DEPARTMENT OF CHEMISTRY

School of Physical Sciences

Central University of Kerala

Tejaswini Hills, Periye P.O.

Kasaragod 671320, Kerala

PhD Chemistry Syllabus - 2021

Programme outcome

- Doctoral Research in the Department of Chemistry at Central University of Kerala aims to equip scholars to take–up challenging tasks for the future that ultimately benefits the society

Specific outcome

The programme enables the students to

- Design and conduct original research in their area of specialization
- Attain systematic understanding of a subject and mastery of the skills and methods associated with the subject
- Develop skills for critical analysis, assessment and synthesis of new and complex ideas
- Develop further the progress made in technological, social or cultural terms within an academic and professional context
- Demonstrate the ability to communicate the results of their research in a clear and effective manner
- Demonstrate an understanding and concern for the high ethical standards in research, teaching, and service
- Demonstrate the ability to teach college-level courses in their area of specialization

Participatory learning

- Many workshops, seminars, and conferences are conducted to motivate the PhD scholars to present their work and also to acquire and update knowledge on cutting edge research activities across the globe.

PhD Chemistry Course Structure

Title of the Course	Credit value	Marks		Total
		Continuous Evaluation	End-Semester Evaluation	
Course 1. Research methodology (including quantitative methods and computer application, where relevant)	4	40	60	100
Course 2. Research and Publication Ethics (mandatory as per UGC circular 2019)	2	40	60	100
Course 3. Special Course related to the core area of research	6	40	60	100
Course 4. Course on the specific research proposal including a review of literature (**CHE 7102**)	6	------	100	100

PhD Chemistry

Structure of the common courses

Course Code	**Course Title**	**Contact hrs./wk**				**Credits**
		Lect.	Lab	Tutorial	Total	
CHE 7101	**Research Methodology**	**4**	**-**	**2**	**6**	**4**
CHE 7109	**Research and Publication Ethics**	**4**	**-**	**2**	**6**	**2**

Syllabus in Detail:

CHE-7101 Research Methodology

1. Research Methodology and Data analysis

   Research processes - scientific research formation of the topic, hypothesis, conceptual definitions, operational definition, gathering of data, analysis of data, revising of hypothesis, Conclusion. Literature survey - Journals, books and e-resources. Presentation and publication of research output.

   Errors in chemical analysis, classification of errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean, standard deviation, comparison of results: “t” test, “f” test and “chi” square test, least squares analysis, weighted least squares analysis, regression coefficient, rejection of results, presentation of data.

2. Basic Methods in Chemical Analysis

   Fundamental and over view of FT-IR spectroscopy, CHN analyser, Chromatography (TLC, GC & HPLC), UV-Visible spectroscopy, Fluorescence, Thermal analysis (DSC & TGA), Atomic absorption spectroscopy, X-ray diffraction analysis, Nuclear Magnetic Resonance (NMR) spectroscopy and Mass Spectrometry, computational tools in chemistry.

3. Chemistry Pedagogy

   The student shall involve in a Teaching Assistant (TA) or Tutor for any chemistry course preferably for laboratory courses. The course instructor will closely monitor the work of the Ph. D. student, provide mentoring, finally evaluate him for his pedagogic skills and knowledge of the subject and award a grade.

4. Computer Knowledge in Research

   Operating System-Windows and Linux. Document Preparation-Microsoft Word and LaTex. Web browsing: Various publishers such as ACS, RSC, Wiley, Science Direct, Scopus, Web of Science, UGC-INFLIBNET, Shodh Sindu, Shodh Ganga and Plagiarism software. Chemistry related software: SciFinder, Reaxys, ChemDraw, ISIS Draw etc. Analysis/Plotting Software: EXCEL, ORIGIN, MATLAB, etc. Presentation Tools: Power Point Presentation and LaTex

References

1. C. R. Kothari, Research Methodology Methods and Techniques, 2nd Revised Ed., 1990.
2. Robert V Smith, Graduate Research: A Guide for Students in the Sciences, University of Washington Press, 1998.
3. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) *Instrumental Methods of Analysis* - 7th Ed., Wadsworth Publishing (1988) ISBN 0534081428
4. Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A. *Principles of Instrumental Analysis* Saunders Golden Sunburst Series (1997).
5. Paul D Leedy, Jeanne E Ormrod and Jeanne Ellis Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.

Course Outcome:

By completing this course, students will obtain the following course/learning outcomes:

- Understand philosophy of doctoral research; ethics in research and scientific publishing
- Collect literature and data/materials for specific research problem
- Learn the basic and sophisticated characterization methods required for research

- Learn basic computational tools useful for chemical research
- Learn to use softwares and programs necessary for data analysis, presentation of results and preparation of research reports and scientific publications
- Present and defend results to an audience in a clear manner

CHE 7102: Literature Review

Course on the specific research proposal including a review of the literature

CHE 7103 Instrumental Methods for Chemists

1. Elementary Electronics: Resister, Capacitor, Inductor, Diode, Transistor, Field effect transistor, Transformers, Rectifiers, Voltage Regulator, Readout devices.
2. Chromatography: Thin layer chromatography, Column chromatography, HPLC, Ion – exchange chromatography, Gel Permeation Chromatography and Gas Chromatography.
3. CHNS-Elemental analyzer, FT-IR Spectrophotometer, FT-NMR (1D & 2D), High resolution mass spectrometer and X-ray diffraction techniques.
4. UV-visible Spectrometer, CD Spectroscopy, Steady state and time-resolved spectrofluorimeters.
5. Cyclic voltrametry: Theory and applications.
6. Photoelectron spectroscopy techniques
7. Thermal Methods of Analysis: TG, DTA and DSC.
8. Flame Emission and Atomic Absorption Spectrometer.
9. Optical Microscopes, Confocal Microscopes and Electron microscopes (SEM, FESEM and TEM). Atomic Force Microscopes (AFM) and Scanning Tunneling Microscopes (STM).
10. Computational Methods: Z-matrix, chemical structures drawing and energy optimization Gaussian.

References

1. D. A. Skoog, D. M West, Principles of Instrumental Analysis, 2nd Ed., Saunders college, Philadelphia, 1980.
2. R. L. Pecsok, Modern Methods of Chemical Analysis, John Wiley, 2nd Ed., 1976.
3. R. H. Willard, L. L. Merrit, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, D, Van Nonstrand, N.Y, 1981.

4. F. W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Ed., International Book Company, London, 1983.
5. H. A. Laitinen, W. E. Harris, Chemical Analysis, 2nd Edition, McGraw-Hill, Tokyo, 1975.
6. D. F. Calbreath, Clinical Chemistry- A Fundamental Textbook, 2nd Ed., W. B. Saunders, 1992.
7. K. Wilson, J. Walker, Practical Biochemistry-Principles and Techniques, Cambridge University Press. 1995.

CHE 7104 Photophysics and Dye Sensitized Solar Cells

Fundamental laws of photochemistry, nature of light and matter, Interaction of light with matter, Mechanism of absorption and emission, electronic transitions, selection rules, spectroscopic term symbols, physical properties of electronically excited molecules, Jablonski diagram, photophysical properties of the electronically excited molecules. Photophysical kinetics of bimolecular processes. Electron and energy transfer reactions.

Dye sensitized solar cells (DSSC): Historical back ground, DSSC structure and working principle, working and counter electrodes, sensitizers, redox couple. Past, present and future designing strategies of sensitizers. Perovskite materials and applications in harvesting solar energy.

References

1. Fundamental of Photochemistry -KK Rohatgi Mukherjee
2. Dye Sensitized Solar Cells – Kalyanasundaram K.
3. A New Sight towards Dye Sensitized Solar Cells: Material and Theoretical – Hong Lin

CHE 7105 Inorganic Materials & their Importance in Catalytic Applications

Surface area and porosity measurement – measurement of acidity of surfaces; Support materials – preparation and structure of supports – surface properties, preparation of catalysts – introduction of precursor compound – pre-activation treatment – activation process.

General methods of synthesis of zeolites, mechanism of nuclear formation and crystal growth, structures of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts.

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

References

1. R.B. Anderson, "Experimental methods in catalysis research", Vol I, II, Academic press, NY, 1981.
2. R. Szostak, "Molecular sieves: principles of synthesis and identification", Van Nostrand, NY, 1989.
3. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.
4. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 1-5, Wiley- VCH, Weinheim, 1997.
5. R.J. Farrauto and C.H. Bartholomew, "Fundamentals of Industrial Catalytic Processes", Blackie Academic and Professional – Chapman and Hall, 1997.
6. R. Pearce and W.R. Patterson, "Catalysis and chemical processes", Academic press, Leonard Hill, London, 1981.
7. C.M. Starks, C.L. Liotta and M. Halpern, "Phase Transfer Catalysis – fundamentals, applications and industrial perspectives", Chapman & Hall, New York, 1994.

CHE 7106 – Nanomaterials for Energy and Catalysis

Synthesis of nano materials- physical, chemical, biological and hybrid methods. Fullerenes, carbon nanotubes, Nanocomposites and nanofillers: formation, properties.

Analysis of Nano Materials: spectral methods of analysis such as SEM, TEM, X-ray diffraction etc.

Nano-science, types of nanotubes, molecular computers. Lipids, templates, proteins, optical memory and DNA, information and probes, photodynamic therapy.

Applications: molecular electronics. Biomolecular imaging. Photon trapping, nanoholes and photons, formation imaging, solar absorbers, nanostructural polymers, photonic crystals. Nanostructured materials, energy conversion and storage. Semiconductors, transistors, nanofabrication of quantum computers nanomedicines: medical diagnosis, targeted drug

delivery. Nanosensors, molecular nanomachines, green in nanoscience, nanomaterial applications in environmental chemistry.

References

1. S.C. Tjong "Nanocrystalline Materials: Their Synthesis-Structure-Property Relationships & Applications", Elsevier Ltd, London, 2006.
2. Jose A. Rodríguez, Marcos Fernández-García "Synthesis, Properties and Applications of Oxide Nanomaterials", John Wiley & Sons, Inc, Canada, 2007.
3. C. Brechignac, P. Houdy, M. Lahmani, "Nanomaterials and Nanochemistry",Springer Berlin Heidelberg, New York, 2007.
4. C. C. Koch, I Lya, A. Ovid'ko, S. Seal and S. Veprek "Structural Nanocrystalline Materials Fundamentals and Applications", Cambridge University Press, Cambridge, 2007.
5. M. Wilson, K. Kanengara, G. Smith, M. Simmons and B. Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (I), N.D., 2005.
6. K. J. Klabunde, Nano Materials in Chemistry, John Wiely Sons Inc., 2001.
7. S. K. Kulkarni, Nano Technology Principles and Practices, Capital Publishing Company New Delhi, 2009.

CHE 7107 - Computational Methods in Chemistry

Molecular Mechanics. Potential energy surfaces. Curve crossing Model. Force field. Factors governing barrier heights. Quantum Mechanical and Molecular Mechanics potential functions. MM force fields. Parametrization. Steric energies, Heats of formation and strain. Compu-chem lab: Z-matrix specification, Input for Semi-empirical and *ab-initio* programs. Molecular mechanics program. Analysis of output.

References

1. F. Jensen, Introduction to computational chemistry, Wiley, NY, 2007.
2. D. C. Young, Computational Chemistry, John-Wiley and Sons, NY, 2001.
3. C. J. Cramer, Essentials of Computational Chemistry, John-Wiley & Sons, 2004.
4. U. Burkert and N.L. Allinger: Molecular Mechanics, ACS Monograph, American Chemical Society, 1977.

5. Albright, Burdett and Whanghbo, Approximate Molecular Orbital Theory, Academic Press, 1985.

6. MOPAC 6.0 Manual and computer program, QCPE Ed.

7. PCMODEL Manual and Computer program, Serena Software.

CHE 7108 – Nano chemistry and Toxicology

Synthesis of nano materials-physical, chemical, biological and hybrid methods. Fullerenes, carbon nanotubes, Nanocomposites: formation, properties. Analysis of Nano Materials: Spectral methods of analysis such as SEM, TEM, X-ray diffraction etc.

Medical Applications of Nanobiotechnology:Nanoparticles, Nanoscience in Drug Delivery, and Controlled Release,Green nanoparticle production and characterization; Biocompatbility; Nanomedical applications of green nanotechnology.

Nanomedicines: medical diagnosis, targeted drug delivery. Nanosensors, molecular nanomachines, green chemistry in nanoscience, nanomaterial applications in environmental chemistry.

Nanoremediation: Identification and characterization of Hazardous waste, Nano Pollution, Air-Water - Soil Contaminants, Identification and Characterization of Organic and inorganics, Environmental cleanup technologies.Nanomaterials-Remediation: Nano Membranes.

Basics of Toxicology: Definition, Branches of toxicology, scope and importance. Inorganic and organic toxicants, factors affecting toxicity. Dose response relationships. Biotransformation of toxic substance. Cellular and molecular based assessment of toxicity.

References

1. S. C. Tjong, Nanocrystalline Materials: Their Synthesis-Structure-Property Relationships & Applications, Elsevier Ltd, London, 2006.

2. J. A. Rodríguez, M. Fernández-García, Synthesis, Properties and Applications of Oxide Nanomaterials, John Wiley & Sons, Inc., Canada, 2007.

3. C. Brechignac, P. Houdy, M. Lahmani, Nanomaterials and Nanochemistry, Springer Berlin Heidelberg, New York, 2007.

4. C. C. Koch, I. Lya, A. Ovid'ko, S. Seal, S. Veprek, Structural Nanocrystalline Materials Fundamentals and Applications, Cambridge University Press, Cambridge, 2007.

5. M. Wilson, K. Kanengara, G. Smith, M. Simmons, B. Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (I), N.D., 2005.

6. K. J. Klabunde, Nano Materials in Chemistry, John Wiley sons Inc., 2001.

7. S. K. Kulkarni, Nano Technology Principles and Practices, Capital Publishing Company, New Delhi, 2009.

8. Ballantyne B, Marris T and Turner P (Ed) 1995. General and applied toxicology (Abridged edition) Macmillian.

CHE 7109 Research and Publication Ethics

Course Code: CPE-RPE

Overview

- This course has total 6 units focusing on basics of philosophy of science and ethics, research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

Pedagogy:

- Class room teaching, guest lectures, group discussions, and practical sessions.

Evaluation

- Continuous assessment will be done through tutorials, assignments, quizzes, and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

Course structure

• The course comprises of six modules listed in table below. Each module has 4-5 units.

Modules	Unit title	Teaching hours
Theory		
RPE 01	Philosophy and Ethics	4
RPE 02	Scientific Conduct	4
RPE 03	Publication Ethics	7
Practice		
RPE 04	Open Access Publishing	4
RPE 05	Publication Misconduct	4
RPE 06	Databases and Research Metrics	7
Total		30

Syllabus in detail

THEORY

- **RPE 01: PHILOSOPHY AND ETHICS (3 hrs.)**

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

- **RPE 02: SCIENTIFIC CONDUCT (5hrs.)**

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)

4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

- **RPE 03: PUBLICATION ETHICS *(*7 hrs.)**

1. Publication ethics: definition, introduction and importance
2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types
5. Violation of publication ethics, authorship and contributor ship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals PRACTICE

• RPE 04: OPEN ACCESS PUBLISHING (4 hrs.)

1. Open access publications and initiatives 2. SHERPA/ROMEO online resource to check publisher copyright & self-archiving policies 3. Software tool to identify predatory publications developed by SPPU 4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

• RPE 05: PUBLICATION MISCONDUCT (4hrs.)

A. Group Discussions (2 hrs.)

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs.)

Use of plagiarism software like Turnitin, Urkund and other open source software tools

• RPE 06: DATABASES AND RESEARCH METRICS *(*7hrs.)

A. Databases (4 hrs.)

1. Indexing databases 2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score 2. Metrics: h-index, g index, i10 index, altmetrics

References

1. Bird, A. (2006). *Philosophy of Science.* Routledge.
2. MacIntyre, Alasdair (1967*) A Short History of Ethics*. London. P.
3. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978 9387480865
4. National Academy of Sciences, National Academy of Engineering and Institute of Medicine.

(2009). *On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition.* National Academies Press.
5. Resnik, D. B. (2011). What is ethics in research & why is it important. *National Institute of Environmental Health Sciences*, 1-10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
6. Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179–179. https://doi.org/10.1038/489179a
7. Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019), ISBN:978-81-939482-1-7. http://www.insaindia.res.in/pdf/Ethics Book.pdf

Course Outcome:

By completing this course, students will obtain the following course/learning outcomes:

- Understand ethics and philosophy of doctoral research
- Learn the importance of integrity, honesty, and good research practice in research work
- Understand scientific and publishing misconduct and take measures to avoid it
- Become aware of the importance of ethics in scientific publishing
- Learn to utilize the databases and resources efficiently for research pupose
- Aware of the responsibility for research, results and consequences of research

CHE 7110 Electro-analytical Technique for Energy and Energy storage applications

Working principle of Capacitors, supercapacitors, batteries and fuel cells. Important electroanalytical techniques in Capacitors, supercapacitors, batteries and fuel cells, Trasatti method, Dunn's method and Tafel plot. Basic principles of electrochemistry, Mass transfer by diffusion and migration, general mass transfer equations, Ionic migration and diffusion. Ilkovic equation, polarography, chronoamperometry, chronocoulometry, pulse polarographic methods. Cyclic voltammetry: Nernstian reversible, totally irreversible, quasi-reversible processes, controlled potential methods, electrogravimetry, electroseparation, controlled current methods, coulometric, potentiometric, and amperometric methods.

References

1. B. E. Conway,– Electrochemical Supercapacitors
2. A. J. Bard, L. R. Faulkner, Electrochmical Methods, Fundamentals and applications, John Wiley, 1980.
3. J. O′M. Bockris, A. K. N. Reddy, Electrochemistry, vol. 1 & 2, Plenum, 1973.
4. H. Kissinger, Electroanalytical Techniques, John Wiley, 1998.

Course Outcome:

This course will enable the research scholar to understand the basics and prerequisites required to carry out the research work related to Electro-Analytical Technique for Energy and Energy storage applications

- The basics of electrochemistry will be described in the introduction process.
- The basic parameters to analyzed to interpret the super capacitor performance, fuel cell applications will be discussed
- Various parameters to study the electrochemical reactions will educate the scholar to carry out the research related to electrochemical reactions.