POSTGRADUATE DEPARTMENT OF CHEMISTRY
Value Added Courses

w.e.f. 2020-2021

Sem	Course code	Course Title	Hours	Credit	Marks
I	PGC 421V	Transport properties of Solids	2	2	20
II	PGC 422V	Computational Chemistry	2	2	20
III	PGC 521V	Nanomaterials	2	2	20
IV	PGC 522V	Green Techniques for Organic synthesis	2	2	20

C421V Transport Properties of Solids 2 Hours/2 Credits

Objective

This course highlights the electronic structure of solids, the types of solids based on electrical, thermal, magnetic, dielectric and optical properties. Property based applications of the solid materials will be discussed.

After completion of this course the students will be able to

i. Classify solids into metals, semiconductors and insulators
ii. Measure temperature using thermocouples
iii. Correlate structure of solids with magnetic property
iv. Analyze the uses of solids with dielectric and optical properties
v. Identify functional materials based on structure and properties

Unit 1: Electrical properties 6 hrs

Band theory – k space and Brillouin zones – band structure – types of solids – Hall effect – materials – applications

Unit 2: Thermoelectric properties 6 hrs

Definition – Types: Thomson effect, Peltier effect, Seebeck effect – theory – materials – applications – Demonstration of working of a Type-K thermocouple

Unit 3: Magnetic properties 6 hrs

Theory – types – materials: metals, alloys, metal oxides, spinels, garnets, ilmenites, perovskites, plumbites – applications: structure property correlation

Unit 4: Dielectric properties 6 hrs

Definition – types: Ferroelectricity, Pyroelectricity, Piezoelectricity – theory – materials - applications – virtual experiments on dielectric properties

Unit 5: Optical properties 6 hrs

Optical absorption – Non-linear optical materials – applications – Luminescence – LED – LCD –phosphorescence – phosphor materials – anti-stokes phosphors – Lasers – Ruby lasers – Neodymium lasers – semiconductor lasers

References

1. West A.R., Solid State Chemistry and its Applications, John Wiley and Sons, New York, 1984.
2. Arumugam M, Materials Science, Anuradha Publications, 3rd edition, 2007
3. Hannay N.B., Solid State Chemistry, Prentice Hall of India Private Limited, New Delhi, 1976.

Mapping of Bloom's Taxonomy with Course Outcome

PGC421V	K1	K2	K3	K4	K5
CO1				4	
CO2					5
CO3				4	
CO4				4	
CO5			3		

Mean 4.0

PGC 422V **Computational Chemistry** **2*hrs / 2 cr***

(Lab cum Theory)

Objective

This course is designed to give an overview of computational methods used in chemical research. The knowledge about the computational chemistry is essential to prepare and communicate research articles. This course addresses computer based calculations within chemistry and integrates theoretical aspects with the computational elements.

On successful completion of the course, the student will be able to

i. Construct chemical structures using Avogadro
ii. Describe and Analyze the various chemical properties using MOPAC
iii. Draw and Evaluate various energy parameters through Gaussian
iv. Prepare and analyses spectra and bonding analysis using Gaussian
v. Survey the research papers through software using Mendeley

Unit 1: AVOGADRO **6 Hrs**
Introduction- Building Molecules - Tools - Display Types - Menus - Extension Menu - Optimizing Geometry - Introduction to Molecular Mechanics

Unit 2: MOPAC **6 Hrs**
Introduction- Point Group Analysis- Heat of Formation **-**Vibrational Parameters (Rotational Constants, ZPE, Modes of Vibrations)**-** Bond Order Calculations**-** pka of an Acid - Calculations using Hamiltonian.

Unit 3: GAUSSVIEW and GAUSSIAN-I **6 Hrs**
Introduction - Create Input Files - Submit Calculations - Visualize Output- Basis Sets – Single-Point Energy - Potential Energy Surface - Optimizing Molecule - Potential Energy Surface Scan, Transition States - Reaction Pathways - Thermodynamic Quantities - Relative Energies**.**

Unit 4: GAUSSIAN-II **6 Hrs**
IR, Raman, NMR and UV Spectral Analysis - Natural Bond Orbitals - Molecular Orbitals - Molecular Electrostatic Potential Map- Contour Plot – Solvent Effect.

Unit 5: REFERENCE COLLECTION AND MANAGEMENT SOFTWARE **6 Hrs**
Introduction to Online Chemical Database Search - Searching and Downloading Research Papers Using Keywords in Scopus - Science Direct - Google Scholar - Reaction Search - Product Search - Reactant Search - Structure Search Using Sci-Finder.
Introduction to Mendeleyand its Applications.

References:

1. Avogadro an open source molecular builder and visualization tool. http://avogadro.cc
2. M. D. Hanwell et al., Journal of Cheminformatics, 2012, 4, 17
3. MOPAC2016, James J. P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA http://OpenMOPAC.net
4. J. B. Foresman and A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, 3rd ed., Gaussian, Inc.: Wallingford, CT, 2015.http://gaussian.com
5. http://endnote.com , http://mendeley.com, http://scifinder.cas.org, http://scholar.google.com

PGC422V	K1	K2	K3	K4	K5	K6
CO1			3			
CO2			3			
CO3					5	
CO4			3			
CO5				4		

Mean 3.6

PGC 521V **Nanomaterials** **2 hr / 2 credit**

Objective

This course reflects the diversity of recent advances in nanomaterials, and nanochemistry with a broad perspective that will be useful for post graduate students. This course deals with new methods of synthesis to novel applications of existing methods to gain understanding of the material and/or structural behavior of advanced systems.

Upon completion of the course, the students will be able to

i. Explore the applications of biopolymers and biodegradable materials.
ii. Describe information on emerging technologies of manufacturing thin natural fibers based on the principle of electrospinning process.
iii. Develop new vapour deposition processes, treatments and coatings that can be combined to produce films with composition gradients or periodic multilayers.
iv. Relate the structure-directing role of nanoporous materials and their applications.
v. Construct a complementary image of the target functional molecule by polymerising monomers

Unit 1: Chitosan/Carbon Nanotube Composites **6 hrs**

Introduction on chitosan and carbon nanotube nanofluids – Preparation methods of Chitosan and carbon nanotube nano-composites – Properties and characterization of nanocomposites – Covalent modification of multi walled nano tubes (MWNT) and low molecular weight chitosan (LCMS) - Layer by layer self-assembly - Demonstration of preparation of nanomaterial.

Unit 2: Electrospun Biodegradable Nanofibers **6 hrs**

Electrospinning and Lamination process-Electrospinning set up – Parameters on electrospunnanofibres – solution properties –processing conditions for electrospinning – interpretation of electrospunfibres – virtual lab on electrospinning process

Unit 3: Nanostructured coatings **6 hrs**

Methodology for making superhard nanostructured coatings – Plasma activated chemical vapour deposition – Physical vapour by sputtering and cathodic arc – Physical vapour deposition by ion beam sputtering– Virtual lab on vapour deposition techniques

Unit 4: Nanoporous materials **6 hrs**

Methods of synthesis – Crystallization process of exemplified by zeolites – Role of inorganic cations and organic species – Organic species and template effect – Application of zeolitic materials – Characterization of mesoporous silica – Demonstration of template synthesis

Unit 5: Nanomolecular imprinting **6 hrs**

General principles of nanomolecular imprinting- Role of complexation sites during the imprinting process - Procedures and methods for molecular imprinting – Structure and properties of the polymer matrix – Applications of nanomolecular imprinting – virtual lab on nanomolecular imprinting

References:

1. Handbook of research on nanomaterials, Nanochemistry and smart materials, A. K. Hagi, G. E. Zaikov, *Nova Biomedical*, **2013**, Nova Science Publishers, Inc. New York.
2. Nanomaterials and Nanochemistry, C. Brechignac, P. Houdy, M. Lahmani, *Springer*, **2007**, Springer Berlin Heidelberg New York

PGC521V	**K1**	**K2**	**K3**	**K4**	**K5**	**K6**
CO1				**4**		
CO2		**2**				
CO3			**3**			
CO4			**3**			
CO5			**3**			

Mean 3.0

PGC522V Green Techniques for Organic synthesis 2 hr / 2 credit

Objective

The course deals with various Green techniques for organic synthesis. Each of the topics covered in this syllabus demonstrates not merely an advance in the discovery, demonstration, and development of a moleculeor synthetic pathways, but also an advance in the design thinking behind the chemistry.

At the end of the course, students will be able to:

i. Identify the alternative approaches to chemical media
ii. Analyze the processes with optimal environment effect
iii. Apply the techniques for reduction of hazardous waste
iv. Predict the greener alternative to solvents
v. Analyze the potential applications of various green synthetic technology and apply them in organic synthesis.

Unit1: Solvent free & Microwave-assisted synthesis 6 hrs
Introduction, Ball Milling, Types of Ball Mills, Kinetics and Thermodynamics of Solvent-Free Reactions, Hard-Soft Acid-Base Theory,Stereoselectivity, Catalysis, Isolation Techniques, Microwave-Assisted MCR Synthesis, Synthesis of Peptides, SiC Reactors and Continuous Flow Synthesis, Nanomaterial Synthesis

Unit2: Ultrasonic &Photochemical synthesis 6 hrs
Introduction, Cavitation principle in ultrasonic reactions, name reactions, Photochemical synthesis and Rearrangement of Open-Chain Compounds, Reactions of Olefins, Ar-H Functionalization, Synthesis of 3,4,5,6 & larger Membered Rings.

Unit3: Pot economy synthesis 6 hrs
Introduction, Multicomponent Reactions, Name Reaction, One-Pot and Multi-Step Reactions, Two, Three-Step Reaction Sequences, More Than Three-Step Reaction Sequences, One-Pot Asymmetric Synthesis, Transition-Metal Catalysis, Organocatalysis, Chiral Pool-Based One-Pot Synthesis

Unit4: Solid supported synthesis 6 hrs
Introduction, Techniques of Solid-Phase Supported Synthesis, Recent Advances in Linkers for Solid-Supported Synthesis, Solid-Phase Supported Synthesis of Natural Products, Solid-Supported Organometallic Chemistry, Solid-Phase Synthesis of Peptides, Solid-Phase Supported Stereoselective Synthesis, Microwave-Assisted Solid-Phase Synthesis, Solid-Phase Supported Reagents in Organic Synthesis.

PGC8

Unit5: Light Fluorous synthesis 6 hrs

Introduction, “Heavy” Versus “Light” Fluorous Chemistry, The Green Chemistry Aspects of Fluorous Synthesis, Fluorous Solid-Phase Extraction (F-SPE) to ReduceWaste, Recycling Techniques, Monitoring Reactions, Fluorous Linker-Facilitated Synthesis, Fluorous Techniques for Discovery Chemistry, Fluorous Ligands for Metal Catalysis,FluorousOrganocatalysis, Fluorous Reagents, Fluorous Scavengers, Fluorous Linkers, Fluorous Mixture Synthesis (FMS).

References

1. Berkeley W Cue& Wei Zhang, Green techniques for organic synthesis and medicinal chemistry, Wiley publications, 2nd edition, 2018.
2. Roger Arthur Sheldon, Isabel Arends, Ulf Hanefeld, Green Chemistry and Catalysis, Wiley-VCHPublications, 2007.
3. James H. Clark, Duncan Macquarrie, Handbook Of Green Chemistry And Technology, Blackwell Publishing, 2002.
4. V. K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, Kluwer Academic Publications, 2004.
5. AlvisePerosa, FulvioZecchini, PietroTundo, Methods and Reagents for Green Chemistry, John Wiley & Sons, Inc., 2007.
6. Miguel De La Guardia & Salvador Garrigues, Handbook of Green Analytical Chemistry, John Wiley & Sons, Ltd. 2012.

PGC522V	K1	K2	K3	K4	K5	K6
CO1				4		
CO2			3			
CO3				4		
CO4				4		
CO5				4		

Mean 3.8