposites, hybrid composites, functionally graded composites, smart and functional composites.

CHE(NCL):2-037: Carbon allotropes: 1-0-0-1

Synthesis, characterization, structure, properties and applications of: Diamond, Graphite, Amorphous carbon, Charcoals, Fullerene and related compounds, Carbon nanotubes, Graphene.

CHE(NCL):2-038: Organic spectroscopy applications: 2-0-0-2

Mass spectroscopy, IR spectroscopy, Proton magnetic resonance spectroscopy, Structural assignment by employing NMR techniques, Carbon-13 NMR spectroscopy, Introduction COSY, HSQC, HMBC, NOESY, ROESY, Structural elucidation using 2D-NMR methods

CHE(NCL):2-039: Surface characterization techniques: 2-0-0-2

XPS, LEED, XAS, SEM, AFM, TEM, NSOM, SPR, SERS, static and dynamic contact angle measurements, Ellipsometry.

300 Level courses

CHE(NCL):3-001: Mathematical Methods: 2-0-0-2

Determinants and Matrices : Orthogonal Matrices, Hermitian Matrices, Unitary Matrices, Diagonalisation of Matrices, Vector analysis : Scalar and Vector product, Triple scalar and vector product, Gradient, Divergence, Curl, Vector Integration, Gauss Theorem, Stokes Theorem. Vector Analysis in Curvilinear coordinates and Tensors, Infinite Series: Fundamental Concepts, Convergence tests, Taylors expansion, Power Series, Special Functions: Gamma Function, The Beta Function, Differential Equations: Series Solution-Frobenius Method, Bessel Functions, Legendre Functions, Hermite Functions, Laguerre Functions, Fourier Series, Applications of Fourier Series, Fourier Transforms

CHE(NCL):3-002: Numerical Methods: 2-0-0-2

Fortran and Linux basics, Solution to the linear algebraic equations, Eigen Values problems, Interpolation and extrapolation, Random number and sorting, Minimization and maximization of functions, Modeling of data

CHE(NCL):3-003: Electronic structure theory: 2-0-0-2

Post-Hartree-Fock methods: Moller-Plesset perturbation theory (MP2, MP3, and MP4), Configuration Interaction (CI), Coupled-Cluster single double (triple) (CCSD(T))–performance of various methods for the prediction of van der Waal and hydrogen bonding interactions, spectral properties. Density functional theory based methods: Hybrid and Minnesota functional – Application of DFT methods (excitation energy calculations). Density functional methods with Dispersion correction (Grimme's approaches). Car-Parrinello Molecular Dynamics (CPMD) and Born-Oppenheimer Molecular Dynamics (BOMD).

CHE(NCL):3-004: Molecular modeling and simulation: 2-0-0-2

Molecular Mechanics: Features of molecular mechanics - Force Fields: Bonds structure and bending angles, Electrostatic Vander Waals and non-bonded interactions, Hydrogen bonding - Derivatives of molecular mechanics energy function - Calculating thermodynamic properties - Force Field for inorganic systems - Energy minimization, Molecular Dynamics Simulation: Molecular Dynamics using simple models, Molecular Dynamics with continuous potentials, Solvent effects, Conformational changes, Thermostats, Barostats, Lincs and shake algorithms, Monte Carlo simulation Methods, sorption, Applications of Molecular Modeling

CHE(NCL):3-006: Computational materials design: 2-0-0-2

Solids, Drude and Sommerfield theories of metals, Kronig-Penning model, Tight-Binding approximation, band structure, density of states, prediction of electrical and magnetic properties, Prediction of properties of organic molecules and polymers, Introduction to Multiscale Modeling and Simulations and applications. Monte Carlo simulation in various ensembles, Gas sensing properties of various porous materials using grand canonical Monte Carlo method, Dissipative particle dynamics, Mesoscale dynamics and applications.

CHE(NCL):3-008: Carbohydrate chemistry: 2-0-0-2

Mono and disaccharides, polysaccharides, Bacterial polysaccharides, starch and cellulose, derivatives of cellulose, Protecting groups, Glycosylation reactions, Dynamics and interactions, carboxy methyl cellulose and gun cotton, structure, Conformational analyses, glycoconjugates, Immunology of carbohydrates.

CHE(NCL):3-015: Chemistry and biology of Heterocycles: 2-0-0-2

Privileged heterocycles, Electronic properties, reactivity (electrophilicity and nucleophilicity), Synthetic methodologies, Biological properties of Natural products and drug candidates, Biosynthesis, Dimeric compounds and related stereochemistry

CHE(NCL):3-023: Homogeneous Catalysis: 1-0-0-1

Organometallic Catalysis, Applications in organic synthesis: Olefin Isomerization, C-C Coupling reactions: Heck, Suzuki, Stille and Sonogashira reactions, Alkene and Alkyne Metathesis, C-Heteroatom coupling: Hydroamination, Olefin Oxidation, C-H activation, Oxidation reactions, hydrogenation of Alkenes, Industrial Applications.

CHE(NCL):3-028: Materials and devices for energy conversion: 2-0-0-2

Design of organic and Inorganic semiconductors, Approaches to process organic semiconductors by covalent and non covalent modifications, band edges and band gaps, Modulation of charge transport properties, kinetics of electron transfer, Design of small molecule dyes for DSSC, Electron transfer at interfaces, Transistors and solar cells, Fabrication of Devices, Device characterisation using dark current, IV curves under illumination, IPCE, Calculation of Voc, Jsc, Vpp, Ipp, FF and Pmax. hybrid solar cells

CHE(NCL):3-029: Functional Ceramics: 1-0-0-1

Advanced Electronic Ceramics, high temperature ceramic super conductors, Dielectric ceramics, microwave ceramics, low k materials, SOFC materials, solid-ionic conductors, phosphor materials, Impedance analysis, varistors, sensors, ceramic magnets, thermal shock resistance and super plastic ceramics.

CHE(NCL):3-030: Modern Magnetic Materials: 1-0-0-1

Types of magnetism, molecular field theory, measurement techniques, magnetoresistance (AMR, GMR, CMR, TMR), hard and soft magnets, New magnetic materials, applications.

CHE(NCL):3-031: Porous structures: 2-0-0-2

Definitions, Micro-Porous and Mesoporous Solids, Structural Chemistry of Zeolite Framework Types, MOFs, COFs, Synthesis, Structure Determination, Role of the Structure-directing Agents, The Chemistry of Microporous Framework Solids, Adsorption and Diffusion, Catalytic Applications, hydrogen storage, separation, CO₂ sequestration, sensors,

CHE(NCL):3-034: Electrochemical power sources: 2-0-0-2

Energy scenario, emissions and global warming, fuel cells, Thermodynamic potentials, electrochemical processes and electrode kinetics, Proton exchange membranes, proton conducting mechanisms, recent advances, Operating conditions, overview of characterization techniques, technical aspects, advantages, materials, significances and challenges, Materials for supercapacitor applications, recent advances in the system development, battery vs. supercapacitor, modern technologies, challenges and prospects.

CHE(NCL):3-035: Alternate energy materials: 2-0-0-2

Energy scenario, Non-renewable and renewable energy sources; description of renewable sources and their importance. Technologies for biomass energy conversion, Solar energy, Wind Turbines, Geothermal Technologies; Applications; Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.

CHE(NCL):3-037: Hydrogen generation and storage: 2-0-0-2

Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.

CHE(NCL):3-046: Polymers and Colloidal Solutions: 2-0-0-2

Intermolecular forces and potentials, Overview of Statistical physics, DLVO theory, charged colloids, Poisson Boltzmann theory, Debye radius, Bjerrum length, electrophoresis, zeta potential, diffusion, Hydrodynamic interactions. Brief overview of Phase transitions in hard sphere colloids, Random walk, self avoiding random walk, flexible polymers, persistence length, Excluded volume interactions, Polymer solutions in the dilute limit/semi-dilute limit, Entropy of mixing, theta temperature, rubber elasticity, Polyelectrolytes, polymer at surfaces: Brushes, polymer dynamics.

CHE(NCL):3-048: Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2

Controlled or Living Radical Polymerization, TEMPO-mediated polymerization and atom Transfer radical Polymerization (ATRP), Kinetics of ATRP, Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide mediated polymerization (NMP), Ring opening Metathesis polymerization (ROMP), living ROP, Macromolecular architectures using controlled living polymerizations

CHE(NCL):3-051: X-Ray Diffraction and Structure of Solids: 2-0-0-2

Introduction to X-ray crystallography, Crystal growth, evaluation and mounting, Symmetry and space group determination, Background theory for data collection, Data collection using four-circle diffractometers, Area detectors, Crystal lattices, Structure factors, Crystal symmetry, Structure solutions, Structure refinement, An introduction to maximum entropy, Least squares fitting of parameters, Practical aspects of structure refinement, Crystallographic Database, Structure solution from Powder Diffraction Data

CHE(NCL):3-052: NMR spectroscopy: 2-0-0-2

Quantum Mechanics of NMR, Multinuclear NMR spectroscopy, Periodic table of NMR, Heteronuclear double resonance experiments, Magnetization transfer and signal enhancement, NMR of diamagnetic and paramagnetic compounds, Multidimensional NMR: 2D NMR, 1H-1H correlations, Heteronuclear Correlation Spectroscopy, 2D Exchange (EXSY), 2D NOESY, ROESY, DOSY Structure elucidation of small molecules, NMR of macromolecules, Multidimensional NMR Spectra, NMR Spectroscopy of Solids, 2D experiments in solids, semi rigid systems: HR MAS, Magnetic Resonance Imaging: In Vivo NMR, Imaging, MRI, functional MRI, NMR imaging of materials.

CHE(NCL):3-053: Mass spectrometry applications: 2-0-0-2

Applications to analyze molecular, macromolecular and biological samples, Sample Preparation Protocols, Drug Metabolism and Pharmacokinetics (DMPK), Development of Quantitative analytical methods using mass spectrometry, Application to some model drugs, Metabolomics, Proteomics, GC-MS, LC-MS, MALDI-TOF, GC-TOF, TOF/TOF MS, LC-ESI-MS, Protein Database search (MASCOT), Clinical Mass Spectrometry,

CHE(NCL):3-055: Small Angle Scattering Techniques: 2-0-0-2

SAXS and Fourier Transforms, General Theorems in Small Angle Scattering: Particulate systems: Porod and Guinier regimes, Pair density distribution functions, Single particle form factor for spheres, rods and plates, polydispersity, Structure factors for equilibrium

concentrated particulate systems, measured structure factors for systems exhibiting polydispersity, Two phase systems: General Theorems, Detailed analysis of scattering from lamellar systems, relevance to semicrystalline polymers.

400 level courses

Compulsory courses

CHE(NCL):4-001: Project proposal writing & presentation: 0-0-4-2

CHE(NCL):4-002: Project proposal writing & presentation: 0-0-4-2

CHE(NCL):4-003: CSIR-800: 0-0-8-4

CSIR-Institute of Minerals and Materials Technology

Course No: CHEM (IMMT) -1-001 Research Methodology, LTPC: 2-0-0-2

1. Research Methodology - Introduction

Meaning, Concept, Need

Historical Research

Survey Research

Experimental Research

Fundamental and Applied Research

2. Literature Search & Review of Literature

3. Research Tools

Measurement of Variables

Presentation of Data

Statistical Techniques – All Basic Techniques, Null hypothesis, Error Analysis, Interval estimation, Statistical Significance, Examples: Analysis of variance (ANOVA), Chi-squared test, Correlation, Factor analysis, Mann–Whitney U, Mean square weighted deviation (MSWD), Pearson product-moment correlation coefficient, Regression analysis, Spearman's rank correlation coefficient, Student's t-test and z-test, Time series analysis

Statistical Packages:

MS Excel - Introduction, Getting Data into Excel, Activating the Data-Analysis Tools, Using Excel to Determine a Confidence Interval, Using Excel for t-Tests of Hypotheses, The t-Test for Independent Samples, The t-Test for Dependent (and Matched-Pair) Samples, Using Excel for ANOVA, Using Excel for Correlation, Using Excel for Linear Regression, Using Excel for Chi-Square Tests, The Chi-Square Goodness-of-Fit Test and the Chi-Square Test of Association

MATLAB - Introduction and Key Features, Developing Algorithms and Applications, Analyzing and Accessing Data, Visualizing Data, Performing Numeric Computation, Publishing Results and Deploying Applications

4. Research Types and Methods

Observation Method

Questionnaire Method

Interview Method

Experimental Method

5. Research Process

Designing a Research: Characteristics, Purpose

Research Plan

Analysis and Testing

Quantitative Methods and Data Analysis

Qualitative Analysis

6. Communicating Research Results

Journal paper

Thesis

Project proposal

Report

Web publishing

Seminar and Oral presentations

7. Research Ethics and Plagiarism

8. Case Studies

Reference Books

- Applications of Research Methodology EMERALD GROUP PUBLISHING - 978-0-7623-1295-5
Applied Computer Science Pertti Järvinen: On Research Methods. Tampere: Opinpajan Kirja, ISBN 952-99233-1-7.
- Blessing, L. T. M. and A. Chakrabarti, "DRM, a Design Research Methodology", Springer, 2009.
- Bolker, Joan (1998). Writing Your Dissertation in Fifteen Minutes a Day: A Guide to Starting, Revising, and Finishing, Holt Paperbacks, ISBN 080504891X
- Booth, W. C. G. G. Colomb and J. M. Williams, "The Craft of Research", Third Edition, University of Chicago, 2008.
- Campbell, Donald T. and Stanley, Julian (1963). Experimental and Quasi-experimental Designs For Research, ISBN 0395307872. (Very old, but still relevant)
- Carey, S. S. "A Beginner's Guide to Scientific Method", Third Edition, Wadsworth, 2003.
- Christensen, L. B.; R. B. Johnson and L. A. Turner, "Research Methods, Design, and Analysis", Eleventh Edition, Allyn & Bacon, 2010.
- Cook, Thomas, K. and Campbell, Donald T. (1979). Quasi-Experimentation: Design and Analysis Issues for Field Settings, Houghton Mifflin Company, ISBN-10 0395307902
- Creswell, J. W. and V. L. P. Clark, "Designing and Conducting Mixed Methods Research", Second Edition, Sage, 2010.
- Creswell, J. W. "Research Design : Qualitative, Quantitative, and Mixed Methods Approaches", Third Edition, Sage, 2011. (Indian Edition exists)
- Creswell, John W. (2002). Research Design: Qualitative, Quantitative, and Mixed Methods Approaches (2nd Edition), Sage Publications, ISBN 0761924426
- Creswell, John W. (2004). Educational Research: Planning, Conducting, and Evaluating Quantitative and Qualitative Research, Prentice Hall; 3rd edition. ISBN 0136135501
- Denzin, Norman K. and Yvonna S. Lincoln (eds) (). The SAGE Handbook of Qualitative Research, Sage Publications. ISBN 0761927573
- Dey, I. (1993). Qualitative Data Analysis. Routledge, London.
- Essence of Research Methodology: A Concise Guide for Master and PhD Students in Management Science SPRINGER-VERLAG BERLIN 978-3-540-71658-7
- Field, A. P. (2005). Discovering statistics using SPSS (second edition). London: Sage publications. ISBN 0-7619-4452-4. (Good introduction to statistics book for beginners, and help with SPSS too).
- Fowler, Floyd, J. (2001) Survey Research Methods, Sage Publications, ISBN 0761921915
- Fraenkel, J., & Wallen, N. (2006). How to Design and Evaluate Research in Education with PowerWeb (6th ed.) New York: McGraw-Hill.
- George, E. P.; William G. Hunter; J. Stuart Hunter and William Gordon Hunter (2005). Statistics for Experimenters: Design, Innovation, and Discovery, 2nd edition. John Wiley & Sons, ISBN 0471718130.
- Hoepfl, Marie C. (1997). Choosing Qualitative Research: A Primer for Technology Education Researchers, Journal of Technology Education, Volume 9, Number 1. HTML.
- Kothari, C. R. "Research Methodology : Methods and Techniques", Second Edition, Wishwa Prakashan / New Age International, 1990.
- Kumar, R. "Research Methodology : A Step-by-Step Guide for Beginners", Third Edition, Sage, 2010/2011. (Indian Edition exists)
- Leedy, P. D., & Ormrod, J. E. (2005). Practical Research: Planning and Design (8th ed.). Upper Saddle River, NJ: Pearson Education. ISBN 0131108956
- Locke, L. F; S. J. Silverman and W. W. Spirduso, "Reading and Understanding Research", Third Edition, Sage, 2009.
- Managing Science: Methodology and Organization of Research SPRINGER 978-1-4419-7487-7
- Marczyk, G. R; D. DeMatteo and D. Festinger, "Essentials of Research Design and Methodology", Wiley, 2005.
- Marder, M. P. "Research Methods for Science", CUP, 2011.

Marshall, C. & Rossman, G. B. (1995) , Designing Qualitative Research, second edition, Sage, London

Merriam, Sharan B. (1997) Qualitative Research and Case Study Applications in Education, Jossey-Bass, ISBN 0787910090

Miles, Matthew B. and Michael Huberman. (1994) Qualitative Data Analysis: An Expanded Sourcebook, Sage Publications. ISBN 0803955405

Newman, Lawrence (2003). Basics of Social Research: Quantitative and Qualitative Approaches. Allyn & Bacon, ISBN 0205355781

Newman, Lawrence (2005). Social Research Methods: Qualitative and Quantitative Approaches, 6th edition. Allyn & Bacon, ISBN 0205457932

O'Leary, Z. "The Essential Guide to Doing Your Research Project", Second Edition, Sage, 2009/2011. (Indian Edition exists)

Peters (1997) Getting What You Came For: A Smart Student's Guide to Earning a Masters or Ph.D.

Phillips, E. M. and D. S. Pugh, How to get a Ph.D.?(UBSPD, New Delhi, 1993).

Robson, C. "Real World Research", Third Edition, Wiley, 2011.

Rozakis, L. E. "The Complete Idiot's Guide to Research Methods", Alpha, 2004.

Salkind, N. J. "Exploring Research", Seventh Edition, Prentice-Hall, 2008.

Salkind, N. J. (Editor), "Encyclopedia of Research Design", Sage, 2010. (in 3 volumes, 1776 pages, ISBN 978-1-4129-6127-1.

Saravanavel, P. Research Methodology (Kitab Mahal,Allahabad, 1987).

Self-study of Practice as a Genre of Qualitative Research - Theory, Methodology, and Practice SPRINGER 978-1-4020-9512-2

Single, P. B. and R. M. Reis, "Demystifying Dissertation Writing : A Streamlined Process from Choice of Topic to Final Text", Stylus, 2009.

Spangenburg , R. and D. K. Moser, The Historyof Science in the Eighteenth Century (UniversityPress, Hyderabad, 1999)

Stake, Robert Earl (1995). The Art Of Case Study Research, Sage Publications, ISBN 080395767X

Steiner, E. (1988). Methodology of Theory Building. Sydney: Educology Research Associates.

Turabian, K. L.; W. C. Booth, G. G. Colomb, J. M. Williams, "A Manual for Writers of Research Papers, Theses, and Dissertations", Seventh Edition, University of Chicago, 2007.

Vogt, W. P. "Quantitative Research Methods for Professionals", Allyn & Bacon, 2006.

Walliman, N. "Your Research Project", Third Edition, Sage, 2011. (Second edition is available in Indian Rupees through Vistaar Publications)

Woods, G. "Research Papers For Dummies", For Dummies/Wiley, 2002.

Yin, R.K. (2002) Case Study Research - Design And Methods. Third edition. Sage Publications, ISBN 0761925538 (first edition was in 1984).

CHEM (IMMT)-1-002 Materials Characterization Technique LTPC: 3-0-2-4

Size and surface area analysis; Interaction of X-rays with matter, diffraction techniques and applications; Optical principles of microscopy; electron diffraction, imaging (various contrasts), determination of crystal structure, burgers vector, electron beam-specimen interactions and other applications of Transmission Electron Microscopy; Applications of Scanning Electron Microscopy and, Electron Probe Micro-Analyser; Principles of Quantitative Microscopy: Overview of other characterization techniques such as Auger electron spectroscopy, Scanning Tunneling Microscopy, Atomic Force Microscopy.

Course Coordinator: Dr. B. K. Mahapatra

200 Level

CHEM (IMMT)-2-001 Advanced Materials Chemistry LTPC: 3-0-2-4

Synthesis and methodology:

Synthesis of various types of materials such as nanomaterials and nanocomposites, functional and layered materials, hybrid materials mesoporous organosilica (PMS), functionalization of mesoporous silica, titania, zirconia, ceria, iron oxide, metal-organic frame work and other oxide, sulphide and phosphate based materials by wet chemical, sol-gel, radiolysis, microwave, combustion, sonochemical, Hydrothermal and solvothermal, template assisted. Nanoparticle fabrications through different phases i.e., nucleation, aggregation, agglomeration, Ostward ripening.

Properties:

Chemical, Structure and texture, optical, magnetic and electronic properties.

Applications:

Catalysis, photocatalysis, electrocatalysis, fuel cells, energy generation and storage, sensors and biosensors, pollution control and abatement.

Course Coordinator: Dr. K. M. Parida

Reference Texts:

Handbook of Layered Materials, S. M. Auerbach, K. A. Carrado, P. K. Dutta , CRC Press; 1 edition (2004) ISBN-13: 978-0824753498

Advanced Catalysts and Nanostructured Materials: Modern Synthetic Methods, W. R. Moser, 2nd Edn, Academic Press, ISBN-13: 978-0125084604

Chemistry of Advanced Materials: An Overview, L. V. Interrante (Ed.), M. J. Hampden-Smith (Ed.), Wiley (1997), ISBN: 978-0-471-18590-1.

Solid State and Materials Chemistry (Second edition) Wiley By Anthony R. West

Principles and Practice of Heterogeneous Catalysis, VCH, Weinheim J. M. Thomas and W.J. Thomas

Introduction to Nanotechnology, Wiley-Interscience, Charles P. Poole, Jr. and Frank J. Owens

Recent trends in Catalysis, Narosa Publishing House, Ed. V. Murugan, B. Arabindoo and M. Palanichamy

Introduction to Surface Chemistry and Catalysis, Wiley Interscience, G.A. Somorjai.

Catalysis and surface characterization, Ed. T. J. Dines, C.H. Rochester and J. Thomson, Royal Society of Chemistry.

Heterogeneous Catalysis by Organic complexes, Vol. II, M.M.T. Khan, A.E. Martell, Academic Press.

Nano Surface Chemistry, Ed. M. Rosoff, Marcel Dekker Inc.

Material Concepts in Surface Reactivity and Catalysis, H. Wise, J. Omdar, Academic Press.

Surface and Nanomolecular Catalysis, Ed. R. Richards, Taylor and Francis

Advanced Materials in Catalysis, Ed. J.J. Burton, R.L. Garten, Academic Press.

Catalysis Science and Technology, ED. J.J. Anderson and M. Boudart, Springer-Verlag.

Photocatalysis Science and Technology, Ed. M. Kaneko and I. Okura, Springer

Fuel Cell Fundamentals, Wiley, 2nd Edn., Ryan O'Hayre, Suk-Won Cha, Whitney Colella and Fritz B. Prinz.

Fuel Cell Science: Theory, Fundamentals and Biocatalysis, Ed. By Andrzej, Wieckowski and Jens K Nørskov, Wiley.

CHEM (IMMT)-2-002 Environmental Science LTPC: 3-0-2-4

Energy and Environment: Basic concepts of energy and environment in mineral, metallurgical and chemical industry

Pollutant source and control: Air, water and solid waste pollution and their control measure.

Cleaner production and life cycle analyses: Reuse/ recycle/ recovery/ source reduction/ raw material substitutions, Basics of EIA and Environmental audit, Public participation in environmental decision making, Life Cycle Analyses, steps and tools, Emerging technologies for sustainable environmental management, Identification and evaluation of emerging environmental issues in air, water, waste water and solid waste.

Biological waste treatment: Qualitative and quantitative characterization of waste, Waste disposal, Principle of Biological treatment like aerobic and anaerobic treatment systems, Suspended and attached Biological waste water treatment system.

Advanced wastewater system: Root zone technology, Wetlands, Centralized versus decentralized systems.

Environmental chemistry: Chemical equilibrium and kinetics fundamentals, Acidity, alkalinity, buffers and buffer intensities, EH-pH diagram, Solubility diagrams, Oxidation and reduction reactions.

Course Coordinator: Dr. G. Roy Chaudhury

Reference Texts:

Modeling of Chemical Kinetics and Reactor Design: A.K. Coker

Chemical Reaction Engineering: O. Levenspiel

Modern Electrochemistry Part-I and II: J.O. Bockris and A.K.N. Reddy

Rate Processes of Extractive Metallurgy: H.Y. Sohn and M.E. Wadsworth

Corrosion Prevention and Protection-Practical solution: V.S. Satri, E. Gali and M. Elboudjaini

Air pollution and Health in rapidly developing countries: G. McGranahan and F. Murray

Water Pollution: B. Allard, O. Hutzinger and D. Barcelo

Encyclopedia of Environmental Science and Engineering: J. R. Pfafflin and E.N. Ziegler

Elements of Environmental Engineering: K.N. Duggal

Handbook of solid waste management and waste minimization technology: N.P. Cherimisinoff

Industrial and Hazardous waste treatment: N.L. Nemerow and A. Dasgupta

Waste water treatment and disposal: Metcalfe and Eddy

300 Level

CHEM (IMMT)-3-001 Advanced Chemistry for Hydro & Electrometallurgy LTPC: 3-0-2-4

Leaching: Atmospheric leaching, Pressure leaching, Bio leaching, Optimisation of process parameters,

Solid liquid separation: Concepts of solid liquid separation, Thickening and thickener design, Counter-current decantation, Flocculation, Filtration and centrifugation,

Solvent Extraction: Basic principle of solvent extraction, Partion coefficient and distribution ratio, Separation coefficient, Types of extractants and extraction mechanism of metals,

Membrane Separation Technique: Salient features of membrane separation, Different types of membrane separation, Supported liquid membrane, Extraction mechanism of liquid membrane, hollow fiber membrane, Reverse osmosis, Nano-filtration, Ultra-filtration,

Transport equations.

Electro Chemistry: Principles of Electrowinning, Effect of impurities on electrowinning, electrorefining, Preparation of energy materials, electro organic Chemicals, Electro-inorganic Chemicals, Fused salt electrolysis.

Course Coordinator: Dr. K. Sarangi

Reference Textbooks:

Hydrometallurgy in extraction processes C.K.Gupta and T.K.Mukherjee, Vol 1 and Vol 2., ISBN No 084936804-9 (Vol 1) and 084936805-7 (Vol 2)

Chemical Hydrometallurgy Theory and Principles, A.R.Burkin, ISBN 1860941842

CHEM (IMMT)-3-002 Advanced Self Study on Special topic 4C

CHEM (IMMT)-4-001 Subject Proposal – I LTPC: 0-1-6-4

CHEM (IMMT)-4-002 Subject Proposal – I LTPC: 0-1-6-4

CHEM (IMMT)-4-002 CSIR-800 Societal Programme LTPC: 0-0-8-4

AcSIR New Courses at CSIR-NCL

200 level courses

CHE(NCL):2-040	Organic Biomolecular Chemistry	2-0-0-2
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300 level courses

CHE(NCL):3-060	Operando Surface Techniques	2-0-0-2
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CHE(NCL):3-061	Chromatographic Techniques	2-0-0-2
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CHE(NCL):3-062	Equilibrium and non-equilibrium statistical mechanics for soft matter	2-0-0-2
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CHE(NCL):3-063	Modern Polymerization Methods for Functional Macromolecules	2-0-0-2
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CHE(NCL):2-040	Organic Biomolecular Chemistry	2-0-0-2
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- Peptidomimetics, Molecular Recognition & Self-assembly
- The Bio-organic Chemistry of Carbohydrates
- Nucleic acids
- Chemistry of Lipids
- Organic Medicinal Chemistry and Drug Discovery Processes
- Bioactive Natural Products

CHE(NCL):3-060	Operando Surface Techniques	2-0-0-2
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- Surface electron spectroscopy techniques: XPS, EELS, XAS
- Surface spectroscopy and microscopy tools for catalysis- applications of XPS, XAS, FT-IR, STM etc in exploring catalysis at nanoscale
- Surface science techniques at operando conditions –bridging the pressure gap
- Electronic structure of surfaces – techniques for probing electronic structure with examples
- Nanoscale catalysis and applications

CHE(NCL):3-061

Chromatographic Techniques

2-0-0-2

- General concepts in column chromatography (band broadening, resolution, theories of chromatography)
- Gas chromatography (column in GC, GC instrumentation, GC detectors)
- Liquid chromatography (retention mechanisms in LC, method development, LC instrumentation and pumps, LC detectors, hyphenated techniques)
- Supercritical fluid chromatography
- Electromigration techniques
- Preparative chromatography
- Chiral separations.

CHE(NCL):3-062 Equilibrium and non-equilibrium statistical mechanics 2-0-0-2
for soft matter

- **Equilibrium Statistical Mechanics**
 - Classical Mechanics
 - Equilibrium Distributions
 - Ergodic Hypothesis
 - Ensembles in Statistical Mechanics
 - Boltzmann Statistics
 - Imperfect Gases: The Virial equations Coefficients
 - Relationship of Thermodynamic Functions to Probability Distribution Functions
 - Static structure factor and direct correlation function.
- **Non-Equilibrium Statistical Mechanics**
 - Linear response theory.
 - Onsagers regression hypothesis
 - Fluctuation dissipation theorem
 - Green-Kubo relation
 - Brownian Motion: The Langevin Equation, Fluctuation-Dissipation Theorem
 - Time-Correlation Function Formalism, Mean square displacement, Velocity Autocorrelation function, Diffusion, friction and Einstein Relationship.

CHE(NCL):3-063

**Modern Polymerization Methods for Functional
Macromolecules**

2-0-0-2

Combination of mechanistically distinct polymerization techniques such as Atom Transfer Radical Polymerization (ATRP), Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide Mediated Polymerization (NMP), Ring Opening Metathesis Polymerization

(ROMP), Living ROP, Metal Catalyzed Polymerization for sequential/tandem polymerization of various incompatible monomers, Heterofunctional initiators, Heterotelechelic polymers.

Incorporation of functionalities into polymers using Click Chemistry, for example azide-alkyne, thiol-ene, thiol-yne, nitroxide-radical, nitrile oxide-alkyne addition, cycloaddition reactions, metal-free click chemistry, imine/hydrazone formation, thiol-disulfide exchange, isocyanate-hydroxyl coupling, photochemical conjugation.

Use of click reactions in combination with above polymerization techniques for synthesis of functional macromolecular architectures such as cyclic polymers, star polymers, graft and brush copolymers, dendritic polymers, linear-dendritic copolymers, cyclic linear copolymers. Polymer origami. Conjugation of biomacromolecules with polymers using click chemistry. Modular transformation of polymers.

Rapid prototyping, electrophoretic casting, electro-spinning. Green strength, drying, binder burnout, green machining, sintering. Sol-gel processing, Thermal and plasma spraying, Thick and thin film coatings – PVD and CVD techniques. Vapor infiltration techniques.

Metals processing: Metal Casting – sand, permanent, pressure, centrifugal and investment processes. Deformation processing - stress during various metal working operations, friction and its role in bulk metal forming operations, microstructural evolution during deformation processing, superplastic forming; Sheet metal forming, enhancement of sheet metal formability; Fundamentals of powder processing of metals, solid and liquid state sintering, driving force and mechanism of sintering

Polymer Processing: Compounding of plastics and rubbers, fabricating processes like compression, transfer, injection and blow moulding, extrusion, calendaring, thermoforming, roto molding, casting, sintering and compaction, dip coating, RTM, RIM, RRIM, post forming and finishing operations.

Composite Processing - Hand lay-up, Filament Winding, Pultrusion, Resin Transfer Molding, Processing Science of Reactive Polymer composites - Process steps for production, Selection of processing conditions Toolings, and equipments, Carbon- Carbon Composites –Processing, thermal and mechanical properties, Quality control

CHE(NIIST):3-364

Advanced Functional Materials

2-0-0-2

Advanced Functional Ceramic Coatings and Thin Films-Co-precipitation, Solgel processing, coating techniques, rheology of coating precursors, functional coatings, wetting and non wetting surfaces, coating characterizations, multilayered coatings, nanocomposites, porous ceramics ceramic membranes, organic-inorganic nano hybrids

Advanced Electronic Ceramics and Applied Superconductors-Dielectric ceramics, microwave ceramics, low k materials, SOFC materials, solid-ionic conductors, phosphor materials, Impedance analysis, varistors, sensors, superconductivity and high temperature ceramic super conductors.

Advanced High Temperature Ceramics-Engineering Ceramics – Properties and applications of Al_2O_3 , SiC, Si_3N_4 , zirconia, mullite, Al_2TiO_5 , rare earth phosphates, B_4C , Cubic Born nitride, thermal shock resistance and super plastic ceramics Functionally Graded Materials, Shape Memory Alloys, Piezoelectric materials, biomimetic functional materials.

CHE(NIIST):3-365

Surface Science and Technology

2-0-0-2

Importance of Surface Science and Technology- Atomic and electronic structure of surfaces - surface degradation of metals, ceramics and polymers and their control measures.

Surface and Coating Technologies-Selection of Coating and Surface Technologies, Surface Coating processes: Electroless deposition- Electro deposition - Chemical vapour deposition - Physical vapour deposition - Thermal spraying - Flame Spraying -Plasma spraying - surface heat treatments and hardening – Carburising – Nitriding -Anodising - Laser surfacing – Sputtering - Ion Plating -Sol-gel Coating - Hot-dip Coating - surface alloying - self-cleaning surfaces - surface functionalization - self assembly - Brazed and welded coating methods - Thin film technologies - Other advanced surface techniques - Testing methods and assessment of coatings - Coatings for Aerospace

structures and components. Surface Coating Materials: Metallic, ceramic, polymer and composite coatings, nanomaterial coatings, superhard and functional and functionally graded coatings.

Corrosion and its control - Corrosion processes, Corrosion problems in the aerospace industry, General corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, influence of deposits and anaerobic conditions, Exfoliation, corrosion. Corrosion control. High temperature oxidation and hot corrosion, Corrosion / mechanical property interactions. Paint and paint systems.

Tribology-Friction, Lubrication and wear of surfaces, coefficient of friction, Types of wear- Abrasive, erosive and sliding wear, interactions between machine parts and environments, failure mechanisms of wear, Interaction between wear and corrosion, Testing methods and control measures of wear.

CHE(NIIST):3-365

ADVANCED DYE-REMOVAL TECHNOLOGIES

1-0-2-2

Introduction, different types of organic synthetic-dyes, their physical and chemical properties, applications, significance of dye-removal technology.

Different methods of dye-removal from aqueous solutions and industry waste-water:

Physical methods, membrane filtration, nano-filtration, reverse osmosis, electrocatalysis, adsorption, different types of adsorbents, adsorption kinetics models, adsorption isotherm models, adsorption capacity, advantages and limitations

Chemicals methods, coagulation, flocculation, flotation, precipitation and filtration, electrofloatation, electrokinetic coagulation, conventional oxidation, oxidizing agents, ozone, hydroxyl radicals, advanced oxidation process, Fenton-reaction, irradiation, photocatalysis, advantages and limitations

Biological methods, fungal decoloration, microbial degradation, adsorption by microbial biomass, bioremediation systems, advantages and limitations

New emerging dye-removal technologies and other recent developments

Experimentation with the selected dye-removal technologies

CSIR-Central Institute of Mining and Fuel Research

BARWA ROAD, DHANBAD, JHARKHAND – 826 015, INDIA

Website: www.cimfr.nic.in

Foreseeing the role of mining in general and coal in particular for the national development and to play a greater role for achieving energy security in the country, *Central Institute of Mining and Fuel Research* (CIMFR), Dhanbad was formed in April 2007 after integrating the core competencies of erstwhile Central Fuel Research Institute (CFRI, established in 1946) and Central Mining Research Institute (CMRI, established in 1956), two national laboratories of CSIR with a mission "*to be a Global Leader and Path Setter in Mining and Fuel Research*". After consolidation, the widened bandwidth of the institute covers the complete mining cycle starting from Coal quality evaluation, Mining (production, productivity, safety and conservation), Processing/beneficiation, Transportation to Utilization including waste disposal and environmental issues.

The Institute has a present strength of 686 manpower, out of which, there are 164 qualified scientists (around 100 Ph.D. holders) working in almost 50 different research areas. The manpower includes a large contingent of experienced mining and chemical engineers, geologists and chemists besides basic science experts and engineers from other disciplines.

Equipped with different national testing facilities and with ISO 9000:2008 accreditation, CSIR-CIMFR extends R&D studies, testing, evaluation, calibration and consultancy services to mining and allied industries to Indian and Overseas Customers. The major test facilities include explosives and accessories, flame proof and intrinsically safe equipment, physico-mechanical properties of coal and rock, mining and allied industrial components for their safe use in mines and other hazardous areas. The institute has a number of pilot plants to study beneficiation, carbonisation, combustion, gasification and liquefaction of coal and testing facilities for determination of coal characteristics and related parameters.

The research areas include methods of mining especially mass production technology, rock mechanics and ground control, design of mining structures including supports, thick and complex seam mining, mine subsidence, hard roof management, slope stability, blasting, stowing, flyash utilization, mine fire evaluation and control, disaster management in mines, EIA/EMP, ventilation planning and design, coastal placer mining, CBM and CMM, resource quality assessment of coal, coal combustion, beneficiation, carbonization, liquefaction, coal biotechnology, clean coal technology, carbon capture & sequestration, minespoil reclamation, and with state-of-art computational facilities. The institute is also actively involved in metal mining, design of hydro-electric projects, underground space technology, socio-economic development of people residing in mining areas, etc.

The institute aims to provide R&D inputs for the entire coal-energy chain from mining to consumption including development of mineral based industries to reach the targeted production for country's energy security and growth with high standards of safety, economy and cleaner environment.

PhD Programme in Science

Broad Research Areas

- ❖ Coal Science and Coal Geology
- ❖ Coal Beneficiation
- ❖ Combustion Science & Technology
- ❖ Gasification
- ❖ Coal Carbonization
- ❖ Coal Liquefaction
- ❖ Coal Biotechnology
- ❖ Environment and Waste Management

Who can apply:

MSc/MTech/ME/MScTech (Chemistry/ Physics/ Geology/ Environmental Science/ Fuel Science/ Soil Science/ Biotechnology/ Life Sciences/ Chemical Engineering/ Petrochemical Engineering/ Mechanical Engineering/ Fuel & Mineral Engineering/ Environmental Engineering/ Metallurgical Engineering) having a valid National level fellowship (JRF/SRF of various funding agencies, e.g. CSIR, UGC, DBT, DST etc.), INSPIRE or other equivalent fellowships.

List of Courses to be Offered to PhD Programme in Science

COURSE CODE	CSIR (CIMFR) 100 level Courses (001 and 002/003 are compulsory)	L-T-P-C
CHE-CIMFR-1-001	Research Methodology	1-0-0-1
CHE-CIMFR-1-002	Analytical Tools and Instrumentation	1-0-0-1
CHE-CIMFR-1-003	Basic Mathematics and Numerical Methods	1-0-0-1
CHE-CIMFR-1-004	Basic Chemistry for Interdisciplinary Sciences	1-0-0-1
COURSE CODE	CSIR (CIMFR) 200 level Courses (003 and 040 are compulsory)	L-T-P-C
CHE-CIMFR-2-003	Advanced Organic Chemistry	2-0-0-2
CHE-CIMFR-2-040	Advanced Coal Science	2-0-0-2
CHE-CIMFR-2-041	Environmental Chemistry	1-0-2-2
COURSE CODE	CSIR (CIMFR) 300 level Courses	L-T-P-C
CHE-CIMFR-3-060	Coal Geology and Organic Petrology	1-0-2-2
CHE-CIMFR-3-061	Analytical Techniques for Coal and Derivatives	1-0-2-2
CHE-CIMFR-3-062	Coal Beneficiation	2-0-2-3
CHE-CIMFR-3-063	Combustion Science and Technology	2-0-2-3
CHE-CIMFR-3-064	Coal Gasification	2-0-2-3
CHE-CIMFR-3-065	Coal to Liquid (CTL) Technology	2-0-2-3
CHE-CIMFR-3-066	Coal Carbonization	2-0-2-3
CHE-CIMFR-3-067	Coal Biotechnology	1-0-2-2
CHE-CIMFR-3-068	Environmental Management in Coal Industry	2-0-0-2
CHE-CIMFR-3-069	Management of Soil, Water & Air Pollution in Coal Industry	1-0-2-2
CHE-CIMFR-3-070	GHG Emission and Clean Development Strategies	2-0-0-2
COURSE CODE	CSIR (CIMFR) 300 level Courses	L-T-P-C
CHE-CIMFR-4-001	Project proposal writing & presentation	0-0-4-2
CHE-CIMFR-4-002	Project proposal writing & presentation	0-0-4-2
CHE-CIMFR-4-003	CSIR-800	0-0-8-4

quality parameters including petrography on combustion, spontaneous combustion of coal. Oxy fuel combustion, co-combustion, chemical looping combustion, super critical and ultra super critical boiler technology. Combustion products- solids and gases, pollution from coal combustion. Ash deposition characteristics, utilization of fly ash, trace and heavy metals pollution from coal combustion.

CHE-CIMFR-3-064 **Coal Gasification** **2-0-2-3**

Course Coordinators: Mr. S. Dutta and Mr. D. Chavan Prakash

Introduction: chemistry of gasification; pyrolysis; char gasification; factors affecting gasification and kinetics; gasification processes; coal properties on gasification; fluidization; fluidized bed gasifier design; types of gasifiers; major gasification technologies; gasification of high ash Indian coals; gasification applications; syn gas cleaning; present status of international and national gasification scenario.

CHE-CIMFR-3-065 **Coal to Liquid (CTL) Technology** **2-0-2-3**

Course Coordinator: Dr. Sudip Maity

Basics of catalysis, different types of Fischer-Tropsch (FT) catalysts, design, development and synthesis of FT catalysts, historical development of CTL Technology, direct liquefaction (Bergius Process); syngas conversions; Indirect Liquefaction (FT Synthesis); FT reactor design and development, modified FT processes, case studies of CTL plants, bench & pilot scale investigations.

CHE-CIMFR-3-066 **Coal Carbonization** **2-0-2-3**

Course Coordinators: Mr. G.K.Bayen and Mr. Manish Kumar

Caking and coking coals; characteristics; significance of proximate analysis and thermal rheological properties; role of macerals; coal blending for coke making; carbonization at various temperature; thermal characteristics of coal and mechanism of coke formation; design and types of coke oven; cooling / quenching of coke; coke oven by-products; pollution in coke industries and its abatement, operation and troubleshooting in coke oven industries; characterization and evaluation of coke; carbonization technology for future generation and utilization of low grade coal for coke making; stamp charging, partial briquette charging, selective crushing.

CHE-CIMFR-3-067 **Coal Biotechnology** **1-0-2-2**

Course Coordinators: Dr. (Mrs). V. Anguselvi and Mr. R. C. Tripathi

Introduction; structure of low rank coal and biomass (lignin & cellulose, hemicellulose etc), microbial techniques; microbial diversity and characteristic features; microbial classification; extremophiles; bioinstrumentation; fermentation technology; microbial physiology; microbial metabolism; microbial genetics; enzyme technology; bioreactors and application; bio-cleaning, bio-desulphurization of coal, bio-methanation and bio-liquefaction of coal, environmental microbial technology; biostatistics.

CHE-CIMFR-3-068 **Environmental Management in Coal Industry** **2-0-0-2**

Course Coordinators: Dr. L. C. Ram and Dr. N K Srivastava

Introduction, global climate change; eutrophication; bioaccumulation; dispersion of pollutants in soil, water and air; Impact of coal mining and coal processing on environment. Acid mine drainage. Carbon capture and sequestration. Mine spoil reclamation and biodiversity conservation. Waste disposal and management. Fly ash generation, characterisation, leaching. Utilisation of fly ash in agriculture; forestry; reclamation of wasteland and low-lying area. Fly ash in cement industry, clay, tiles, brick making, embankment; land/ mine filling. Management

of coal mine spoil, waste dumps, washery rejects, etc. Environmental hazard and risk assessment. Environmental impact assessment, environmental management plan and environmental auditing.

- CHE-CIMFR-3-069** **Management of Soil, Water & Air Pollution in Coal Industry** **1-0-2-2**
Course Coordinators: Mr. R. C. Tripathi and Dr. R. E. Masto
Soil: concept, properties, classification. Soil pollution; soil erosion and conservation; soil quality assessment, reclamation of coal mine spoil. Source and characteristics of wastewater, sampling and analysis, fundamentals of water treatment, physical, chemical and biological processes and design parameters, sludge stabilization, effluent disposal and reuse, Recycling of water in coal washery, recovery of coal fines. Air pollution; sources; abiotic, biotic and gaseous pollutants; air sampling and monitoring techniques; ambient air and stack monitoring; qualitative and quantitative analyses; environmental health hazards; abatement strategies.
- CHE-CIMFR-3-070** **GHG Emission and Clean Development Strategies** **2-0-0-2**
Course Coordinators: Dr. Pinaki Sarkar and Mr. S. Biswas
Kyoto protocol, national and international protocols and guidelines. Climate change issues. Tire-I, Tire-II and Tier - III approach for GHG emission estimates. Estimation of GHGs in mining and industrial sectors; flue gas cleaning. Carbon footprints and carbon market, CO₂-capture & storage. Uncertainties in emission estimates, development of country specific NCV and CEF for different types of coal and lignite. Clean development mechanism (CDM); sectors eligible for CDM; national CDM authority and guidelines.
- CHE-CIMFR-4-001** **Project Proposal Writing & Presentation** **0-0-4-2**
Course Coordinators: Concerned thesis supervisors
Formulation of a project proposal in specified format in a holistic manner preferably candidate's own research work suitable for submission to appropriate funding agencies.
- CHE-CIMFR-4-002** **Project Proposal Writing & Presentation** **0-0-4-2**
Course Coordinators: Concerned thesis supervisors
Formulation of a complete project proposal in specified format on the related sub-areas of candidate's own research work.
- CHE-CIMFR-4-003** **CSIR 800** **0-0-8-2**
Course Coordinators: Dr. M. S. Alam and Dr. Rajesh Kumar
The students have to undertake a project in rural area for 6-8 weeks in line with CSIR- 800 programme which is primarily prepared at empowering 800 million Indians by way of S & T inventions. The theme for the project may be chosen from CSIR-800 document and as per expertise available at CSIR-CIMFR. Students will choose the topics in consultation with Doctoral Advisory Committee (DAC).

100 level courses

001 and 002 are compulsory

CHE-NEIST-1-001

Research Methodology: 1-0-0-1

Good laboratory practices, Safety in the laboratory, First Aid in the laboratory, Maintenance of laboratory records, Scientific literature management, Communication skills (scientific writing and presentation), Intellectual property management & planning, Ethics in Science, Computer applications and tools, Statistical methods & Data analysis

CHE-NEIST-1-002

Analytical Tools and Instrumentation: 1-0-0-1

Thermal methods (TG, DTG, DTA, TMA, DSC), X-ray methods (XRD, XRF, SAXS), NMR (^1H , ^{13}C) and other Spectroscopic methods (EPR, IR, UV, Fluorescence), Chromatographic methods (TLC, GC, LC), Mass spectroscopy, Electron Microscopy (SEM, TEM), Electron Probe Micro Analysis (EDS, WDS), Quantitative Analysis (AAS, ICP, CHN)

CHE-NEIST-1-004* (*Optional course)

Basic Chemistry for Interdisciplinary sciences: 1-0-0-1

Basics of inorganic, organic, physical and biochemistry, Nomenclature (IUPAC), molarity, molality and normality, types of bonding, Ionic, covalent and non-bonding interactions, Acids and bases, Atomic structure, periodic table and periodic properties, stoichiometry, chemical reactions and kinetics, solvent effects, functional groups in organic compounds, general named reactions and reaction mechanisms, carbohydrates, lipids, proteins, nucleotides, enzymes, photosynthesis

CHE-NEIST-1-005* (*Optional course)

Introduction to Nanoscience and Nanotechnology: 1-0-0-1

General considerations, Introduction, definitions, consequences of size reduction, Properties: structural, thermodynamic, optical, electrical and magnetic properties, Methods of synthesis, Surface modifications, factors governing the stability and assembly, Characterization of nanomaterials, Applications of Nanomaterials

CHE-NEIST-1-006* (*Optional course)

Introduction to Chemical Biology: 1-0-0-1

chemical biology/synthetic biology, Structure, function and chemistry of biological macromolecules including amino acids, proteins, nucleic acids and carbohydrates, Chemical kinetics and thermodynamics in biology, Chemical reactions and chemical diversity in Biology The Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Drugs from Nature, Drug interaction

*Optional courses, over and above minimum requirements if required

200 level courses

001/002/003 compulsory (Core)

CHE-NEIST-2-001

Advanced Physical Chemistry: 2-0-0-2

Thermodynamics and chemical kinetics, Quantum Mechanics, Atomic structure and spectroscopy, Chemical bonding in diatomics, Chemical applications of group theory, Colloids and Surface science, surfactants, Interface and Interfacial properties, Electrochemistry.

CHE-NEIST-2-002

Advanced Inorganic Chemistry: 2-0-0-2

Structure & Bonding in Inorganic Compounds, Chemistry of Coordination Compounds, Symmetry in Chemistry & Group Theory, Main group chemistry, Organometallic chemistry, Electronic Spectra of Transition Metal Compounds, Magneto Chemistry, Metal Cluster Compounds, Inorganic Reaction Mechanism, Electron Transfer Reactions in Metal Complexes, Bioinorganic Chemistry (Metalloenzymes, Metal complexes as oxygen carriers, Photosynthesis), Metal Complexes in Medicinal Chemistry, Catalysis by Inorganic Complexes.

CHE-NEIST-2-003

Advanced Organic Chemistry: 2-0-0-2

Stereochemistry, reaction mechanism, C-C and C-X bond formations, Retrosynthetic analysis, photochemistry, pericyclic reactions, reactive intermediates, Methods of asymmetric synthesis and their application in total synthesis, oxidation-reduction reactions, organocatalysis, metathesis reactions.

CHE-NEIST-2-004

Advanced Analytical Chemistry: 2-0-0-2

Analytical instrumentation, signal and noise, Overview of optical methods of analysis: Components of optical instruments, atomic and molecular spectrometry based on absorption, emission and scattering, Electroanalytical techniques (basic electrochemistry, voltammetry, potentiometry), Analytical separations and introduction to chromatographic methods, GC, LC, Mass spectrometry, electromigration techniques, hyphenated techniques, detectors, Analytical tools for petroleum refining.

CHE-NEIST-2-006

Advanced Organometallic Chemistry: 2-0-0-2

Fundamentals, The 18 Valence Electron Rule; Structure and bonding of organometallic complexes using molecular orbital theory.

σ -Donor Ligands: Transition-Metal-Alkyl and -Aryl compounds; σ -Donor/ π -Acceptor Ligands: Transition-Metal-Alkenyl, -Aryl and -Alkynyl Complexes, Transition-Metal-Carbenes (Fischer and Schrock Carbenes); Metal Carbonyl; Structure, properties and principal reaction types of the above complexes; σ , π -Donor/ π -Acceptor Ligands: Olefin Complexes; Alkyne, Allyl and Enyl Complexes, Complexes of the cyclic C_nH_n

Fundamental Mechanism of Organometallic Transformations: Oxidative addition, Migratory Insertion, β -hydride elimination and reductive elimination; Interaction of C-C and C-H σ -bonds with Transition Metals

CHE-NEIST-2-007

Advanced Coordination Chemistry: 2-0-0-2

Naming of coordination compounds, classification of ligands, chelate and macrocyclic effect, Theories dealing with the formation of Coordination Compounds, Spectrochemical Series; Splitting of d-orbitals, Jahn–Teller Effect; Stability constants of Transition metal complexes and their determination by Job's Method. Spin–Orbit Coupling, Electronic states and term symbols, Selection rules (Laporte and spin selection rule), Interpretation of electronic spectra of Transition metal complexes, Orgel and Tanabe Sugano diagrams. Charge Transfer spectra, Magnetic Properties of Transition elements, Chemistry of Inner Transition Elements.

CHE-NEIST-2-009

Advanced Polymer Chemistry: 2-0-0-2

Techniques of polymerization, polymer characterization techniques, Stereochemistry of Polymers, polymer nano-architectures, random and block copolymers, Liquid Crystalline Polymers, Conducting Polymers, Non-linear Polymers, Polymer Blends and Composites, polymer rheology, inorganic, bio and supramolecular polymers

CHE-NEIST-2-010

Advanced Electrochemistry: 2-0-0-2

Basic electrochemistry concepts, Reference electrodes, Electrochemical Thermodynamics, Kinetics of electron transfer, the Taft equation, Diffusion, Double Layers, electrode Kinetics, the Gibbs adsorption isotherm, the Lippmann equation, infinitely dilute solutions and thermal balance, Electro capillary phenomena, Faradaic vs. capacitive currents, transport properties, potential theory, Electrochemical Techniques, Voltammetry, Reversible and irreversible reactions, Mass transport by convection, rotating electrodes, Equivalent circuits, A.C. voltammetry, Electrolysis methods, Adsorption, Thin layer cells, Electrochemistry of polymers and inorganic solids, Spectroelectrochemistry, Applications.

CHE-NEIST-2-011

Advances in Bioinorganic chemistry: 2-0-0-2

Metal ions in biology, structure and function of metallo-proteins and enzymes, Communication role for metals in biology. Heme and non-heme systems with one-, two- or multi-metal, photosynthesis and photosystem II; O₂-binding, reduction to O₂⁻, O₂²⁻, and O²⁻ species their utilization in hydroxylation and epoxidation; nitrogen fixation, water-oxidation reactions. Synthetic models, Correlation with structure and function of the natural enzymes, design and synthesis, mechanisms. Metal based drugs, Porphyrins, Corrins, hydroporphyrins.

CHE-NEIST-2-012

Advances in hydrocarbon chemistry: 2-0-0-2

Chemistry of crude oil, thermal cracking, visbreaking and coking processes, catalytic cracking, hydro cracking and hydrogen production processes, catalytic reforming process, Chemistry and industrial processes for alkylates, isomerisation processes, Petrochemicals, Basic Building blocks; C₁-Chemistry; Petrochemicals from n-paraffins; Petrochemicals from olefins and aromatics; Refinery-Petrochemical Integration, Future Prospects

CHE-NEIST-2-015

Advanced Catalysis: 2-0-0-2

Homogeneous and heterogeneous catalysis, adsorption, diffusion, kinetics, equilibrium and rate expressions; chiral catalysis, Surface Science in Catalysis, Catalytic Materials; Supports; Active Components, Classes of reactions and types of reactors; Catalyst preparation methods; Characterization of catalysts; Catalysis in super critical media; Brief introduction of organo and electrocatalysis; Structure-activity-property-stability of catalysts,

Catalysts in chemical industry, Catalysis in petroleum refining and petrochemicals; Catalysis in the utilization of renewable feed stocks and concepts of sustainable chemistry.

CHE-NEIST-2-016

Advanced Surface Science: 2-0-0-2

Introduction to Surface Science - Surface phenomena - Adsorption, Desorption, Adsorption Models, Special properties of surfaces and interfaces, Electronic structure of surfaces, Surface modification and its applications, Nanoscale catalysis and applications, Surface spectroscopy and microscopy tools for nanocatalysis

CHE-NEIST-2-018

Advanced Materials Characterization Techniques: 2-0-0-2

Optical Microscopy, Electron microscopy: TEM, HRTEM, SEM, STEM, EDX, FIB, e-beam lithography, Scanning probe microscopy: AFM, STM, MFM, confocal, etc, Raman spectroscopy/microscopy, Thermal analysis techniques, Magnetic measurements, Electrical measurements, Spectroscopic ellipsometry.

CHE-NEIST-2-019

Advances in Nanoscience and Nanotechnology: 2-0-0-2

Low-dimensional structures: Quantum wells, Quantum wires, and Quantum dots, Nano clusters & Nano crystals, fullerenes, carbon nano tubes and graphene, Nano Composites, synthesis and characterization techniques, Properties at Nano Scales and comparison with bulk materials, fabrication techniques, general applications, nanomaterials in biology.

CHE-NEIST-2-021

Advances in Chemical Biology: 2-0-0-2

Amino Acids, Peptides & Proteins, Design of poly peptides, Peptide hormones and their pharmaceutical significance, Peptide mimetics as therapeutics, Chemistry of Carbohydrates, Nucleic acids, Structure & function of DNA and RNA, Nucleic acid mimetics & their therapeutic applications, Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Basic principles of medicinal chemistry, Drugs from Nature, Natural products based drug discovery, Kinetics and thermodynamics of biological process, Enzyme Catalysis, consecutive, parallel and competitive reactions in biological systems, Thermodynamics, allosteric effect in biology, types of bonds, hydration and their specific contribution towards specific thermodynamic parameters, enthalpy or entropy, Scatchard analysis, hill plot analysis.

CHE-NEIST-2-024

Sol-gel chemistry: 2-0-0-2

Introduction, Hydrolysis and condensation reactions, Solution chemistry and physics of intermediates, Role of the anion on the hydrolysis and condensation reactions, Kinetics of Hydrolysis and Condensation, Non-Hydrolytic Sol-Gel Processing, Gelation, Ageing, Drying, Densification, Characterization, Chemistry of Sol-Gel Silicates, Solution chemistry of transition metal alkoxide precursors, Sol-gel synthesis and characterization of important materials, structure-property relationships

CHE-NEIST-2-026

Green chemistry: 1-0-0-1

Green chemistry concepts: Basic understanding, scope and interdisciplinary nature of green chemistry; Environmental factors; Carbon credit, Energy efficiency and atom economy, Catalysis and green chemistry, Alternate reaction media and reaction systems, ionic liquids, supercritical fluids, solventless chemistry.

CHE-NEIST-2-027

Coal chemistry: 2-0-0-2

Mining processes, mine safety, Sampling methods of coal and its importance, Coal classification systems, Physical characterization, proximate analysis, Ultimate analysis, Sulphur analysis, Ash fusion temperature, Low temperature Carbonization, Swell Index, Cracking Index, Thermogravimetric analysis etc, Size Reduction and Size Classification of Coal, Structure of coal, Organic functionality of coal, aromatic Index, Mineral matter content, Mineralogy of coal, Geological origin of coal, petrographic analysis, geochemical processes during mining of coals, Coal Utilization, Coal Conversion processes, Other useful products from coal, Environmental Issues, CO₂ sequestration.

CHE-NEIST-2-028

Alternative feedstock options for petrochemicals: 2-0-0-2

Global scenario of Petrochemicals, Renewable resources; categorization of resources; chemicals from edible renewable resource; Chemicals from non-edible renewable resources; Catalytic reactions (mineral acid, bases; enzymes, homogeneous and heterogeneous catalysts); alternate fuels; fuels derived from renewable resources; biodiesel, bioethanol, biobutanol; Hydrogen generation from renewable feed stocks, Conversion of glycerol; Naphtha as a conventional source, Need for sustainability in production of Petrochemicals, Alternate Options; from Refineries sources, Natural Gas/Methane as an Option and other Non Refinery Sources, CO₂ utilization, Identification and Recommendations based on techno-economic analysis for India.

CHE-NEIST-2-029

Natural products: 2-0-0-2

Carbohydrates and polysaccharides, Structure and functions of important derivatives of monosaccharides, Classification and nomenclature and synthesis of some simple Alkaloids; Terpenoids and Steroids such as pinene; Camphor and Cadenine; α -vetinone; Hirsutene and Abietic acid (Terpenoids); Cholesterol; Testosterone and Andestrone (Steroids) etc. isolation and characterization, elucidation of structure-property relationships. Biosynthesis of steroids, terpenoids, fatty acids, alkaloids and polysaccharides, biosynthesis of natural products

CHE-NEIST-2-030

Ionic liquids: 1-0-0-1

Introduction to ionic liquids, ionic liquids vs. molecular solvents/ionic salts (solids), ionic liquids vs. eutectic mixtures, solvent polarities using different spectral techniques (parameters), physicochemical properties of ionic liquids, effect of functional groups on the properties of ionic liquids, surface active ionic liquids, aggregation behavior of ionic liquids, interaction of ionic liquids with different molecular solvents, interaction of ionic liquids with biopolymers, thermodynamics of the binary mixtures of ionic liquids, structure property relationship in ionic liquids.

CHE-NEIST-2-031

Synthetic methods for organic chemists: 2-0-0-2

Formation of carbon-carbon bond employing various kinds of organometallic reagents, C-C double bonds through different reactions, oxidation, reduction through various kinds of reagents, functional group interconversion, by substitution including protection and deprotection, alkylation of enolates, and other carbon nucleophiles, reaction of carbon nucleophiles with carbonyl compounds, electrophilic addition to C-C multiple bonds, reactions of C-C multiple bonds, Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

CHE-NEIST-2-032

Organic reaction mechanisms: 2-0-0-2

Basics, The concept of Aromaticity, How to write an organic reaction mechanism?, Popular name reactions, Reactive intermediates: Generation, stability, structures and reactivity of carbocation, carbanion, carbene, radicals, benzyne, nitrene, Types of mechanism: classification, limitations examples of aliphatic nucleophilic substitution - aliphatic electrophilic substitution - aromatic nucleophilic substitution - aromatic electrophilic Substitution - types of radical reactions - molecular rearrangements oxidation and reduction; Electrophilic reactions-Friedel crafts reaction, Riemer Tiemann reaction, Beckmann rearrangements; nucleophilic reactions- aldol condensation, perkin reaction, benzoin condensation; free radical reaction-halogenation of alkane, addition of HBr on alkene in presence of peroxide; allylic halogenation - using N-Bromo Succinamide (NBS), thermal halogenation of alkene $\text{CH}_3 - \text{CH} = \text{CH}_2$

CHE-NEIST-2-034

Physical organic chemistry: 2-0-0-2

Hammett concepts-Quantitative structure activity relationships, linear free energy relationships, Molecular mechanics, Semi-empirical and *ab initio* molecular theory, Pericyclic Reactions; Substituent Effects; Frontier Molecular Orbitals, HOMO-LUMO Interactions, Aromaticity, Odd and Even Alternant Hydrocarbons, Pericyclic Reactions The Woodward-Hoffman Rules. Free Energy Changes, Transition State Theory, The Eyring Equation, The Mechanistic Significance of Kinetic versus Thermodynamic Control of Organic Reactions, The Hammond Postulate, The Curtin-Hammett Principle; Kinetic Isotope Effects, The Reactivity-Selectivity Principle, Substituent Effects, Absorption of Light by Organic Molecules, Jablonsky Diagrams, Morse Potential Energy Curves, Common Photochemical Reactions, Photocycloadditions.

CHE-NEIST-2-036

Composite materials: 2-0-0-2

Concept of Composite materials, Various types of composites, Classification based on Matrix Material: Organic Matrix composites, Polymer matrix composites (PMC), Carbon matrix Composites or Carbon-Carbon Composites, Metal matrix composites (MMC), Ceramic matrix composites (CMC); Classification based on reinforcements: Fiber Reinforced Composites, Fiber Reinforced Polymer (FRP) Composites, Laminar Composites, Particulate Composites, Reinforcements/Fibers, Types of fibres, Multiphase fibers, Whiskers and Flakes, Mechanical properties of fibres, Processing of Advanced composites, Metal Matrix Composites: Casting – Solid State diffusion technique, Cladding – Hot isostatic pressing; Ceramic Matrix Composites: Liquid Metal Infiltration – Liquid phase sintering; Carbon – Carbon composites: Knitting, Braiding, Weaving; Polymer matrix composites: Preparation of Moulding compounds and prepregs – hand lay up method – Autoclave method – Filament winding method – Compression moulding – Reaction injection moulding, Processing and characteristics of nanocomposites, hybrid composites, functionally graded composites, smart and functional composites.

CHE-NEIST-2-037

Carbon allotropes: 1-0-0-1

Synthesis, characterization, structure, properties and applications of: Diamond, Graphite, Amorphous carbon, Charcoals, Fullerene and related compounds, Carbon nanotubes, Graphene.

CHE-NEIST-2-038**Organic spectroscopy applications: 2-0-0-2**

Mass spectroscopy, IR spectroscopy, Proton magnetic resonance spectroscopy, Structural assignment by employing NMR techniques, Carbon-13 NMR spectroscopy, Introduction COSY, HSQC, HMBC, NOESY, ROESY, Structural elucidation using 2D-NMR methods

CHE-NEIST-2-039**Surface characterization techniques: 2-0-0-2**

XPS, LEED, XAS, SEM, AFM, TEM, NSOM, SPR, SERS, static and dynamic contact angle measurements, Ellipsometry.

CHE-NEIST-2-040**Oil Field Materials and Operations (2-0-0-2)**

- Oil well drilling, Clay based and oil based drilling fluids, clay structure and chemistry, Drilling Chemicals, Oil well cementing, formation of damage, Oil well simulation, Water injection, polymer flooding, Water shut off, EOR Chemicals, Fracturing Chemicals and Materials, Environmental aspects related to oil field.

300 Level courses

CHE-NEIST-3-005

Computer aided drug design: 2-0-0-2

Definition of a drug molecule and factor affecting their biological activity, definition of chemotherapeutic index, therapeutic index, design of a drug molecule and relationship of functional groups, discovery of new drugs: drug discovery without a lead, lead discovery, random screen, non-random screen, concept of absorption, distribution, metabolism, and excretion (ADME), drug receptors, physicochemical properties, mechanism of a drug action, stereochemistry and drug action, synthetic and natural drugs and their modifications to increase oral bioavailability, chirality and drug action, bioisosterism, drug receptor-interactions, topographical and stereo-chemical considerations, concept of drug resistance, drug synergism, enzyme inhibition and activation, molecular modeling and *insilico* drug design, concept of structure-activity relationship(SAR) and quantitative structure-activity relationship (QSAR), Lipinski rule of five, mechanism of action of some important drug molecules.

CHE-NEIST-3-008

Carbohydrate chemistry: 2-0-0-2

Mono and disaccharides, polysaccharides, Bacterial polysaccharides, starch and cellulose, derivatives of cellulose, Protecting groups, Glycosylation reactions, Dynamics and interactions, carboxy methyl cellulose and gun cotton, structure, Conformational analyses, glycoconjugates, Immunology of carbohydrates.

CHE-NEIST-3-013

Total Synthesis: 1-0-0-1

Synthesis of complex organic molecules – planning and execution; Concepts of Retrosynthetic Analysis and Total synthesis of Natural products; Retrosynthesis; Disconnection; Synthons; Linear and Convergent Synthesis; Photochemistry in total synthesis; MCRs in total synthesis; Breakthrough synthesis – past and present.

CHE-NEIST-3-014

Asymmetric Synthesis: 1-0-0-1

Strategies for the preparation of optically pure compounds; Stereoselective, Enantioselective and Diastereoselective reactions; Stoichiometric asymmetric synthesis- chiral auxiliaries, Evans Aldol and modified versions; Catalytic asymmetric synthesis; Asymmetric Dihydroxylation; Asymmetric Aminohydroxylation; Asymmetric Hydrogenation; Asymmetric allylation, propargylation, and alkylation; Chiral Organocatalysis; Cascade reactions by organocatalysis; Transition Metal based catalysis; Asymmetric amplification and autocatalysis.

CHE-NEIST-3-015

Chemistry and biology of Heterocycles: 2-0-0-2

Privileged heterocycles, Electronic properties, reactivity (electrophilicity and nucleophilicity), Synthetic methodologies, Biological properties of Natural products and drug candidates, Biosynthesis, Dimeric compounds and related stereochemistry

CHE-NEIST-3-017**Fluoro organic chemistry: 2-0-0-2**

Importance of fluorine in organic compounds, Strategies to introduce fluorine/ trifluoromethyl group into organic molecules, Preparation of fluorinated reagents, Preparation of fluorinated carbon materials and their uses, Known fluorinated drugs and their mode of action, Overview on CFCs, HCFCs, HFCs, their preparation and applications, Halon substitutes, Harmful effects of fluorine and inorganic fluorides

CHE-NEIST-3-019**Nutraceuticals: 2-0-0-2**

Raw material preparation, and characterization, extraction of valuable biomolecules, characterization of these molecules with stability study, preparation and formulations for functional foods. Characterization and stability study of nutraceuticals, properties and stability packaging of nutraceuticals.

CHE-NEIST-3-023**Homogeneous Catalysis: 1-0-0-1**

Organometallic Catalysis, Applications in organic synthesis: Olefin Isomerization, C-C Coupling reactions: Heck, Suzuki, Stille and Sonogashira reactions, Alkene and Alkyne Metathesis, C-Heteroatom coupling: Hydroamination, Olefin Oxidation, C-H activation, Oxidation reactions, hydrogenation of Alkenes, Industrial Applications.

CHE-NEIST-3-025**Catalysis for organic synthesis: 1-0-0-1**

A background on fine and specialty chemicals in chemical industry; Concept of atom economy; Homogeneous and heterogeneous catalytic reactions: hydrogenation, hydrogenolysis, dehydrogenation, selective oxidation, alkylation & acylation, isomerization and C-C bond forming reactions, Enzyme catalysis in organic synthesis; Reaction mechanisms

CHE-NEIST-3-029**Functional Ceramics: 1-0-0-1**

Advanced Electronic Ceramics, high temperature ceramic super conductors, Dielectric ceramics, microwave ceramics, low k materials, SOFC materials, solid-ionic conductors, phosphor materials, Impedance analysis, varistors, sensors, ceramic magnets, thermal shock resistance and super plastic ceramics.

CHE-NEIST-3-031**Porous structures: 2-0-0-2**

Definitions, Micro-Porous and Mesoporous Solids, Structural Chemistry of Zeolite Framework Types, MOFs, COFs, Synthesis, Structure Determination, Role of the Structure-directing Agents, The Chemistry of Microporous Framework Solids, Adsorption and Diffusion, Catalytic Applications, hydrogen storage, separation, CO₂ sequestration, sensors,

CHE-NEIST-3-035**Alternate energy materials: 2-0-0-2**

Energy scenario, Non-renewable and renewable energy sources; description of renewable sources and their importance. Technologies for biomass energy conversion, Solar energy, Wind Turbines, Geothermal Technologies; Applications; Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.

CHE-NEIST-3-040

Natural gas to liquid fuels: 2-0-0-2

generation processes; SMR; POx; ATR; DMR and Tri reforming, Syngas conversion processes; FT Synthesis, LTFT, HTFT, Low Pressure versus high pressure FT, Syn-crude up gradation by hydrocracking, methanol synthesis, chemistry of the processes; catalysts, development in reactors; tubular; multitubular; fixed bed; fluidized bed; FFB; CFB, SBCR, variables affecting SCBR, Commercial Processes; MTO; UOP/Hydro MTO; Exxon Mobil MTO; Lurgi MTP, DME Synthesis, status and prospects of DME production; Challenges for DME commercialization, commercialization activities of GTL plants, SSPD, SMDS, AGC- 21 and Gasel Processes.

CHE-NEIST-3-042

Block copolymers: 2-0-0-2

Chain and controlled block copolymerization, monomer reactivity ratios, Copolymer compositions, molecular architecture, blends, grafts, melts, self assembly and phase separation, phase diagram, range of applicability of copolymerization equation; types of copolymerization; Block copolymers with controlled molecular weight, Living Polymerization, block copolymer synthesis, characterization techniques, block copolymers for biomedical and industrial applications, Amphiphilic block copolymer micelles, Block copolymer thin films.

CHE-NEIST-3-045

Conducting polymers: 1-0-0-1

Synthesis and characterization, electrical transport properties, theory of conductivity, doping, electrochromic properties, Classification and types of organic conductors, Structure and properties of conducting charge-transfer salts, Conducting polymers based on organometallic compounds, Applications of conducting polymers, EMI shielding, supercapacitors, sensors

CHE-NEIST-3-046

Polymers and Colloidal Solutions: 2-0-0-2

Intermolecular forces and potentials, Overview of Statistical physics, DLVO theory, charged colloids, Poisson Boltzmann theory, Debye radius, Bjerrum length, electrophoresis, zeta potential, diffusion, Hydrodynamic interactions. Brief overview of Phase transitions in hard sphere colloids, Random walk, self avoiding random walk, flexible polymers, persistence length, Excluded volume interactions, Polymer solutions in the dilute limit/semi-dilute limit, Entropy of mixing, theta temperature, rubber elasticity, Polyelectrolytes, polymer at surfaces: Brushes, polymer dynamics.

CHE-NEIST-3-047

Biodegradable polymers: 2-0-0-2

Polymers from biomass, microbial production, synthetic polymers, structure and properties, Biodegradation mechanism, measurement techniques, processing techniques, sterilization and storage, global standards, market potential, applications.

CHE-NEIST-3-048

Controlled Radical/Living Polymerizations and Macromolecular Architectures: 2-0-0-2

Controlled or Living Radical Polymerization, TEMPO-mediated polymerization and atom Transfer radical Polymerization (ATRP), Kinetics of ATRP, Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide mediated polymerization (NMP), Ring opening Metathesis polymerization (ROMP), living ROP, Macromolecular architectures using controlled living polymerizations

CHE-NEIST-3-051**X-Ray Diffraction and Structure of Solids: 2-0-0-2**

Introduction to X-ray crystallography, Crystal growth, evaluation and mounting, Symmetry and space group determination, Background theory for data collection, Data collection using four-circle diffractometers, Area detectors, Crystal lattices, Structure factors, Crystal symmetry, Structure solutions, Structure refinement, An introduction to maximum entropy, Least squares fitting of parameters, Practical aspects of structure refinement, Crystallographic Database, Structure solution from Powder Diffraction Data

CHE-NEIST-3-052**NMR spectroscopy: 2-0-0-2**

Quantum Mechanics of NMR, Multinuclear NMR spectroscopy, Periodic table of NMR, Heteronuclear double resonance experiments, Magnetization transfer and signal enhancement, NMR of diamagnetic and paramagnetic compounds, Multidimensional NMR: 2D NMR, 1H-1H correlations, Heteronuclear Correlation Spectroscopy, 2D Exchange (EXSY), 2D NOESY, ROESY, DOSY Structure elucidation of small molecules, NMR of macromolecules, Multidimensional NMR Spectra, NMR Spectroscopy of Solids, 2D experiments in solids, semi rigid systems: HR MAS, Magnetic Resonance Imaging: In Vivo NMR, Imaging, MRI, functional MRI, NMR imaging of materials.

CHE-NEIST-3-056**Natural products and drug discovery: 2-0-0-2**

Natural products: Importance, lead, clinical trials in drug discovery research, Case studies of marketed natural product drugs, Synthetic Biology and Genetic engineering in the production of natural product, A brief overview of drug discovery approach, Cause of diseases, Target identification, Target validation, Modeling, Synthesis and SAR, Drug Delivery, Clinical Trials, Etiology, pathogenesis, prevention, drug targets and chemotherapy, drug resistance and remedies of tropical infectious diseases, Etiology and remedies of diseases developed through metabolic disorders.

400 level courses

Compulsory courses

CHE-NEIST-4-001

Project proposal writing & presentation: 0-0-4-2

CHE-NEIST-4-002

Project proposal writing & presentation: 0-0-4-2

CHE-NEIST-4-003

CSIR-800: 0-0-8-4

Central Drug Research Institute CSIR, Lucknow



AcSIR Ph.D. Program
Coursework under Chemical Science

Part A - CHE-CDRI-LEVEL-100 (2 Credits)

Course Title	Category	Code	L-T-P-C
Research Methodology	Compulsory	CHE-CDRI-1-001	1-0-0-1
Analytical Tools and Instrumentation	Compulsory	CHE-CDRI-1-002	1-0-0-1
Basic Chemistry for Interdisciplinary Sciences	Optional	CHE-CDRI-1-004	1-0-0-1
Introduction to Chemical Biology	Optional	CHE-CDRI-1-006	1-0-0-1

***Optional Courses, over and above minimum requirements if required

Part B - CHE-CDRI-LEVEL-200 (6 Credits)

Course Title	Category	Code	L-T-P-C
Advanced Organic Chemistry	Compulsory	CHE-CDRI-2-003	2-0-0-2
Advanced process chemistry	Optional	CHE-CDRI-2-013	2-0-0-2
Advances in Chemical Biology	Optional	CHE-CDRI-2-021	2-0-0-2
Natural Products	Optional	CHE-CDRI-2-029	2-0-0-2
Synthetic Methods for Organic Chemists	Optional	CHE-CDRI-2-031	2-0-0-2
Organic Spectroscopy Applications	Optional	CHE-CDRI-2-038	2-0-0-2

Part C - CHE-CDRI-LEVEL-300 (4 Credits)

Course Title	Category	Code	L-T-P-C
Molecular Modeling and Simulation	Optional	CHE-CDRI-3-004	2-0-0-2
Asymmetric Synthesis	Optional	CHE-CDRI-3-014	1-0-0-1
Chemistry and Biology of Heterocycles	Optional	CHE-CDRI-3-015	2-0-0-2
Homogenous Catalysis	Optional	CHE-CDRI-3-023	1-0-0-1
Natural Products and Drug Discovery	Optional	CHE-CDRI-3-056	2-0-0-2
Green and Sustainable Chemistry	Optional	CHE-CDRI-3-060	2-0-0-2

Part D - CHE-CDRI-Level-400 (8 Credits)

Course Title	Category	Code	L-T-P-C
Project Proposal Writing and Presentation	Compulsory	CHE-CDRI-4-001	0-0-4-2
Project Proposal Writing and Presentation	Compulsory	CHE-CDRI-4-002	0-0-4-2
CSIR-800 Programme	Compulsory	CHE-CDRI-4-003	0-0-8-4

L= Lecture per Week; T= Tutorial; P= Practical; C= Credit

CHE-CDRI-2-031

Synthetic methods for organic chemists

2-0-0-2

Formation of carbon-carbon bond employing various kinds of organometallic reagents, C-C double bonds through different reactions, oxidation, reduction through various kinds of reagents, functional group interconversion, by substitution including protection and deprotection, alkylation of enolates, and other carbon nucleophiles, reaction of carbon nucleophiles with carbonyl compounds, electrophilic addition to C-C multiple bonds, reactions of C-C multiple bonds, Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

CHE-CDRI-2-038

Organic spectroscopy applications

2-0-0-2

Mass spectroscopy, IR spectroscopy, Proton magnetic resonance spectroscopy, Structural assignment by employing NMR techniques, Carbon-13 NMR spectroscopy, Introduction COSY, HSQC, HMBC, NOESY, ROESY, Structural elucidation using 2D-NMR methods

CHE-CDRI-3-056

Natural products and drug discovery

2-0-0-2

Natural products: Importance, lead, clinical trials in drug discovery research, Case studies of marketed natural product drugs, Synthetic Biology and Genetic engineering in the production of natural product, A brief overview of drug discovery approach, Cause of diseases, Target identification, Target validation, Modeling, Synthesis and SAR, Drug Delivery, Clinical Trials, Etiology, pathogenesis, prevention, drug targets and chemotherapy, drug resistance and remedies of tropical infectious diseases, Etiology and remedies of diseases developed through metabolic disorders.

CHE-CDRI-3-060

Green and Sustainable Chemistry

2-0-0-2

Introduction to green chemistry (Concept of Atom Economy), Principles, plans and benefit, Tools of green chemistry, Name reactions using green chemistry concept, Asymmetric green chemistry, Raw materials diversification, Energy production, Waste reduction at source, Direct and Indirect utilisation of CO₂, Biomass exploitation

400 level courses

Compulsory courses

CHE-CDRI-4-001	Project proposal writing & presentation	0-0-4-2
CHE-CDRI-4-002	Project proposal writing & presentation	0-0-4-2
CHE-CDRI-4-003	CSIR-800	0-0-8-4

Fundamental Mechanism of Organometallic Transformations: Oxidative addition, Migratory Insertion, β -hydride elimination and reductive elimination; Interaction of C-C and C-H σ -bonds with Transition Metals

CHE-CLRI -207 **Advanced Coordination Chemistry** **2-0-0-2**

Naming of coordination compounds, classification of ligands, chelate and macrocyclic effect, Theories dealing with the formation of Coordination Compounds, Spectrochemical Series; Splitting of d-orbitals, Jahn–Teller Effect; Stability constants of Transition metal complexes and their determination by Job's Method. Spin–Orbit Coupling, Electronic states and term symbols, Selection rules (Laporte and spin selection rule), Interpretation of electronic spectra of Transition metal complexes, Orgel and Tanabe Sugano diagrams. Charge Transfer spectra, Magnetic Properties of Transition elements, Chemistry of Inner Transition Elements.

CHE-CLRI -208 **Advanced Photochemistry** **2-0-0-2**

Introduction to photochemistry, excited state processes, fluorescence and phosphorescence, quantum yields, charge-transfer spectra, solvatochromism, photochromism, transient absorption techniques, Luminescence emission lifetimes, two- and multiphoton processes, photoinduced energy and electron transfer, FRET, fluorescence polarization, excimers, exciplexes, delayed fluorescence, Photochemistry of Organic chromophores. Photochemistry in organized and confined media.

CHE-CLRI -209 **Advanced Polymer Chemistry** **2-0-0-2**

Techniques of polymerization, polymer characterization techniques, Stereochemistry of Polymers, polymer nano-architectures, random and block copolymers, Liquid Crystalline Polymers, Conducting Polymers, Non-linear Polymers, Polymer Blends and Composites, polymer rheology, inorganic, bio and supramolecular polymers

CHE-CLRI -210 **Advanced Electrochemistry** **2-0-0-2**

Basic electrochemistry concepts, Reference electrodes, Electrochemical Thermodynamics, Kinetics of electron transfer, the Taft equation, Diffusion, Double Layers, electrode Kinetics, the Gibbs adsorption isotherm, the Lippmann equation, infinitely dilute solutions and thermal balance, Electro capillary phenomena, Faradaic vs. capacitive currents, transport properties, potential theory, Electrochemical Techniques, Voltammetry, Reversible and irreversible reactions, Mass transport by convection, rotating electrodes, Equivalent circuits, A.C. voltammetry, Electrolysis methods, Adsorption, Thin layer cells, Electrochemistry of polymers and inorganic solids, Spectroelectrochemistry, Applications.

CHE-CLRI -211 **Advances in Bioinorganic chemistry** **2-0-0-2**

Metal ions in biology, structure and function of metallo-proteins and enzymes, Communication role for metals in biology. Heme and non-heme systems with one-, two- or multi-metal, photosynthesis and photosystem II; O_2 -binding, reduction to O_2^- , O_2^{2-} , and O^{2-} species their utilization in hydroxylation and epoxidation; nitrogen fixation, water-oxidation reactions. Synthetic models, Correlation with structure and function of the natural enzymes, design and synthesis, mechanisms. Metal based drugs, Porphyrins, Corrins, hydroporphyrins.

CHE-CLRI -212 **Advances in hydrocarbon chemistry** **2-0-0-2**

Chemistry of crude oil, thermal cracking, visbreaking and coking processes, catalytic cracking, hydro cracking and hydrogen production processes, catalytic reforming process, Chemistry and industrial processes for alkylates, isomerisation processes, Petrochemicals, Basic Building blocks; C_1 -Chemistry; Petrochemicals from n-paraffins; Petrochemicals from olefins and aromatics; Refinery-Petrochemical Integration, Future Prospects

- CHE-CLRI -213** **Advanced process chemistry** **2-0-0-2**
Integral and Differential analysis; Evaluation of rate equations, unit processes, mass transfer, mass balance, energy balance, fluid flow, Design of homogeneous systems, different types of reactors, green chemistry
- CHE-CLRI -214** **Advanced Materials Science** **2-0-0-2**
Crystal systems and space groups, Close packing and various simple structure types like AB, AB₂, AB₃ and complex structural types ABX₃, AB₂X₄, etc. Factors affecting crystal structures, Common preparative methods; X-ray diffraction and Electron microscopy, Defect structures, colour centers, reciprocal lattices, Properties of solids – Band theory, metals, insulators, semiconductors, dielectric and ferroelectric properties, magnetic properties, optical properties, ionic conduction; structure-processing-property correlations.
- CHE-CLRI -215** **Advanced Catalysis** **2-0-0-2**
Homogeneous and heterogeneous catalysis, adsorption, diffusion, kinetics, equilibrium and rate expressions; chiral catalysis, Surface Science in Catalysis, Catalytic Materials; Supports; Active Components, Classes of reactions and types of reactors; Catalyst preparation methods; Characterization of catalysts; Catalysis in super critical media; Brief introduction of organo and electrocatalysis; Structure-activity-property-stability of catalysts, Catalysts in chemical industry, Catalysis in petroleum refining and petrochemicals; Catalysis in the utilization of renewable feed stocks and concepts of sustainable chemistry.
- CHE-CLRI -216** **Advanced Surface Science** **2-0-0-2**
Introduction to Surface Science - Surface phenomena - Adsorption, Desorption, Adsorption Models, Special properties of surfaces and interfaces, Electronic structure of surfaces, Surface modification and its applications, Nanoscale catalysis and applications, Surface spectroscopy and microscopy tools for nanocatalysis
- CHE-CLRI -217** **Advanced Separation Science and Technology** **2-0-0-2**
Resins and membranes for separations, Classification of membranes; electromembrane Processes; Ion-exchange membranes and their applications, Electrodialysis and related processes. Polymer electrolyte membrane and their applications for fuel cells; Water electrolyzer for hydrogen production; Reverse electrodialysis for non-renewable energy from concentration gradient, reverse osmosis, nanofiltration, ultrafiltration, pervaporation and gas separation: Membrane fouling, concentration polarization and other limitations of Pressure-driven membrane technologies.
- CHE-CLRI -218** **Advanced Materials Characterization Techniques** **2-0-0-2**
Optical Microscopy, Electron microscopy: TEM, HRTEM, SEM, STEM, EDX, FIB, e-beam lithography, Scanning probe microscopy: AFM, STM, MFM, confocal, etc, Raman spectroscopy/microscopy, Thermal analysis techniques, Magnetic measurements, Electrical measurements, Spectroscopic ellipsometry.
- CHE-CLRI -219** **Advances in Nanoscience and Nanotechnology** **2-0-0-2**
Low-dimensional structures: Quantum wells, Quantum wires, and Quantum dots, Nano clusters & Nano crystals, fullerenes, carbon nano tubes and graphene, Nano Composites, synthesis and characterization techniques, Properties at Nano Scales and comparison with bulk materials, fabrication techniques, general applications, nanomaterials in biology.
- CHE-CLRI -220** **Advances in soft matter chemistry** **2-0-0-2**
Condensed Matter, Colloids, Characterization of colloids by light scattering and electric-field based techniques, Micelles, Self-assembled systems, Molecular gels, Lyotropic liquid crystalline phases, One-, Two- and Three-dimensionally ordered phases, Thermotropic Liquid crystals textures and their identification, characterization of mesophases, Description of order parameter, Phase transitions.

- CHE-CLRI -221** **Advances in Chemical Biology** **2-0-0-2**
Amino Acids, Peptides & Proteins, Design of poly peptides, Peptide hormones and their pharmaceutical significance, Peptide mimetics as therapeutics, Chemistry of Carbohydrates, Nucleic acids, Structure & function of DNA and RNA, Nucleic acid mimetics & their therapeutic applications, Chemistry of Enzymes, Lipids, Fats & Steroids, Drug discovery, Basic principles of medicinal chemistry, Drugs from Nature, Natural products based drug discovery, Kinetics and thermodynamics of biological process, Enzyme Catalysis, consecutive, parallel and competitive reactions in biological systems, Thermodynamics, allosteric effect in biology, types of bonds, hydration and their specific contribution towards specific thermodynamic parameters, enthalpy or entropy, Scatchard analysis, hill plot analysis.
- CHE-CLRI -222** **Advanced Biomaterials** **2-0-0-2**
Definition of biomaterials, Surface property requirements of biomaterials, Types of materials used in medicine, Synthesis and surface characterization, Biology of wound healing, foreign body response and tissue remodeling, Molecular and cellular interactions of materials with biological environment, Degradation and long term fate of materials used in medicine, Requirements of biomaterials for biomedical implants, surface coatings, wound dressings, sutures, cardiovascular devices, ophthalmology, dentistry, orthopedics and cosmetic surgeries, Applications in drug delivery and tissue engineering, Standard protocols for testing the efficacy and efficiency of biomaterials, The regulatory environment for biomaterials, Some concepts for design development of common biomaterials.
- CHE-CLRI -223** **Rare Earth Chemistry** **2-0-0-2**
Lanthanides and actinides, Electronic structure, periodic properties, extraction, separation, solution chemistry, coordination compounds, spectroscopy, luminescence, magnetism, dyes and pigments, trans-uranium elements, nuclear technology, displays and energy related applications.
- CHE-CLRI -224** **Sol-gel chemistry** **2-0-0-2**
Introduction, Hydrolysis and condensation reactions, Solution chemistry and physics of intermediates, Role of the anion on the hydrolysis and condensation reactions, Kinetics of Hydrolysis and Condensation, Non-Hydrolytic Sol-Gel Processing, Gelation, Ageing, Drying, Densification, Characterization, Chemistry of Sol-Gel Silicates, Solution chemistry of transition metal alkoxide precursors, Sol-gel synthesis and characterization of important materials, structure-property relationships
- CHE-CLRI -225** **Combinatorial chemistry** **1-0-0-1**
Principles and techniques of combinatorial chemistry, Popular organic reactions in combinatorial chemistry. solid-phase organic synthesis, Solution-phase parallel synthesis, mixture-based compound libraries, principles of compound library design, natural product and natural product-like libraries, case studies of combinatorial chemistry in drug discovery
- CHE-CLRI -226** **Green chemistry** **1-0-0-1**
Green chemistry concepts: Basic understanding, scope and interdisciplinary nature of green chemistry; Environmental factors; Carbon credit, Energy efficiency and atom economy, Catalysis and green chemistry, Alternate reaction media and reaction systems, ionic liquids, supercritical fluids, solventless chemistry.
- CHE-CLRI -229** **Natural products** **2-0-0-2**
Carbohydrates and polysaccharides, Structure and functions of important derivatives of monosaccharides, Classification and nomenclature and synthesis of some simple Alkaloids; Terpenoids and Steroids such as pinene; Camphor and Cadenine; α -vetinone; Hirsutene and Abietic acid (Terpenoids); Cholesterol; Testosterone and Andestrone (Steroids) etc.

isolation and characterization, elucidation of structure-property relationships. Biosynthesis of steroids, terpenoids, fatty acids, alkaloids and polysaccharides, biosynthesis of natural products

CHE-CLRI -230 **Ionic liquids** **1-0-0-1**

Introduction to ionic liquids, ionic liquids vs. molecular solvents/ionic salts (solids), ionic liquids vs. eutectic mixtures, solvent polarities using different spectral techniques (parameters), physicochemical properties of ionic liquids, effect of functional groups on the properties of ionic liquids, surface active ionic liquids, aggregation behavior of ionic liquids, interaction of ionic liquids with different molecular solvents, interaction of ionic liquids with biopolymers, thermodynamics of the binary mixtures of ionic liquids, structure property relationship in ionic liquids.

CHE-CLRI -231 **Synthetic methods for organic chemists** **2-0-0-2**

Formation of carbon-carbon bond employing various kinds of organometallic reagents, C-C double bonds through different reactions, oxidation, reduction through various kinds of reagents, functional group interconversion, by substitution including protection and deprotection, alkylation of enolates, and other carbon nucleophiles, reaction of carbon nucleophiles with carbonyl compounds, electrophilic addition to C-C multiple bonds, reactions of C-C multiple bonds, Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

CHE-CLRI -232 **Organic reaction mechanisms** **2-0-0-2**

Basics, The concept of Aromaticity, How to write an organic reaction mechanism?, Popular name reactions, Reactive intermediates: Generation, stability, structures and reactivity of carbocation, carbanion, carbene, radicals, benzyne, nitrene, Types of mechanism: classification, limitations examples of aliphatic nucleophilic substitution - aliphatic electrophilic substitution - aromatic nucleophilic substitution - aromatic electrophilic Substitution - types of radical reactions - molecular rearrangements oxidation and reduction; Electrophilic reactions-Friedel crafts reaction, Riemer Tiemann reaction, Beckmann rearrangements; nucleophilic reactions- aldol condensation, perkin reaction, benzoin condensation; free radical reaction-halogenation of alkane, addition of HBr on alkene in presence of peroxide; allylic halogenation - using N-Bromo Succinamide (NBS), thermal halogenation of alkene $\text{CH}_3 - \text{CH} = \text{CH}_2$

CHE-CLRI -233 **Dyes and pigments** **1-0-0-1**

Colour and constitution, chromogen and chromophore. Classification of dyes based on structure and mode of dyeing, Chemistry of some important dyes, NIR reflecting dyes, Dyes for solar cells

CHE-CLRI -234 **Physical organic chemistry** **2-0-0-2**

Hammett concepts-Quantitative structure activity relationships, linear free energy relationships, Molecular mechanics, Semi-empirical and *ab initio* molecular theory, Pericyclic Reactions; Substituent Effects; Frontier Molecular Orbitals, HOMO-LUMO Interactions, Aromaticity, Odd and Even Alternant Hydrocarbons, Pericyclic Reactions The Woodward-Hoffman Rules. Free Energy Changes, Transition State Theory, The Eyring Equation, The Mechanistic Significance of Kinetic versus Thermodynamic Control of Organic Reactions, The Hammond Postulate, The Curtin-Hammett Principle; Kinetic Isotope Effects, The Reactivity-Selectivity Principle, Substituent Effects, Absorption of Light by Organic Molecules, Jablonsky Diagrams, Morse Potential Energy Curves, Common Photochemical Reactions, Photocycloadditions.

CHE-CLRI -235 **Thermodynamics and Statistical Mechanics** **2-0-0-2**

Introduction: Thermodynamics – A Macroscopic Theory of Matter; Laws of Thermodynamics, Ideal Gas Laws, Specific Heat Capacities; Concept of Free Energy, Hamiltonian Mechanics, Equilibrium Distributions and Ergodic Hypothesis, Ensembles, Thermodynamic Functions and the Distribution Function, $g(r)$, Imperfect Gases, Kinetic Theory of Gases, Time Dependent Processes, Phase Transitions

CHE-CLRI -236 **Composite materials** **2-0-0-2**

Concept of Composite materials, Various types of composites, Classification based on Matrix Material: Organic Matrix composites, Polymer matrix composites (PMC), Carbon matrix Composites or Carbon-Carbon Composites, Metal matrix composites (MMC), Ceramic matrix composites (CMC); Classification based on reinforcements: Fiber Reinforced Composites, Fiber Reinforced Polymer (FRP) Composites, Laminar Composites, Particulate Composites, Reinforcements/Fibers, Types of fibres, Multiphase fibers, Whiskers and Flakes, Mechanical properties of fibres, Processing of Advanced composites, Metal Matrix Composites: Casting – Solid State diffusion technique, Cladding – Hot isostatic pressing; Ceramic Matrix Composites: Liquid Metal Infiltration – Liquid phase sintering; Carbon – Carbon composites: Knitting, Braiding, Weaving; Polymer matrix composites: Preparation of Moulding compounds and prepregs – hand lay up method – Autoclave method – Filament winding method – Compression moulding – Reaction injection moulding, Processing and characteristics of nanocomposites, hybrid composites, functionally graded composites, smart and functional composites.

CHE-CLRI -238 **Organic spectroscopy applications** **2-0-0-2**

Mass spectroscopy, IR spectroscopy, Proton magnetic resonance spectroscopy, Structural assignment by employing NMR techniques, Carbon-13 NMR spectroscopy, Introduction COSY, HSQC, HMBC, NOESY, ROESY, Structural elucidation using 2D-NMR methods

CHE-CLRI -239 **Surface characterization techniques** **2-0-0-2**

XPS, LEED, XAS, SEM, AFM, TEM, NSOM, SPR, SERS, static and dynamic contact angle measurements, Ellipsometry.

properties, Prediction of properties of organic molecules and polymers, Introduction to Multiscale Modeling and Simulations and applications. Monte Carlo simulation in various ensembles, Gas sensing properties of various porous materials using grand canonical Monte Carlo method, Dissipative particle dynamics, Mesoscale dynamics and applications.

CHE-CLRI -307 **Multiphase reaction kinetics** **1-0-0-1**

Mass transfer theories, Multi phase reactors, Multi phase reactors selection criteria; Mass transfer coupled with chemical reaction; measurement of gas-liquid parameters, Reaction in porous catalysts; effective diffusivity and structure of porous catalysts, Important design parameters for gas-liquid and solid reactors, Reactor modeling in petroleum refining industry, Modeling of catalytic sweetening, isomerisation, hydro treating, and FT synthesis.

CHE-CLRI -308 **Carbohydrate chemistry** **2-0-0-2**

Mono and disaccharides, polysaccharides, Bacterial polysaccharides, starch and cellulose, derivatives of cellulose, Protecting groups, Glycosylation reactions, Dynamics and interactions, carboxy methyl cellulose and gun cotton, structure, Conformational analyses, glycoconjugates, Immunology of carbohydrates.

CHE-CLRI -309 **Biophysical chemistry** **2-0-0-2**

Physico Chemical properties of Water, State of Water in biostructures & its significance, Lipids & Proteins, Membrane organization & stability, Protein lipid interactions, Phase properties of biological membranes, Transport across the membrane, Osmosis, molecular basis of aqueous channels, Structural level of proteins & stabilizing forces, Conformational analysis of polypeptides, Ramachandran plot, Double helical structure of DNA, Conformational parameters of Nucleic acids & their constituents, Types & structure of RNA, mRNA, rRNA, tRNA, Protein-ligand and DNA-protein interactions.

CHE-CLRI -310 **Physics and chemistry of collagen** **2-0-0-2**

Molecular Structure of Collagen, Native collagen fibrils, X-ray Diffraction studies of collagen, Electron microscopic appearance of collagen, synthetic collagen-like polypeptides, Chemistry of Collagen and its Distribution, Biosynthesis of Collagen, Crosslinking, Degradation, Isolation and Characterization of Collagen, Physico-Chemical Techniques for Collagenous Matrices, Microscopy and other Non-invasive methods.

CHE-CLRI -311 **Marine Natural products** **2-0-0-2**

Polysaccharide contents of various seaweeds, Phaeophyceae and Rhodophyceae, Bioactive compounds from halophytic plants and marine algae/seaweeds, Gelling polysaccharides, extraction from natural sources, characterization and properties. Preparation of polysaccharide based biodegradable materials, hybrid composites, stimuli responsive materials. Applications of polysaccharide based materials. Biosynthesis of bioactive polysaccharides, steroids, fatty acid derivatives and alkaloids.

CHE-CLRI -312 **Supramolecular chemistry** **2-0-0-2**

Nature of supramolecular interactions, role of various non-covalent interactions, multiple hydrogen bonding motifs, Stability of H-bonds, Jorgensen model for H-bonding, supramolecular synthons, dimensions of supramolecular chemistry, Janus molecules. Photoresponsive molecules and self-assembly, Molecular recognition, classification of supramolecular host-guest complexes, supramolecular self-assembly, supramolecular polymers, molecular capsules, self-assembled dendrimers, self-assembled nanotubes, low molecular weight organogels. Characterization techniques of self-assemblies, supramolecular sensors.

- CHE-CLRI -313** **Total Synthesis** **1-0-0-1**
Synthesis of complex organic molecules – planning and execution; Concepts of Retrosynthetic Analysis and Total synthesis of Natural products; Retrosynthesis; Disconnection; Synthons; Linear and Convergent Synthesis; Photochemistry in total synthesis; MCRs in total synthesis; Breakthrough synthesis – past and present.
- CHE-CLRI -314** **Asymmetric Synthesis** **1-0-0-1**
Strategies for the preparation of optically pure compounds; Stereoselective, Enantioselective and Diastereoselective reactions; Stoichiometric asymmetric synthesis-chiral auxiliaries, Evans Aldol and modified versions; Catalytic asymmetric synthesis; Asymmetric Dihydroxylation; Asymmetric Aminohydroxylation; Asymmetric Hydrogenation; Asymmetric allylation, propargylation, and alkylation; Chiral Organocatalysis; Cascade reactions by organocatalysis; Transition Metal based catalysis; Asymmetric amplification and autocatalysis.
- CHE-CLRI -315** **Chemistry and biology of Heterocycles** **2-0-0-2**
Privileged heterocycles, Electronic properties, reactivity (electrophilicity and nucleophilicity), Synthetic methodologies, Biological properties of Natural products and drug candidates, Biosynthesis, Dimeric compounds and related stereochemistry
- CHE-CLRI -316** **Agrochemicals** **2-0-0-2**
Biochemistry in agriculture, Carbohydrates, Proteins, Lipids, Vitamins and Minerals and Enzymes, Soil science, guidelines on agricultural crops micronutrients and fertilizers, Chemistry of pesticides, synthesis, formulations, mode of action, toxicology, resistance and residual analysis, Methodologies for the synthesis of agrochemicals and other relevant organic molecules, chemistry in Integrated Pest Management, Semiochemicals, insect growth regulators, botanical pesticides and other biotechnological approaches, Analysis of agrochemicals and residues - Botanical pesticides, hormones, pheromone, kairomones and plant volatiles
- CHE-CLRI -317** **Fluoro organic chemistry** **2-0-0-2**
Importance of fluorine in organic compounds, Strategies to introduce fluorine/ trifluoromethyl group into organic molecules, Preparation of fluorinated reagents, Preparation of fluorinated carbon materials and their uses, Known fluorinated drugs and their mode of action, Overview on CFCs, HCFCs, HFCs, their preparation and applications, Halon substitutes, Harmful effects of fluorine and inorganic fluorides
- CHE-CLRI -318** **Corrosion science** **2-0-0-2**
Basic aspects, Forms of corrosion, Atmospheric corrosion and protective coatings, Immersion corrosion and electrochemical protection, Corrosion monitoring, impedance spectroscopy, harmonics and NDT techniques.
- CHE-CLRI -319** **Nutraceuticals** **2-0-0-2**
Raw material preparation, and characterization, extraction of valuable biomolecules, characterization of these molecules with stability study, preparation and formulations for functional foods. Characterization and stability study of nutraceuticals, properties and stability packaging of nutraceuticals.
- CHE-CLRI -321** **Ionic liquids for lubricants** **1-0-0-1**
Lubrication by Ionic liquids and its structural correlation, Ionic liquids interaction with surfaces, synthetic oil lubricants, synthesis of lubricating ionic liquids, effect of alkyl chain length and anions, IL lubrication oils at variable temperatures, thin films, heat capacity and

thermal properties, viscosity and wetting properties, ionic liquids as additives for lubricants, comparison with conventional hydrocarbon oils, Case studies.

CHE-CLRI -322 **Applications of ionic liquids** **1-0-0-1**

Introduction to task specific ionic liquids, self-assembly of ionic liquids in aqueous/non aqueous media and synthesis of nanomaterials therein, ionic liquids in catalysis, extraction of metal ions, ionic liquids and biopolymers: dissolution, regeneration and ionic-gel formation, processing of lignocellulosic biomass using ionic liquids, clean separation of various fractions of biomass and recovery of valuable chemicals using ionic liquids, application of ionic liquids in electrochemistry, separation of azeotropic mixtures using ionic liquids, organic reactions in ionic liquids.

CHE-CLRI -323 **Homogeneous Catalysis** **1-0-0-1**

Organometallic Catalysis, Applications in organic synthesis: Olefin Isomerization, C-C Coupling reactions: Heck, Suzuki, Stille and Sonogashira reactions, Alkene and Alkyne Metathesis, C-Heteroatom coupling: Hydroamination, Olefin Oxidation, C-H activation, Oxidation reactions, hydrogenation of Alkenes, Industrial Applications.

CHE-CLRI -325 **Catalysis for organic synthesis** **1-0-0-1**

A background on fine and specialty chemicals in chemical industry; Concept of atom economy; Homogeneous and heterogeneous catalytic reactions: hydrogenation, hydrogenolysis, dehydrogenation, selective oxidation, alkylation & acylation, isomerization and C-C bond forming reactions, Enzyme catalysis in organic synthesis; Reaction mechanisms

CHE-CLRI -328 **Materials and devices for energy conversion** **2-0-0-2**

Design of organic and Inorganic semiconductors, Approaches to process organic semiconductors by covalent and non covalent modifications , band edges and band gaps, Modulation of charge transport properties, kinetics of electron transfer, Design of small molecule dyes for DSSC, Electron transfer at interfaces, Transistors and solar cells, Fabrication of Devices, Device characterisation using dark current, IV curves under illumination, IPCE, Calculation of Voc, Jsc, Vpp, Ipp, FF and Pmax. hybrid solar cells

CHE-CLRI -329 **Functional Ceramics** **1-0-0-1**

Advanced Electronic Ceramics, high temperature ceramic super conductors, Dielectric ceramics, microwave ceramics, low k materials, SOFC materials, solid-ionic conductors, phosphor materials, Impedance analysis, varistors, sensors, ceramic magnets, thermal shock resistance and super plastic ceramics.

CHE-CLRI -331 **Porous structures** **2-0-0-2**

Definitions, Micro-Porous and Mesoporous Solids, Structural Chemistry of Zeolite Framework Types, MOFs, COFs, Synthesis, Structure Determination, Role of the Structure-directing Agents, The Chemistry of Microporous Framework Solids, Adsorption and Diffusion, Catalytic Applications, hydrogen storage, separation, CO₂ sequestration, sensors,

CHE-CLRI -332 **Biomaterials for targeted therapeutics** **2-0-0-2**

Rational design and engineering of lipid-based targeted drug delivery vehicles and their therapeutic applications - Design of polymeric micelles as nano drug carriers - Design of polymer-based nanometric targeted delivery systems and their therapeutic applications - Set-backs and unmet challenges – Cancer and its Hall Marks - Principles of designing anti-cancer therapeutics – Molecular basis of lung, breast, melanoma and prostate cancers – Rationale for selecting leading pathways in cancer therapy – Nuclear hormone receptors as targets in cancer therapy – Rationale for design of cancer therapy against multiple pathways – Concept of designing hybrid molecules as a dual strategy – Use of nanotechnology in cancer therapy – Concept of cancer stem cells and design of cancer stem cell therapeutics.

- CHE-CLRI -346** **Polymers and Colloidal Solutions** **2-0-0-2**
Intermolecular forces and potentials, Overview of Statistical physics, DLVO theory, charged colloids, Poisson Boltzmann theory, Debye radius, Bjerrum length, electrophoresis, zeta potential, diffusion, Hydrodynamic interactions. Brief overview of Phase transitions in hard sphere colloids, Random walk, self avoiding random walk, flexible polymers, persistence length, Excluded volume interactions, Polymer solutions in the dilute limit/semi-dilute limit, Entropy of mixing, theta temperature, rubber elasticity, Polyelectrolytes, polymer at surfaces: Brushes, polymer dynamics.
- CHE-CLRI-347** **Biodegradable polymers** **2-0-0-2**
Polymers from biomass, microbial production, synthetic polymers, structure and properties, Biodegradation mechanism, measurement techniques, processing techniques, sterilization and storage, global standards, market potential, applications.
- CHE-CLRI -348** **Controlled Radical/Living Polymerizations and** **2-0-0-2**
Macromolecular Architectures
Controlled or Living Radical Polymerization, TEMPO-mediated polymerization and atom Transfer radical Polymerization (ATRP), Kinetics of ATRP, Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide mediated polymerization (NMP), Ring opening Metathesis polymerization (ROMP), living ROP, Macromolecular architectures using controlled living polymerizations
- CHE-CLRI -349** **Pi-conjugated polymers** **2-0-0-2**
Synthesis and characterization, electronic and optical properties, energy band structure, Display Materials: Organic Light Emitting Diodes, Organic thin film transistors, device preparation, working principle, advantages, drawbacks; Organic photovoltaics, OFETs, device preparation and characterization, factors influencing efficiency, stability.
- CHE-CLRI -350** **Liquid Crystals** **2-0-0-2**
Liquid crystal phases, classification, Chiral liquid crystalline phases, Ferroelectric liquid crystalline phases, discotic liquid crystalline phases, Characterization techniques, Surface Alignment of Liquid Crystals, Dichroic LCs, Polycatenar mesogenes, Display and photovoltaic applications.
- CHE-CLRI -351** **X-Ray Diffraction and Structure of Solids** **2-0-0-2**
Introduction to X-ray crystallography, Crystal growth, evaluation and mounting, Symmetry and space group determination, Background theory for data collection, Data collection using four-circle diffractometers, Area detectors, Crystal lattices, Structure factors, Crystal symmetry, Structure solutions, Structure refinement, An introduction to maximum entropy, Least squares fitting of parameters, Practical aspects of structure refinement, Crystallographic Database, Structure solution from Powder Diffraction Data
- CHE-CLRI -352** **NMR spectroscopy** **2-0-0-2**
Quantum Mechanics of NMR, Multinuclear NMR spectroscopy, Periodic table of NMR, Heteronuclear double resonance experiments, Magnetization transfer and signal enhancement, NMR of diamagnetic and paramagnetic compounds, Multidimensional NMR: 2D NMR, 1H-1H correlations, Heteronuclear Correlation Spectroscopy, 2D Exchange (EXSY), 2D NOESY, ROESY, DOSY Structure elucidation of small molecules, NMR of macromolecules, Multidimensional NMR Spectra, NMR Spectroscopy of Solids, 2D experiments in solids, semi rigid systems: HR MAS, Magnetic Resonance Imaging: In Vivo NMR, Imaging, MRI, functional MRI, NMR imaging of materials.

400 level courses

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CHE-CLRI -401	Project proposal writing & presentation	0-0-4-2
CHE-CLRI -402	Project proposal writing & presentation	0-0-4-2
CHE-CLRI -403	CSIR-800	0-0-8-4